FEATURE SELECTION VIA JOINT LIKELIHOOD

A thesis submitted to the University of Manchester
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Abstract

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We study the nature of filter methods for feature selection. In particular, we examine information theoretic approaches to this problem, looking at the literature over the past 20 years. We consider this literature from a different perspective, by viewing feature selection as a process which minimises a loss function. We choose to use the model likelihood as the loss function, and thus we seek to maximise the likelihood. The first contribution of this thesis is to show that the problem of information theoretic filter feature selection can be rephrased as maximising the likelihood of a discriminative model.

From this novel result we can unify the literature revealing that many of these selection criteria are approximate maximisers of the joint likelihood. Many of these heuristic criteria were hand-designed to optimise various definitions of feature "relevancy" and "redundancy", but with our probabilistic interpretation we naturally include these concepts, plus the "conditional redundancy", which is a measure of positive interactions between features. This perspective allows us to derive the different criteria from the joint likelihood by making different independence assumptions on the underlying probability distributions. We provide an empirical study which reinforces our theoretical conclusions, whilst revealing implementation considerations due to the varying magnitudes of the relevancy and redundancy terms.

We then investigate the benefits our probabilistic perspective provides for the application of these feature selection criteria in new areas. The joint likelihood

automatically includes a prior distribution over the selected feature sets and so we investigate how including prior knowledge affects the feature selection process. We can now incorporate domain knowledge into feature selection, allowing the imposition of sparsity on the selected feature set without using heuristic stopping criteria. We investigate the use of priors mainly in the context of Markov Blanket discovery algorithms, in the process showing that a family of algorithms based upon IAMB are iterative maximisers of our joint likelihood with respect to a particular sparsity prior. We thus extend the IAMB family to include a prior for domain knowledge in addition to the sparsity prior.

Next we investigate what the choice of likelihood function implies about the resulting filter criterion. We do this by applying our derivation to a cost-weighted likelihood, showing that this likelihood implies a particular cost-sensitive filter criterion. This criterion is based on a weighted branch of information theory and we prove several novel results justifying its use as a feature selection criterion, namely the positivity of the measure, and the chain rule of mutual information. We show that the feature set produced by this cost-sensitive filter criterion can be used to convert a cost-insensitive classifier into a cost-sensitive one by adjusting the features the classifier sees. This can be seen as an analogous process to that of adjusting the data via over or undersampling to create a cost-sensitive classifier, but with the crucial difference that it does not artificially alter the data distribution.

Finally we conclude with a summary of the benefits this loss function view of feature selection has provided. This perspective can be used to analyse other feature selection techniques other than those based upon information theory, and new groups of selection criteria can be derived by considering novel loss functions.

Declaration

No portion of the work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

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And finally thanks to my parents, my brother Matt and Sarah, without whom I would not be capable of anything.

Notation

d	Dimension of the feature space (*i.e.* the number of features)
N	Number of datapoints
Y	Random variable denoting the output
X_i, X	Random variable denoting the i'th input/feature, and the joint random variable of all the features $X_1, \ldots, X_d$
$\|Y\|$	The number of states in Y
y, y^i, $\hat{y}$	A label $y \in Y$, the i'th datapoint's label, and a predicted label
$\mathbf{x}$, $\mathbf{x}^i$	A feature vector $\mathbf{x} \in X$, and the i'th datapoint's feature vector
$\mathbf{w}$, $w(y)$	A $\|Y\| - 1$ dimensional non-negative weight vector, a weight function based upon the label y
$\mathcal{D}$	A dataset of N $\{\mathbf{x}$,y$\}$ tuples
$\boldsymbol{\theta}$, θ_i	A d-dimensional bit vector, and the i'th element of the vector, $\theta_i = 1$ denotes the i'th feature is selected
$\neg\boldsymbol{\theta}$	The logical inverse of $\boldsymbol{\theta}$, *i.e.* the unselected features
$X_{\boldsymbol{\theta}}$, $\mathbf{x}_{\boldsymbol{\theta}}$	The selected subset of features $X_{\boldsymbol{\theta}} \subseteq X$, and a feature vector $\mathbf{x}_{\boldsymbol{\theta}} \in X_{\boldsymbol{\theta}}$
λ, τ	Generative parameters for creating $\mathbf{x}$, discriminative parameters for determining y from a particular $\mathbf{x}$
$p(y)$, $\hat{p}(y)$	A true probability distribution, and an estimated distribution
$q(y\|\mathbf{x}, \tau)$	The probability of label y conditioned on $\mathbf{x}$ from a predictive model using parameters τ
$\mathcal{L}$, $-\ell$	The likelihood function, and the negative log-likelihood
S	The selected feature set — equivalent to $X_{\boldsymbol{\theta}}$
$J(X_j)$	Scoring criterion measuring the quality of the feature X_j
$\boldsymbol{\theta}^t$	The selected feature vector at time t

Chapter 1

Introduction

If we wish to make a decision about an important subject, the first step is often to gather data about the problem. For example, if we need to decide which University to study at for a degree, it would be sensible to gather *relevant* information like the courses offered by different Universities, what the surrounding environment is like, and what the job prospects are for graduates of the institutions. If we instead chose to base our decision on *irrelevant* information like the colour of the cars parked outside each University, then our choice would not be well informed and the course might be entirely unsuitable. The problem of choosing what information to base our decisions on must be solved before we can even attempt the larger problem of making a decision. The task of automatically making decisions falls under the remit of *Artificial Intelligence*, and specifically the field of *Machine Learning*. Machine Learning is about constructing models which make predictions based upon data, and in this thesis we focus on that first step in producing a prediction, namely selecting the relevant data.

In this chapter we motivate the problem of feature selection, giving a brief introduction to the relevant topics and explaining the importance of the problem. We state the specific questions that this thesis answers, explaining the relevancy of those questions to the field. We then provide a brief outline of the thesis structure, and detail the publications which have resulted from this thesis.

1.1 Prediction and data collection

In this section we will look at the process of making a prediction at a high level. We consider the problem of predicting what university undergraduate

course would best suit a particular student. As we outlined above, a crucial first step is deciding what data we should base our predictions on. In this task basing our predictions on the colour of houses in southern Peru is unlikely to give much insight, but basing our predictions on that student's strengths and the qualities of the university would allow a much improved prediction. Therefore choosing the inputs (also known as *features*) to a learning algorithm is as important as the choice of learning algorithm, as without good inputs nothing can be learned. Once we have selected a set of appropriate inputs, it is possible to analyse those choices and decipher how each input relates to the thing we wish to predict. *Feature selection* is the process of finding those inputs and learning how they relate to each other.

If we consider the task of feature selection, we can separate out features into three different classes: relevant, redundant and irrelevant (we will give precise definitions of each of these concepts in Chapter 3). Relevant features are those which contain information which will help solve the prediction problem. Without these features it is likely we will have incomplete information about the problem we are trying to solve, therefore our predictions will be poor. As mentioned previously, the proportion of graduates who have jobs or gone on to further study would be a very relevant feature when choosing a degree course. Redundant features are those which contain useful information that we already know from another source. If we have two features, one which tells us a university has 256 Computer Science (CS) undergraduates, and the other tells us the same university has more than 200 CS undergraduates, then the second is clearly redundant as the first feature tells us exactly how many students there are (assuming both features give true information). If we didn't know the first feature, then the second would give useful information about the popularity of the CS course, but it doesn't add any extra information to the first feature. Irrelevant features are those which contain no useful information about the problem. It is easy to think of irrelevant features for any given problem, for example the equatorial circumference of the Moon is unlikely to be relevant to the problem of choosing a degree course. If we could go through our data, and label each feature relevant, redundant or irrelevant then the feature selection task would be easy. We would simply select all the relevant features, and discard the rest. We could then move on to the complex problem of learning how to predict based upon those features.

Unfortunately, as with many things in machine learning, the high level view

sounds simple but the details of implementing such a process can be very hard. In the extreme examples described above it was simple to determine if a feature was relevant, irrelevant, or redundant in the presence of other features. In real problems it is usually much more difficult. For example, if one of our features is the number of bricks in the Computer Science building at the university, will that feature help us decide if the Computer Science undergraduate course will be good? Intuitively we might expect this feature to be irrelevant, but this is not necessarily the case. We might imagine that a large number means there is a large CS building, (hopefully) full of fascinating lectures and the latest in computer hardware. Equally the number could be very small, if the building is modern and built from glass and steel, and yet still contain the truly relevant (but hard to quantify) things which will make a good undergraduate course. The number could also be somewhere in the middle, indicating a smaller building with fewer students. This feature could *interact* with other features we have collected, changing the meaning of that feature. Our prospective undergraduate could prefer going to a large department with many students, where there is more potential for socialising and working with different people. Or they could prefer a small department which is less busy and where it is possible to know all the students and staff. These two features (the number of bricks, and our prospective student's preference) interact, so a student who wants a large department might prefer a course with a large number of bricks (or a very small number) denoting a large CS building. The student who favours a small department might prefer a course with a medium number of bricks, denoting a smaller CS building. However without considering both of these features *together* our feature selection process might believe the number of bricks to be irrelevant, as small, medium and large values all lead to good and bad choices of undergraduate course, because the choice also depends on the student's preference.

Determining if a feature is redundant is an equally hard problem. In our example if we knew both the number of bricks and the amount of floor space in the CS building we might think the former is redundant in the presence of the latter. In the previous example we simply used the number of bricks as a proxy for the size of the building, so knowing the size of the building surely makes that feature redundant? As always the answer is not quite so simple, as very small numbers of bricks also told us that the building might be modern and made from steel. Our new feature of the size of the building does not provide that

information, and so does not make the number of bricks completely redundant.

If analysing features to determine these properties is so difficult for humans, how can we construct algorithms to perform the task automatically? The standard approach is to use *supervised learning* where we take a dataset of features, label them with the appropriate class, and then try to learn the relationship between the features and the class. In our example we would measure all of the features for each different university course, gather a sample of prospective undergraduates, survey their preferences for courses and finally record their choice of course and whether they were happy with that choice. For each student we would have a list of features pertaining to their chosen university course, their individual preferences, and a label which stated if they were happy with the course. We then test each feature to see how relevant it is to the happiness of the student. The choice of the relevancy test (or *selection criterion*) is one of the principle areas of research in feature selection, and forms the topic of this thesis.

One further question we might ask is why analyse the features at all. Surely if we find a sufficiently sophisticated machine learning algorithm to make our prediction about the choice of course then we do not need to separately analyse the features. While many modern machine learning methods are capable of learning in the presence of irrelevant features, this comes at the expense of extra run time and requires additional computer power. In addition to these strictly computational benefits, there are also reductions in cost by not collecting the irrelevant features. If collecting each feature has a material or time cost (such as interviewing lecturers at a university, or surveying the surrounding towns), then if we do not need those features we can avoid that collection cost. We can see that even if we assume our learning algorithm can cope with irrelevant features there are benefits to removing them through feature selection.

1.2 Research Questions

The literature surrounding feature selection contains many different kinds of selection criteria [50]. Most of these criteria have been constructed on an ad-hoc basis, attempting to find a trade off between the relevancy and redundancy of the selected feature set. The heuristic nature of selection criteria is particularly apparent in the field of information theoretic feature selection, upon which this

thesis focuses. There has been little work which aims to derive the optimal feature selection criterion based upon a particular evaluation measure that we wish to minimise/maximise (*e.g.* we might wish to minimise the number of mistakes our prediction algorithm makes when given a particular feature set). Therefore the first question is "Can we *derive* a feature selection criteria which minimises the error rate (or a suitable proxy for the error rate)?". Having achieved this we wish to understand the confusing literature of information theoretic feature selection criteria, by relating them to our optimal criterion. The next question is therefore "What *implicit* assumptions are made by the literature on information theoretic criteria, and how do they relate to the optimal criterion?". Once we have understood the literature we should look at what other benefits a principled framework for feature selection might provide, and how we could extend the framework to other interesting areas, such as cost-sensitivity. We therefore ask one final question, "How should we construct a cost-sensitive feature selection algorithm?".

1.3 Contributions of this thesis

This thesis focuses on filter feature selection criteria, specifically those which use information theoretic functions to score features. The main contribution is an interpretation of this field as approximate iterative maximisers of a discriminative model likelihood. We provide a summary of the contributions here, with a more thorough description given in the Conclusions chapter (Chapter 8).

- A derivation of the optimal information theoretic feature selection criterion which iteratively maximises a discriminative model likelihood (Chapter 4).
- Theoretical analysis of a selection of information theoretic criteria showing how they are approximations to the optimal criterion derived in Chapter 4. This leads to an analysis of the assumptions inherent in these criteria (Chapter 5).
- Empirical study of the same criteria, showing how they behave in terms of stability and accuracy across a range of datasets (15 UCI, 5 gene expression, and 2 from the NIPS-FS Challenge). This study shows how the different criteria respond to differing amounts of data, and how the theoretical points influence empirical performance (Chapter 5).

- An investigation into the use of priors with information theoretic criteria, in particular showing a Markov Blanket discovery algorithm to be a special case of the iterative maximisers from Chapter 4, using a specific sparsity prior. We then extend this algorithm to include domain knowledge (Chapter 6).
- A derivation of cost-sensitive feature selection, from a weighted form of the conditional likelihood which bounds the empirical risk. Development of approximate criteria which maximise this likelihood, and produce cost-sensitive feature sets (Chapter 7).
- Proofs for two important properties of the Weighted Mutual Information, namely non-negativity and a version of the chain rule (Chapter 7).
- An empirical study of cost-sensitive feature selection, showing how it can be combined with a cost-insensitive classification algorithm to produce an overall cost-sensitive system (Chapter 7).

1.4 Structure of this thesis

In Chapter 2 we present the background material in Machine Learning, classification and Information Theory which is necessary to understand the contributions of the thesis. We cover the different evaluation metrics we use to measure the performance of our feature selection algorithms, and the simple classifiers we use to produce predictions based upon the feature sets. We look at the problem of cost-sensitive classification, where some kinds of errors are more costly than others, and review the common approaches used for solving those problems. Finally we review Information Theory as a way of measuring the links between two random variables.

In Chapter 3 we present the literature surrounding feature selection itself, which provides the landscape for the contributions of this thesis. We look at the state-of-the-art in information theoretic feature selection, and how researchers have attempted to link together the complex literature. We review feature selection algorithms which incorporate domain knowledge, and those which can cope with cost-sensitive problems. Finally we look at the related area of Bayesian Networks and specifically structure learning, which has many links to the topic of feature selection particularly when using Information Theory.

In Chapter 4 we present the central result of this thesis, namely a derivation of information theoretic feature selection as the optimisation of a discriminative model likelihood. We then derive the appropriate update rules which select features to maximise this likelihood.

In Chapter 5 we use the derivation from the previous chapter to unify the literature in information theoretic feature selection, showing that many of the common criteria are in fact approximate maximisers of the discriminative model likelihood. We state the *implicit* assumptions made by these criteria, and investigate the impact of these assumptions on the empirical performance of the selection criteria across a wide range of problems.

In Chapter 6 we look at the benefits our probabilistic framework gives, focusing on how to use it to incorporate domain knowledge into the feature selection process. We find that a well-known structure learning algorithm can be interpreted as yet another maximiser of our discriminative model likelihood, under a specific sparsity prior. We extend that algorithm to incorporate other kinds of domain knowledge, showing how it improves the performance even when half the "knowledge" is incorrect.

In Chapter 7 we look at what happens to the feature selection criteria if we change the underlying likelihood. Specifically we investigate a cost-sensitive likelihood, and derive cost-sensitive feature selection criteria based upon a weighted variant of information theory. We prove several results related to the weighted information measure to ensure its suitability as a feature selection criteria, before benchmarking the new cost-sensitive criteria on a variety of problems.

In Chapter 8 we conclude the thesis, reviewing the material presented and looking at how this has contributed to the field of feature selection. We suggest several interesting future directions for feature selection which have arisen during the course of this research.

1.5 Publications and Software

The work presented in this thesis has resulted in several publications with one further paper currently in preparation:

[14] — G. Brown, A. Pocock, M.-J. Zhao and M. Luján. Conditional Likelihood Maximisation: A Unifying Framework for Information Theoretic Feature Selection. *Journal of Machine Learning Research (JMLR), 2012.*

[88] — A. Pocock, M. Luján and G. Brown. Informative Priors for Markov Blanket Discovery. *15th International Conference on AI and Statistics (AISTATS 2012).*

[87] — A. Pocock, N. Edakunni, M.-J. Zhao, M. Luján and G. Brown. Information Theoretic Feature Selection for Cost-Sensitive Problems. *In preparation, 2012.*

Chapters 4 and 6 are expanded versions of the material presented in the AISTATS paper [88]. Chapter 5 is an updated version of the material presented in the JMLR paper [14]. The JMLR paper also presents an earlier version of the derivation given in Chapter 4. Chapter 7 is an expanded version of the material of the paper in preparation [87].

Other published work

In collaboration with other members of the iTLS project, several other papers were published which contain work which is not relevant to this thesis.

[89] — A. Pocock, P. Yiapanis, J. Singer, M. Luján and G. Brown. Online Non-Stationary Boosting. In J. Kittler, N. El-Gayar, F. Roli, editors, *9th International Workshop on Multiple Classifier Systems, (MCS 2010).*

[57] — N. Ioannou, J. Singer, S. Khan, P. Xekalakis, P. Yiapanis, A. Pocock, G. Brown, M. Luján, I. Watson, and M. Cintra. Toward a more accurate understanding of the limits of the TLS execution paradigm. *2010 IEEE Symposium on Workload Characterisation, (IISWC 2010).*

[98] — J. Singer, P. Yiapanis, A. Pocock, M. Luján, G. Brown, N. Ioannou, and M. Cintra. Static Java program features for intelligent squash prediction. *Statistical and Machine learning approaches to ARchitecture and compilaTion (SMART10).*

Software

To support the experimental studies in this thesis several libraries were developed:

- **MIToolbox:** A mutual information library for C or MATLAB, provides common information theoretic functions such as Entropy, Mutual Information. Also includes an implementation of Rényi's entropy and divergence. Available at MLOSS (`http://mloss.org/software/view/325/`).

- **JavaMI:** A reimplementation of MIToolbox in Java. Available here (`http://www.cs.man.ac.uk/~pococka4/JavaMI.html`).
- **FEAST:** A feature selection toolbox for C or MATLAB, provides implementations of all the algorithms considered in Chapter 5. Available at MLOSS (`http://mloss.org/software/view/386/`).
- **Weighted MIToolbox/Weighted FEAST:** A weighted information theory library for C or MATLAB. Available once the corresponding paper is published or upon request (forms an update to MIToolbox).

Chapter 2

Background

In the previous chapter we briefly investigated the notions of feature selection and prediction. We now provide a fuller treatment of those areas, and providing the background material necessary to understand the ideas presented in this thesis. We also introduce much of the common notation used throughout the thesis. As this material is common to many branches of machine learning it forms the basis of many textbooks, the particular references used for this chapter (unless otherwise stated) are Bishop [10], Duda *et al.* [35] and over & Thomas [24].

We begin by revisiting the classification problem in Section 2.1, giving a formal definition of the problem before detailing some of the common methods for evaluating classification problems. We also explore the notions of likelihood and probabilistic modelling, which are central to the results in the later chapters. We review the literature around cost-sensitive classification algorithms in Section 2.2. Finally we introduce Information Theory in Section 2.3, and explore the two variants we use in this thesis, Shannon's original formulation of Entropy and Information [97], and Guiaşu's formulation of the Weighted Entropy [46]. We then review the links between information theory and the classification problem in the current literature.

2.1 Classification

The most common task in machine learning is predicting an unknown property of an object. We base the predictions on a set of inputs or *features*, and the predictions themselves come in two main kinds. Classification is the process of predicting an integer or categorical label from the features. Regression is

the process of predicting a real-numbered value from the features. Whilst these processes are similar, as regression can be seen as classification in an ordered space, the two processes are usually treated separately. For the remainder of this thesis we will focus on classification problems.

We can formally express a classification problem as an unknown mapping $\phi : X \to Y$ from a d-dimensional vector of the real numbers, $X \in \mathbb{R}^d$, to a member of the set of class labels, $Y \in \{y_1, y_2, \cdots\}$. The problem for any given classification algorithm is to learn the general form of this mapping. In supervised learning tasks we learn this mapping from a set of data examples which have been labelled beforehand. This is a difficult task as labelled data is more expensive to acquire than unlabelled data, as it requires more processing (and usually some human oversight). Each data example forms a tuple $\{\mathbf{x}, y\}$ of a feature vector $\mathbf{x}$ and the associated class label y. In general we will assume our data is *independently and identically distributed* (i.i.d.) which means that each training example tuple is drawn independently from the same underlying distribution. We can think of this mapping as producing a decision boundary which separates the feature space into subspaces based upon what class label is mapped to a subspace. A classification model is the estimated mapping function f, which takes in $\mathbf{x}$ and some parameters τ and returns a predicted class label $\hat{y}$,

$$\hat{y} = f(\mathbf{x}, \tau). \tag{2.1}$$

The task is then to find the model parameters τ which give the best predictions $\hat{y}$. We will look at how to measure the quality of the predictions in more detail later.

In general we wish to minimise the number of parameters which are fitted by the classification algorithm. This is an application of Occam's Razor, we wish to find the simplest rule which explains all the data, as we expect this will lead to the best performance on unseen data. As the number of parameters increases there are more different ways to fit the available training data, and any given classification rule (which is a function of the parameters) becomes more complex. In Figure 2.1 we can see two example classification boundaries which separate the circles and stars. The solid line is a linear boundary, and thus has few parameters (as any straight line in d dimensions has $d + 1$ parameters). This line does not perfectly separate the two classes, it incorrectly classifies 6 training examples. The dashed line is a non-linear boundary, and thus has comparatively many

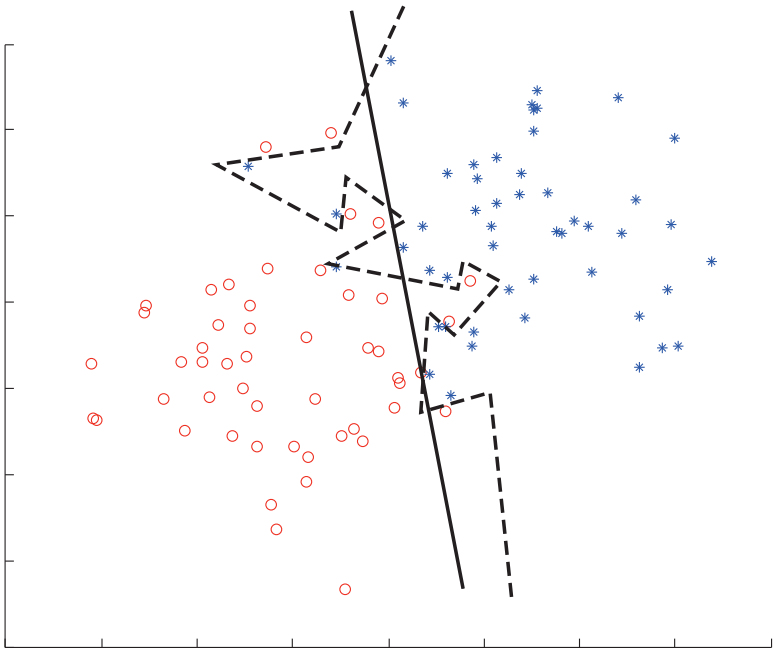


Figure 2.1: Two example classification boundaries. The solid line is from a linear classifier, and the dashed line is from a non-linear classifier.

parameters to control the different line segments. This line perfectly separates the two classes on the training data, but we would expect it to perform poorly on testing data as it has *overfit* to the training data. Each class in the figure is drawn from a 2-dimensional Gaussian distribution with unit variance, if we drew some testing data from those Gaussians the non-linear boundary would perform very poorly compared to the linear one. This phenomenon of overfitting is something which feature selection can help reduce, as it reduces the dimension of the problem which in turn reduces the potential for overfitting.

We can measure the performance of classification algorithms in multiple different ways, with the most common being the *error rate*, *i.e.* the number of misclassified examples divided by the total number of examples tested. Using $\hat{y}^i$ to denote the predicted label for the ith example and y^i to denote the corresponding true label we express the error rate for a dataset $\mathcal{D}$ and model f as,

$$\text{err}(\mathcal{D}, f) = \frac{1}{N} \sum_{i=1}^{N} 1 - \delta_{y^i, \hat{y}^i} \tag{2.2}$$

where $\delta_{y^i, \hat{y}^i}$ is the Kronecker delta function, which returns one if the arguments are identical (*i.e.* if $y^i = \hat{y}^i$), and zero otherwise (*i.e.* $y^i \neq \hat{y}^i$). The *Bayes Error*

		True Label	
		+	-
Prediction	+	TP	FP
	-	FN	TN

Table 2.1: Summarising different kinds of misclassification.

(or Bayes Rate) of a dataset or problem is the error achieved by the optimal classifier and represents the theoretical minimum error for that dataset. It is usually described as a function of the noise in the data, and thus noisy datasets where the unknown mapping ϕ contains an additional random element in general have higher Bayes error. Alternatively the features $\mathbf{x}$ may not have sufficient discriminative power to determine the class label, which also results in a high Bayes error. The Bayes error of a problem is difficult to determine but there exists a bound on it in terms of estimable values (see Section 2.3.2).

The error rate masks several important properties of the classification performance that we may wish to examine separately. To explain this we introduce the notions of *true positives*, *true negatives*, *false positives* and *false negatives*. The definitions below strictly apply in two class problems, but in Chapter 7 we will use multi-class versions by defining one class to be the positive class, and the remaining classes defined as the negative classes. In two class problems we usually refer to one class as the positive class, and the other as the negative class, with the positive class denoting the one we are interested in (*e.g.* in a medical situation the positive class is presence of disease, and the negative class is the absence of disease).

Definition 1. ***Types of classification.***
True Positive: *A true positive (TP) is a correctly predicted positive example.*
True Negative: *A true negative (TN) is a correctly predicted negative example.*
False Positive: *A false positive (FP) is an incorrect prediction that an example was positive, when it in fact was negative. Also known as a Type I error.*
False Negative: *A false negative (FN) is an incorrect prediction that an example was negative, when it in fact was positive. Also known as a Type II error.*

The different kinds of classifications are neatly summarised in Table 2.1. From these definitions we can define several new functions which we will use to measure different aspects of classification performance. Many of these functions treat the positive class differently to the negative class (or classes in the case of multi-class

problems), so throughout the thesis we will take care to define the positive class when using these measures. These functions come in pairs, and we first detail the *precision* and *recall*.

Definition 2. ***Precision and Recall.***
Precision*: the fraction of predicted positives which are actually positive.*

$$Precision = \frac{TP}{TP + FP} \tag{2.3}$$

Recall*: the fraction of actual positives which are correctly predicted positive.*

$$Recall = \frac{TP}{TP + FN} \tag{2.4}$$

The precision and recall can be used in multi-class problems to measure the predictive performance of the classifier for a particular class, as they do not require the calculation of the number of true negatives, which is not well defined for multi-class problems. Another common pair of error functions are the *sensitivity* and *specificity*.

Definition 3. ***Sensitivity and Specificity.***
Sensitivity*: the fraction of actual positives which are correctly predicted positive. Also known as the true positive rate.*

$$Sensitivity = \frac{TP}{TP + FN} \tag{2.5}$$

Specificity*: the fraction of actual negatives which are correctly predicted negative. Also known as the true negative rate.*

$$Specificity = \frac{TN}{TN + FP} \tag{2.6}$$

We note that the sensitivity and recall are different names for the same function, but in this thesis we will use the appropriate name depending on the other measure in use. There are two further functions that we will use to evaluate classification performance, the *balanced error rate* and the *F-Measure* (or F-score).

Definition 4. ***Balanced Error Rate and F-Measure.***
Balanced Error Rate (BER)*: the mean of the sensitivity and specificity.*

$$BER = \frac{Sensitivity + Specificity}{2} \tag{2.7}$$

***F-Measure**: The F-Measure (technically the F_1-Measure[1]) is the harmonic mean of the precision and the recall. Written in terms of true positives, false positives and false negatives it is,*

$$F\text{-}Measure = \frac{2 \times TP}{2 \times TP + FN + FP} \tag{2.8}$$

The balanced error rate is useful to determine the classification performance when the data has a *class-imbalance*, *e.g.* there are many more negative examples than positive examples. The F-Measure is useful to summarise the predictive performance of a particular class, as it takes into account the true positives, the false positives, and the false negatives.

2.1.1 Probability, Likelihood and Bayes Theorem

If we base our decisions on the output of a classifier we would like to know how confident the classifier is that the prediction is correct. We denote the confidence in the occurrence of an event x by its *probability* $0 \leq p(x) \leq 1$, with 1 denoting we are certain this event will occur and 0 denoting we are certain this event will not occur. We can construct a *distribution* of probabilities for a variable X (denoted $p(X)$) by incorporating all the possible states or events $x \in X$ and normalising them so the sum of the probabilities is 1. If we have a classifier which predicts a particular $y \in \{y_1, y_2\}$ with $p(y) = 0.51$, then it has a low confidence in that prediction, yet it is still the most likely prediction. If our classifier predicts y with $p(y) = 0.9$ then it is more certain that y is the correct class label. Of course our classifier makes predictions based upon the input we give it, so our probability should be conditioned on the data, *i.e.* we should calculate $p(y|\mathbf{x})$ where $\mathbf{x}$ is our test datapoint. This denotes the *conditional probability*, the probability of the outcome y when the value $\mathbf{x}$ is known. Again a distribution over the conditional probabilities can be formed, $p(Y|\mathbf{x})$, denoting the probabilities of each of the class labels based upon our test datapoint. This can be normalised over all the possible distributions for the different values of $\mathbf{x}$, resulting in $p(Y|X)$ which is the conditional probability distribution over all the possible states of Y, for all possible states of X. These distributions do not take into account the likelihood of a particular value of X, which is important to the expected performance of

[1]The F-Measure is usually parameterised as the F_β measure, where β controls the relative weighting of the precision and recall.

any given classifier. If our classifier performs well on the majority of data, but poorly on rare examples (*i.e.* ones with a small $p(\mathbf{x})$) then it will perform well in expectation. Similarly, good performance across most of the states of X does not guarantee good performance in expectation if the classifier is poor at predicting in the most common states. To incorporate this information we need a *joint probability* $p(y, \mathbf{x})$, which is the probability of both events y and $\mathbf{x}$ happening together. The joint probability distribution over Y and X can be constructed from $p(Y|X)$ by multiplying by $p(X)$, so

$$p(X, Y) = p(Y|X)p(X). \tag{2.9}$$

We can now construct one of the most important formulae in Machine Learning, *Bayes' Theorem* (or Bayes' Rule), which we can use to convert probabilities we can estimate from the data into the probability of a particular class label given that data. Bayes' Theorem follows from the commutativity of probability (*i.e.* $p(x, y) = p(y, x)$) and the definition of joint probability given in Equation (2.9), resulting in,

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}. \tag{2.10}$$

We can estimate the probability of the data, $p(X)$, and the probability of the class label, $p(Y)$, from our training dataset. We can also estimate $p(X|Y)$ by partitioning the dataset by class label and separately estimating $p(X|Y = y)$ for each y. Then we can use Bayes' Theorem to produce the probability of each of the possible labels for a particular datapoint $\mathbf{x}$. In the context of Bayes' Theorem we call $p(Y)$ the *prior*, which reflects our belief in the probability of Y *a priori* (*i.e.* before seeing any data), and we call $p(Y|X)$ the *posterior*, which reflects our updated belief in the probability of Y once we have seen the data X. If we use Bayes' Theorem and return the most likely class label as our prediction, we have chosen the mode of the distribution $p(Y|X)$ which is the *maximum a posteriori* (MAP) solution. This is an alternative to the *Maximum Likelihood* solution, which is simply the largest $p(X|Y)$, otherwise known as the model likelihood. We return to the concept of the MAP solution in Chapter 4 where we explore the MAP solution to the feature selection problem.

In general we do not have access to the true probability distribution p, and so this needs to be estimated from our training data. There are many different approaches to this estimation process but in this thesis we will focus on discrete

probability distributions rather than probability densities, and thus we use simple histogram estimators. These count the number of occurrences of a state in a dataset, and return the normalised count as a probability. This approach returns the correct distribution in the limit of infinite data, and is a reasonable approximation with finite data. As the distribution becomes higher dimensional (*e.g.* as we model more and more features) our estimate of the distribution takes longer to converge to the true distribution. This problem is commonly known as the "curse of dimensionality" [35], and is the reason many machine learning algorithms seek low dimensional approximations to the true joint distribution $p(x, y)$. Other approaches commonly used involve assuming each distribution follows a particular functional form, such as a Gaussian, and then estimating the parameters which control that distribution by fitting it to the data (*e.g.* the mean and the variance for the Gaussian distribution). This approach is more popular when taking the fully Bayesian approach to modelling a system [10], where everything is expressed in terms of a probability distribution or density, and there are no hard values returned. We will look at the Bayesian approach to modelling systems more in Chapter 3 when we look at Bayesian Networks.

When dealing with classification algorithms we often have parameters we can tune to alter the behaviour of the algorithm. These are referred to as "hyperparameters" of the model, in contrast to the model parameters which are fit by the training process. We would like to express the probability of our model parameters given the data, and to optimise those parameters to maximise the probability, which in turn minimises our error rate. When used in this way we refer to the *likelihood*, $\mathcal{L}$, of the data given the parameters, where parameters with higher likelihood fit the data better. We then construct our prior distribution over the parameters and use Bayes' Theorem to calculate the probability of our parameters given the data.

The likelihood of a model is a central concept in this thesis, as it represents how well a model fits a given dataset. The likelihood of a set of model parameters is

$$\mathcal{L}(\tau) = \prod_{i=1}^{N} q(y^i, \mathbf{x}^i|\tau). \tag{2.11}$$

Here q is our predictive model which returns a probability for a given $\{y^i, \mathbf{x}^i\}$ pair, based upon the parameters τ. The likelihood takes the form of a product of these probabilities over the datapoints due to the i.i.d. assumption made about the

dataset. It is often useful to incorporate a measure of how likely the parameters τ are *a priori*, to incorporate domain knowledge about the parameter settings, or to explicitly include Occam's razor by preferring smaller numbers of parameters. We call a likelihood which includes this prior distribution over τ, $p(\tau)$, the joint likelihood of a model,

$$\mathcal{L}(y, \mathbf{x}, \tau) = p(\tau) \prod_{i=1}^{N} q(y^i, \mathbf{x}^i | \tau). \tag{2.12}$$

Maximising this value means we find the parameters τ that both model the data, and are a priori most likely. We use a variant of this joint likelihood in Chapter 4 to investigate feature selection.

In classification problems we care about maximising the *discriminative* performance, *i.e.* how well our model predicts y^i from a given $\mathbf{x}^i$. This is represented by the *conditional likelihood* of the labels with respect to the parameters,

$$\mathcal{L}(\tau | \mathcal{D}) = \prod_{i=1}^{N} q(y^i | \mathbf{x}^i, \tau). \tag{2.13}$$

We look at cost-weighted versions of this likelihood in Chapter 7.

2.1.2 Classification algorithms

In this thesis we focus on the selection of the inputs into a classification algorithm, rather than the construction of new classification algorithms. We thus briefly discuss the classifiers we use to benchmark our feature selection algorithms.

The k-Nearest Neighbour (k-NN) algorithm [23] is conceptually the simplest of all classification algorithms. It searches for the k nearest neighbours of the test datapoint in the training data, and then returns the most popular label amongst those neighbours. If there is a tie for the most popular class then it chooses between them at random. The notion of "nearest" is determined by the choice of distance metric, though the most commonly used is the Euclidean distance. Whilst it is a simple classifier to describe, it draws complex non-linear decision boundaries, and requires the storage of all of the training data in the classifier. In this sense it is a very complex classifier as each training datapoint is an extra d parameters in the model (one for each dimension or feature). This means it does not provide a compact representation of the training data, which

could be analysed to deduce properties of the problem space. However it makes very few assumptions about the distribution of the data, beyond the presence of "smoothness" in the label space (*i.e.* examples which are close together have the same labels).

A common probabilistic technique is the Naïve Bayes classifier [35]. The classifier is based on an approximation of Bayes Rule, given in Equation (2.10), which makes it tractable with small amounts of data. Bayes Rule gives the optimal classification boundary, but calculating the terms involved is intractable due to the amount of data required to estimate each term. When generating classifications (instead of finding the probability of each class) the denominator is unnecessary, all that is required is to find the y s.t. $p(X|Y = y)p(Y = y)$ is maximal. Unfortunately even the $p(X|Y = y)$ term is difficult to estimate when there are tens of features, or each feature is multinomial/real valued. This is where the naïve assumption is required, which states that $p(X|Y = y)$ can be approximated by assuming all the features X_j are jointly independent given the label Y, *i.e.* all the features are class conditionally independent of each other. The classification rule can then be rewritten as follows

$$\arg\max_{y \in Y} \{p(Y = y) \prod_{i=1}^{d} p(X_i|Y = y)\}. \tag{2.14}$$

The conditional independence factorises the joint distribution into the product of marginal distributions for each feature. As we shall see when we consider feature selection, the assumption of class-conditional independence is not generally a valid one, and thus the Naïve Bayes classifier is suboptimal in many cases. However it provides surprisingly good classification performance even when the naïve assumption is provably untrue [33]. In addition, it is fast to train on a given dataset, and is equally fast at classifying a test dataset. In the next chapter we will look at Bayesian Networks, and see how the Naïve Bayes classifier can be interpreted as a simple Bayesian Network.

Support Vector Machines (SVMs) [22] are an optimal way of drawing a linear classification boundary which maximises the *margin* (the distance between the classification boundary and the closest datapoints of each class). The problem of finding the maximum margin boundary is solved by identifying the *support vectors* which control the position of the boundary (usually the examples on the convex hull of each class). SVMs have become ubiquitous in Machine Learning,

as the problem formulation has a convex solution (so there is a unique minima) which can be found using quadratic programming solvers so the optimal solution is always returned. While the SVM only finds linear boundaries and thus has insufficient complexity to model non-linear functions, it is possible to transform the feature space into a higher dimension which might permit a linear solution. This is called the *kernel trick* as the mapping is done through a kernel function, and it is a powerful property of the SVM algorithm. When the (high-dimensional) linear boundary is mapped back into the original (low-dimensional) space it produces a non-linear boundary, though one which is still optimal in terms of the margin. The SVM is a two-class classifier, in contrast to the k-NN and Naive Bayes methods described above which can deal with multi-class problems, though there are extensions to the SVM which give multi-class classifiers.

These are the three classifiers we will use throughout the remainder of the thesis, though of course there exist many other classifiers tailored to different problems. One important class of algorithms are *ensemble techniques* which combine multiple classification models into one classification system [66]. We refer the reader to Kuncheva [66] for more detail on ensemble algorithms, but note that these algorithms are popular when dealing with complex cost-sensitive classification problems and we now review the literature surrounding cost-sensitive problems.

2.2 Cost-Sensitive Classification

In many classification problems one kind of error can be more costly than other kinds, *e.g.* false negatives are usually much more costly than false positives in medical situations, as the cost of not treating the disease is generally higher than the cost of unnecessary treatment. If we have asymmetric costs (where one class is more important than another) we would like to train a classifier which could focus on correctly classifying examples of that class. A closely related problem is classifying in unbalanced datasets, where there are vastly more examples of one class than another. In these datasets it is simple to achieve a low error rate by continually predicting the majority class, though the classifier has learned little about the structure of the problem beyond the asymmetry in the class priors.

2.2.1 Bayesian Decision Theory

We can formalise the problem of cost-sensitive classification by constructing it as a decision theory problem, using Bayesian Decision Theory [35]. This provides a formal language for making optimal predictions given that some errors are more costly than others. The standard approach for specifying these costs is through a *cost matrix*. In decision theoretic terminology, the expected loss of a prediction procedure $p(y|\mathbf{x})$ is the *conditional risk*:

$$R(\hat{y}|\mathbf{x}) = \sum_{y \in Y} c(\hat{y}, y) p(y|\mathbf{x}). \tag{2.15}$$

Here $c(\hat{y}, y)$ is the entry in the cost matrix associated with predicting class $\hat{y}$ given that the true class is y. The *Bayes risk*, is achieved by predicting the class label which minimises the conditional risk $R(\hat{y}|\mathbf{x})$. This is the optimal prediction in terms of reducing the misprediction costs. Elkan [38] shows that in two-class problems the cost matrix is over-specified as there are only 2 degrees of freedom, each of which controls the cost for mispredicting one label. While the cost matrix approach is simple to understand it has some restrictions, as it does not allow the costs to be example dependent. Elkan proposed a more general framework [38, 114] which gives each example a weight based upon how important it is to classify correctly. This allows the weight to be a function of both y and $\mathbf{x}$, allowing it to vary with the value of the features as well as the label. This approach can be extended to the multi-class case by giving each example a vector of $|Y| - 1$ weights, where $|Y|$ is the number of classes.

2.2.2 Constructing a cost-sensitive classifier

There are many examples of cost-sensitive classifiers, where the cost matrix or some function thereof is incorporated into the final decision rule. A very simple strategy to minimise risk is to tune a threshold on class probability predictions, encouraging more predictions of a particular (costly) class, though this does tend to introduce false positives. Dmochowski *et al.* [31] showed that adjusting the threshold is an optimal solution to the problem if and only if the classification model is sufficiently expressive to fit the true underlying process which generated the data.

A more popular strategy is perturbing the data so that a *cost-insensitive*

classifier trained on the new data behaves like a *cost-sensitive* classifier trained on the original data. Examples of this are the widely used SMOTE technique [19], and the Costing ensemble algorithm [114]. These approaches resample the data according to the cost of each example, before training a standard (cost-insensitive) classifier on the newly resampled data. However, this strategy has the consequence of distorting the natural data distribution $p(x, y)$, and so the supplied training data will not be i.i.d. with respect to the testing data, potentially causing problems with overfitting. The MetaCost algorithm [32] relabels the data based upon an ensemble prediction and the risk, before training a standard classifier on the relabelled data. We can view these approaches as distorting how the classifier "sees" the world – encouraging it to focus on particular types of problems in the data. The popular LibSVM [17] implementation of the SVM classifier uses an analogous system where the internal cost function of the classifier is changed so some examples are more costly to classify incorrectly.

Dmochowski *et al.* [31] investigate using a weighted likelihood function to integrate misclassification costs into the (binary) classification process. Each example is assigned a weight based upon the tuple {$\mathbf{x}$,y}, and the likelihood of that example is raised to the power of the assigned weight. They prove that the negative weighted log likelihood forms a tight, convex upper bound on the empirical loss, which is the expected conditional risk across a dataset. This property is used to argue that maximising the weighted likelihood is the preferred approach in the case where the classifier cannot perfectly fit the true model. We will look at this weighted likelihood in more detail in Chapter 7.

2.3 Information Theory

If we wish to investigate the relationship between two variables, we first need to decide upon an appropriate measure of similarity or correlation. We would like this measure to be a function of the interaction between the variables, rather than a function of their values, and we would also like it measure as many different kinds of interaction as possible, rather than measuring a single kind of interaction, such as the linear correlation measured by Pearson's Product-Moment Correlation Coefficient [85]. We could think of this measure as the amount of shared information between two variables, as variables which are identical share exactly the same information. However to develop this idea we first need to quantify

information. The area of mathematics which deals with measuring information is innovatively named *Information Theory*.

In Information Theory, the essential quantity of information is taken to be the reduction in uncertainty in one variable when another is known. Thus before we can define information we need to define the uncertainty in a random variable, and the uncertainty in that variable when another is known. We can then define the reduction in uncertainty and thus the information content.

2.3.1 Shannon's Information Theory

Claude Shannon developed the first comprehensive set of answers to these questions in 1948, in his landmark paper "A Mathematical Theory of Communication" [97]. He defines three crucial measures which form the basis of much of the rest of the work we present in this thesis. They are the Entropy, $H(X)$, for a random variable X, the Conditional Entropy of X given another random variable Y, $H(X|Y)$, and the Mutual Information between two variables, $I(X;Y)$. All three are non-negative quantities. A detailed treatment of these three concepts is given in Cover and Thomas [24]. In this thesis we will work with discrete random variables, and so we give definitions for the discrete entropies and mutual informations. When working with continuous random variables the summations over possible states are replaced with integrations over the support of the random variable.

The Entropy of a random variable X, measures the uncertainty about the state of a sample x from X. The entropy of X is defined in terms of the probability distribution $p(x)$ over the states of X as follows,

$$H(X) = -\sum_{x \in X} p(x) \log p(x). \tag{2.16}$$

The logarithm base defines the units of entropy, with $\log_2$ using bits, and $\log_e$ using nats. In general the choice of base does not matter provided it is consistent throughout all calculations. In this thesis we will calculate entropy using $\log_2$ unless otherwise stated. High values of entropy mean the state of x is very uncertain (and thus highly random), and low values mean the state of x is more certain (and thus less random). Entropy also increases with the number of possible states of X, as if X has 4 states there are more possibilities for the state of x than if X had 2 states. Entropy is maximised when all states of X are equally likely,

as then the state of x is most uncertain/hardest to predict, and $H(X) = \log |X|$ where $|X|$ denotes the number of states of X.

The Conditional Entropy of X conditioned on Y measures the expected uncertainty of the state of a sample of x when Y is known. It is averaged over the possible states of Y so it gives a useful measure in the abstract when Y is unknown. This has two equivalent definitions, in terms of the joint probability distribution $p(x, y)$,

$$H(X|Y) = \sum_{y \in Y} p(y) H(X|Y = y) \tag{2.17}$$

$$= -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log p(x|y). \tag{2.18}$$

The conditional entropy can also be defined as the entropy of the joint variable XY minus the entropy of Y,

$$H(X|Y) = H(XY) - H(Y). \tag{2.19}$$

The conditional entropy is upper bounded by the marginal entropy, and lower bounded by 0.

$$0 \leq H(X|Y) \leq H(X) \tag{2.20}$$

This lower bound is attained when knowledge of Y enables perfect prediction of the state of X, and the upper bound is reached when X and Y are independent.

By itself the conditional entropy tells us little about the interaction between two variables, we need to know the entropy of X before we can derive any useful information. The difference between the entropy and the conditional entropy for a pair of variables is called the Mutual Information, $I(X; Y)$. It measures the average reduction in uncertainty in the state of X when the state of Y is known, and thus the increase in information. The mutual information is a symmetric measure, in that $I(X; Y) = I(Y; X)$, *i.e.* the information gained about X when Y is known is equal to the information gained about Y when X is known. This leads to several equivalent definitions for the mutual information,

$$I(X; Y) = H(X) - H(X|Y) \tag{2.21}$$

$$= H(Y) - H(Y|X) \tag{2.22}$$

$$= H(X) + H(Y) - H(XY) \tag{2.23}$$

The mutual information can also be expressed as the KL-Divergence[2] between the joint distribution $p(x, y)$ and the product of both marginal distributions $p(x)p(y)$, defined as follows

$$I(X;Y) = \sum_{x \in X} \sum_{y \in Y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)}. \tag{2.24}$$

With this formulation we can see how the mutual information reaches its maximal and minimal values more easily. The maximal value is the minimum of the two entropies $H(X)$ and $H(Y)$, and occurs when knowledge of one variable allows perfect prediction of the state of the other. In the above equation this is due to $p(x, y)$ becoming equal to either $p(x)$ or $p(y)$ for all values, and then the KL-Divergence cancels down to Equation (2.16), the standard entropy. The minimal value is 0, which occurs when X and Y are independent. In the above equation this causes $p(x, y)$ to factorise into $p(x)p(y)$, thus the fraction is unity, and the logarithm becomes zero. In the field of feature selection it is common to use a normalised function of the mutual information, termed the *Symmetric Uncertainty*. This is the mutual information between the two variables normalised by the sum of their marginal entropies, therefore

$$SU(X;Y) = \frac{I(X;Y)}{H(X) + H(Y)} \tag{2.25}$$

It is commonly advocated instead of the mutual information as unlike the mutual information it is not biased towards high arity variables, and is thus useful when comparing the scores for variables with differing numbers of states.

There is one final commonly used concept in Information Theory, the Conditional Mutual Information between two variables, conditioned on a third. The most common definition is in terms of the chain rule of mutual information, which describes how the information content of a pair of variables can be broken down in several equivalent ways,

$$\begin{aligned} I(XZ;Y) &= I(Z;Y) + I(X;Y|Z) && (2.26)\\ &= I(X;Y) + I(Z;Y|X) && (2.27)\\ &= I(X;Y) + I(Z;Y) - I(X;Z) + I(X;Z|Y). && (2.28) \end{aligned}$$

[2]The KL-Divergence is also referred to as the *relative entropy*.

The conditional mutual information measures the dependency between two variables when the state of a third is known, and is defined in terms of an expected KL-Divergence as follows,

$$I(X;Y|Z) = \sum_{z \in Z} p(z) I(X;Y|Z=z) \tag{2.29}$$

$$= \sum_{z \in Z} p(z) \sum_{x \in X} \sum_{y \in Y} p(x,y|z) \log \frac{p(x,y|z)}{p(x|z)p(y|z)}. \tag{2.30}$$

Unlike the conditional entropy, the conditional mutual information can be larger than the unconditioned mutual information. This is due to a *positive interaction* between the variables, where the dependency between two variables is increased by the knowledge of the state of a third. Again like the mutual information, the conditional mutual information is zero when the two variables are independent, conditioned on the presence of the third variable. The maximal value of the conditional mutual information is the minimum of the two *conditional entropies* $H(X|Z)$ and $H(Y|Z)$, again achieved when knowledge of one variable (and the conditioning variable) allows perfect prediction of the state of the other. We will see an important use of the conditional mutual information when we investigate structure learning in Bayesian Networks in the next chapter. In Chapters 4 and 5 we will see how the conditional mutual information is particularly important in the context of filter feature selection.

2.3.2 Bayes error and conditional entropy

One of the reasons for the popularity of Information Theory in Machine Learning is the existence of bounds on the Bayes Error of a classification problem, defined in terms of the Conditional Entropy. There exists both an upper and lower bound in terms of the conditional entropy and the range between these bounds shrinks as the conditional entropy decreases. The lower bound was proved by Fano in 1961 [39], and the upper bound was proved by Hellman and Raviv in 1970 [55]. They form the informal basis for the use of mutual informations as feature selection criteria, which we explore in the next chapter. We will derive an alternate justification for the use of mutual information based criteria in Chapter 4.

For a two class problem the Bayes error is bounded by the conditional entropy

as follows:

$$\frac{H(Y|X)-1}{\log|Y|} \leq e_{\text{bayes}} \leq \frac{1}{2}H(Y|X). \tag{2.31}$$

With these bounds we can see that the conditional entropy represents the constraint placed upon the class label by the data. If the data does not constrain the choice of class label then for any given feature vector, there may be multiple different classes which could be assigned, so there is still a large amount of uncertainty in the choice of class label, and thus the Bayes error will be high. If the data tightly constrains the choice of class label then on average a given feature vector will only have one possible class, and thus the Bayes error will be low. Therefore a large value of $H(Y|X)$ implies the features alone do not have enough information to create a good classification boundary, whereas a small value of $H(Y|X)$ implies the features contain sufficient information to produce a good boundary.

We can see the link between mutual information and feature selection by considering how the mutual information decomposes into sums of entropies, as in Equation (2.21). As the entropy of the class label $H(Y)$ is constant, maximising the mutual information $I(X;Y)$ between the features and the class label is equivalent to minimising the conditional entropy $H(Y|X)$, which in turn minimises the Bayes Error. Therefore finding a feature set X_θ which maximises $I(X_\theta;Y)$ will minimise the bound on the Bayes rate, and thus provide an informative feature set for any future classification process. We will look at the literature in information theoretic feature selection more closely in the next chapter, before deriving a more concrete link between the mutual information and the classification process in Chapter 4.

One further important point about the conditional entropy is that it is the limit of the scaled conditional log-likelihood of the labels given the data,

$$\lim_{N\to\infty}\frac{1}{N}\log\prod_{i=1}^{N}p(y^i|\mathbf{x}^i) = H(Y|X). \tag{2.32}$$

This assumes that the distribution p is perfectly estimated, which is in general untrue. Estimating these information theoretic quantities is a topic we review in the next section, whilst we return to the link between likelihood and information theory in Chapter 4.

2.3.3 Estimating the mutual information

The problem of calculating mutual informations reduces to that of *entropy estimation*, and in turn to the problem of estimating probability distributions. A thorough review of this topic is available in Paninski [83], and we provide a brief summary of the relevant issues in this section. We begin with some extra notation, introducing $\hat{p}$ to denote a probability distribution which has been estimated from a dataset sampled from the true distribution p. We can write the mutual information as the expected logarithm of a ratio of probabilities:

$$I(X;Y) = E_{xy}\Big\{ \log \frac{p(x,y)}{p(x)p(y)} \Big\}. \tag{2.33}$$

We can estimate this from data, as the Strong Law of Large Numbers assures us that the sample estimate using $\hat{p}$ converges *almost surely* to the expected value — for an i.i.d. dataset of N observations (x^i, y^i),

$$I(X;Y) \approx \hat{I}(X;Y) = \frac{1}{N}\sum_{i=1}^{N} \log \frac{\hat{p}(x^i,y^i)}{\hat{p}(x^i)\hat{p}(y^i)}. \tag{2.34}$$

In order to calculate this we need the estimated distributions $\hat{p}(x,y)$, $\hat{p}(x)$, and $\hat{p}(y)$. The computation of entropies for continuous or ordinal data is highly non-trivial, and requires an assumed model of the underlying distributions — to simplify experiments throughout this thesis, we use discrete data and estimate distributions with *histogram estimators* using fixed-width bins. The maximum likelihood estimate of the probability of an event $p(X = x)$ is given by the frequency of occurrence of the event $X = x$ divided by the total number of events (i.e. datapoints). There exist many other methods for estimating entropy, though they fall into two main approaches: plug-in estimators which first estimate the probability distributions $\hat{p}$, and direct entropy estimators which calculate the entropy from data without constructing probability distributions (*e.g.* Póczos and Schneider [90]). For more information on alternative entropy estimation procedures, we refer the reader to Paninski [83].

At this point we must note that the approximation above holds *only* if N is large *relative to the dimension of the distributions over x and y.* For example if x, y are binary, $N \approx 100$ should be more than sufficient to get reliable estimates; however if x, y are multinomial, this will likely be insufficient. If we wish

to measure the information between a set of variables $X_{\boldsymbol{\theta}}$ and a particular target variable then the quality of our estimate depends on the number of states in our set $X_{\boldsymbol{\theta}}$. As the dimension of the variable $X_{\boldsymbol{\theta}}$ grows then the necessary probability distributions become more high-dimensional, and hence our estimate of the mutual information becomes less reliable. This in turn causes increasingly poor judgements in any process we might base upon the mutual information. For precisely this reason, the feature selection literature contains many low-dimensional approximations to the complex high-dimensional mutual information. We review a selection of these approximations in Section 3.2, and a unification of these various criteria (found in Chapter 5) forms a substantial part of the contributions of this thesis.

For the remainder of this thesis, we use notation $I(X;Y)$ to denote the ideal case of being able to compute the mutual information, though in practice on real data we use the finite sample estimate $\hat{I}(X;Y)$.

2.4 Weighted Information Theory

We now briefly explore Guiaşu's formulation of Information Theory as an alternative way of measuring the uncertainty in a random variable, incorporating a measure of how important or costly each state is. This topic has received little attention in the literature, and one of the contributions of Chapter 7 will be a more thorough treatment of the weighted mutual information.

The weighted entropy was first defined as the "Quantitative-Qualitative measure of information" by Belis and Guiaşu [8]. It was termed this as it incorporated "qualitative" measures of the importance of a state into the "quantitative" measure of the entropy, using the probabilities of each state. An extensive theoretical treatment of the subject was written by Guiaşu [46] where the measure is renamed the Weighted Entropy. It is defined for a variable X with respect to the distribution $p(x)$ and a set of weights $w(x) \geq 0$ as follows,

$$H_w(X) = -\sum_{x \in X} w(x)p(x)\log p(x). \tag{2.35}$$

Due to the presence of the weights, it is no longer bounded with respect to the number of states in X, but by $w_{max}\log|X|$, where w_{max} denotes the largest weight in w. This measure is non-negative like the Shannon Entropy, and reduces to the

Shannon Entropy when all the weights are equal to one. The weights w do not have to be normalised into the range $0 \leq w \leq 1$, though any such normalisation will not change the relative values of the entropy, due to the linearity of expectation.

To ensure that H_w conforms to the axioms of an entropy measure (as listed in Guiaşu [46]) the weights for joint events must be constructed in a specific way. For any joint event $E \cup F$ the weight $w(E \cup F)$ is defined in terms of the probabilities *and* the weights of the individual events E and F. In general $w(E \cup F)$ is defined as follows,

$$w(E \cup F) = \frac{p(E)w(E) + p(F)w(F)}{p(E \cup F)}. \tag{2.36}$$

We can express this definition in a more useful form, with respect to distributions over the states $x \in X$ and $y \in Y$ as follows,

$$w(x)p(x) = \sum_{y \in Y} p(x, y)w(x, y). \tag{2.37}$$

It is this property of the weights which allows the definition of a conditional entropy as the joint entropy minus a marginal entropy,

$$\begin{aligned} H_w(X, Y) &= H_w(Y|X) + H_w(X) \\ &= H_w(X|Y) + H_w(Y). \end{aligned} \tag{2.38}$$

This is in contrast to other extensions to entropy such as Rényi's [92] or Tsallis' [105], which do not lead to natural definitions of the conditional entropy as a function of the joint distribution. It is precisely this marginalisation property of the conditional entropy which ensures the three definitions of the (Shannon) mutual information given in Equations (2.21—2.24) are equivalent.

In the same book [46] Guiaşu briefly defines a "weighted entropic measure of cohesion", which is the sum of two marginal weighted entropies, minus the joint weighted entropy. Luan *et al.* [75] also defined a similar quantity as the "Quantitative-Qualitative measure of mutual information", and Schaffernicht and Gross [96] define this quantity as the Weighted Mutual Information. This latter term is the one we will use throughout this thesis. The weighted mutual

information is defined as,

$$\begin{aligned} wI(X;Y) &= H_w(X) + H_w(Y) - H_w(X,Y) \\ &= H_w(Y) - H_w(Y|X) \\ &= \sum_{x\in X}\sum_{y\in Y} w(x,y)p(x,y)\log\frac{p(x,y)}{p(x)p(y)}. \end{aligned} \tag{2.39}$$

The final definition is in the form of a weighted relative entropy [102], between $p(x,y)$ and $p(x)p(y)$. However there is a flaw with this weighted information measure, which was shown for the weighted relative entropy by Kvålseth in 1991 [68], namely that the measure can take negative values, *i.e.* for some X and Y, $wI(X;Y) < 0$. This is a problem with the weighted mutual information which has restricted its use in the literature, as there is no intuitive understanding of what a negative information might mean. We provide examples of situations with negative weighted mutual informations in Chapter 7 and there define an new weighted information measure which is provably non-negative.

2.5 Chapter Summary

In this chapter we reviewed the background knowledge of Machine Learning, classification and Information Theory necessary to understand the contributions in the remainder of this thesis. We also looked at cost-sensitive learning approaches based upon manipulating the data, or altering the output of the classification system. In summary:

- We looked at the classification process, several common algorithms (SVM, k-NN, and Naïve Bayes), and various different metrics for evaluating classification performance.
- We looked at the central role of probability theory in machine learning, and how it measures the certainty of a prediction. We also reviewed the notion of model likelihood and how it measures classification performance.
- We investigated cost-sensitive classification, looking at the Bayes Risk and how different approaches seek to minimise it. We looked at the two main approaches, data manipulation and classifier manipulation, noting the trade-offs made by each approach.

- Finally we looked at Information Theory, examined the basic methods of measuring information, and saw the strong links between information theoretic values and classification performance. We also looked briefly at an extension of information theory which incorporates weights, leading to a measure of how costly the uncertainty in a variable is.

In the next chapter we have a detailed review of the literature in feature selection and structure learning which gives the landscape in which the contributions exist, detailing the state of the art in feature selection and pinpointing areas where this thesis advances the state of the art.

Chapter 3

What is feature selection?

In this chapter we review the literature surrounding feature selection. We begin by introducing the topic of feature selection, detailing the major concepts and approaches. In Section 3.1 we explore the three main paradigms for feature selection: filters, wrappers and embedded methods. We present a detailed review of the literature surrounding information theoretic filter feature selection in Section 3.2. We look at more general feature selection approaches which include prior knowledge in Section 3.3, and feature selection in multi-class spaces in Section 3.4. In Section 3.5 we explore Bayesian Networks as a way of modelling systems, and investigate how learning the structure of a Bayesian Network is a special case of the feature selection problem. Finally we detail the main algorithms for structure learning in Section 3.6, looking at the differences between global and local algorithms, and those which use conditional independence tests versus those which optimise a function of the network.

3.1 Feature Selection

Feature Selection is the process of determining what inputs should be presented to a classification algorithm. Originally feature selection was performed by domain experts as they chose what properties of an object should be measured to try and determine the class label. Modern classification problems attempt to collect all possible features, (*e.g.* in gene expression tasks, many thousands of genes are tested) and then use a statistical feature selection process to determine which features are relevant for the classification problem. In Chapter 6 we develop a novel method for integrating domain experts back into the feature selection

process.

Feature selection algorithms of all kinds rely upon a single assumption about the data, that the feature set contains *irrelevant* and/or *redundant* features. Irrelevant features contain no useful information about the classification problem, and redundant features contain information which is already present in more informative features. If we can select a feature set which does not include these irrelevant or redundant features then we can reduce the collection cost of the feature set, and we can investigate the remaining *relevant* features to determine how they relate to the class label. We may also improve classification performance by reducing the potential for overfitting when shrinking the feature set. These heuristic notions of relevancy and redundancy were formalised by Kohavi & John [62] into three classes: strongly relevant, weakly relevant, and irrelevant. In the definitions below, X_i indicates the ith feature in the overall set X, and $X_{\setminus i}$ indicates the set $\{X \setminus X_i\}$, *i.e.* all features *except* the ith.

Definition 5. Strongly Relevant Feature [62]
Feature X_i is strongly relevant *to Y iff there exists an assignment of values x_i, y, $x_{\setminus i}$ for which $p(X_i = x_i, X_{\setminus i} = x_{\setminus i}) > 0$ and $p(Y = y|X_i = x_i, X_{\setminus i} = x_{\setminus i}) \neq p(Y = y|X_{\setminus i} = x_{\setminus i})$.*

Definition 6. Weakly Relevant Feature [62]
Feature X_i is weakly relevant *to Y iff it is not strongly relevant and there exists a subset $Z \subset X_{\setminus i}$, and an assignment of values x_i, y, z for which $p(X_i = x_i, Z = z) > 0$ such that $p(Y = y|X_i = x_i, Z = z) \neq p(Y = y|Z = z)$.*

Definition 7. Irrelevant Feature [62]
Feature X_i is irrelevant *to Y iff it is not strongly or weakly relevant.*

The strongly relevant features are not redundant as each one contains useful information that is not present in any other combination of features. The weakly relevant features contain information which is either already present in the strongly relevant features, or exists in other weakly relevant features. The irrelevant features contain no useful information about the problem. We would like a feature selection algorithm to return the set of strongly relevant features, plus a (potentially empty) subset of the weakly relevant features, excluding the irrelevant features. Unfortunately these definitions do not lend themselves to the construction of a feature selection algorithm, as they require checking exponentially many combinations of features to ascertain weak relevancy. They also

are quite abstract quantities, and we will relate their notions of relevancy and irrelevancy to concrete information theoretic quantities in Chapter 5.

We now introduce a small amount of notation and thus formally define the feature selection problem. Throughout this thesis we will use $\boldsymbol{\theta}$ as a binary vector of length d where d is the number of features, $\theta_i = 1$ means the i'th feature is selected and $\theta_i = 0$ means it is ignored. We shall define $\neg\boldsymbol{\theta}$ as the negation of the vector $\boldsymbol{\theta}$, thus denoting the unselected features. We formally define feature selection by stating the mapping $\phi : X \to Y$ uses a subset of the features $\boldsymbol{\theta}^{rel}$, with the remaining features $\neg\boldsymbol{\theta}^{rel}$ being redundant or irrelevant. Therefore $\phi : X \to Y$ is equivalent to $\phi' : X_{\boldsymbol{\theta}^{rel}} \to Y$ where $X_{\boldsymbol{\theta}^{rel}}$ is the subset of X containing the features selected by $\boldsymbol{\theta}^{rel}$. The concept of sparsity in the statistics literature [10] is related to the process of feature selection. A sparse solution to a prediction problem means that few of the features are involved in the prediction, hence we can think of feature selection as enforcing sparsity on the solution. The term arises from matrices where a sparse matrix is one with few non-zero elements. In our case we say $\boldsymbol{\theta}$ is sparse if it has few set bits, thus the feature set selected by $\boldsymbol{\theta}$ is also sparse. The choice of search function is important in feature selection problems as the space of possible feature subsets is the powerset of the dimension, thus the number of possible feature sets is 2^d. Therefore examining all possible feature sets is intractable for any reasonably sized problem.

Feature selection algorithms are a subset of the more general *feature extraction* algorithms. Feature extraction techniques produce a new feature set by processing the original set. This can be by combining multiple features, or projecting the feature set into a higher or lower dimensional space. Such techniques are useful when the classification algorithm cannot understand the current representation, *e.g.* we can see the kernel trick in SVM classifiers as a form of feature extraction (see Section 2.1.2). In feature selection we extract features by returning a relevant subset of the input feature set. For the remainder of this thesis we will focus on feature selection algorithms, of which there are three main kinds: filters, wrappers and embedded methods. Filters and wrappers are defined by two things, the evaluation function or *criterion* which scores the utility of a feature or a feature set (which we term J), and the search algorithm which generates new candidate features or feature sets for evaluation. We show the general form of a filter or wrapper algorithm in Algorithm 1. Embedded methods are feature selection techniques which are integrated into a particular classification algorithm therefore

Algorithm 1 The general form of a filter/wrapper

Require: A dataset $\mathcal{D}$, with features X and label Y
  Initialise candidate feature subset S
  while Stopping criterion == False **do**
    Propose new candidate subset S' based on S
    Evaluate $J(S')$
    if $J(S') > J(S)$ **then**
      $S = S'$
    end if
  end while

separating out the evaluation function from the search procedure is more difficult. We explore the main differences between the three approaches below.

3.1.1 Filters

Filter approaches use a measure of relevancy or separation between the candidate feature or feature set and the class label as the scoring function for that feature or feature set. These measures range from simple correlation measures such as Pearson's Correlation Coefficient [85], through complex correlation measures such as the mutual information (discussed in Section 2.3), to complex measures of inter and intra class distances, used in the Relief algorithm [60]. All these measures return a number which represents the strength of the relationship between the candidate feature set and the class label. This relationship might be a measure of information, or a measure of the separability of the classes based on that feature set. Other common measures, are based upon probabilistic independence, which is a topic we discuss in more detail in Section 3.5. Much of the early work in filter feature selection focused on different kinds of distance or divergence metrics, both probabilistic and based directly upon the data [30]. We call the scoring function a *feature selection criterion*, and the study of the criteria based on information theoretic measures is the topic of this thesis.

Filter algorithms can be further divided into those which measure univariate relationships or multivariate relationships. Univariate measures only consider the relationship between the candidate feature and the class label, ignoring any interactions with the previously selected features. In contrast, multivariate methods measure the relationship in the context of previously selected features. This can either increase or decrease the strength of the relationship between the candidate

feature and the class label, but (in general) better represents how it would work in a classifier. A more detailed review of scoring criteria is found in Duch [34]. In this thesis we focus on a set of filter algorithms which use variations on information theoretic measures (see Section 2.3 for a description of Information Theory) to measure the interaction between features, and to measure the correlation with the class label. We review the information theoretic filter literature in more detail in Section 3.2.

The scoring criteria is coupled with a search method which describes how the candidate feature sets are selected (see Reunanen [93] for a review of search strategies for both filter and wrapper approaches). The complexity of the scoring criteria usually dictates the complexity of the search method, as univariate criteria will not benefit from complex search methods, due to their inability to consider feature interactions. Many common filters (*e.g.* Relief [60] or mRMR [86]) use greedy forward or backward searches, testing each feature in turn for inclusion (exclusion) and adding (removing) the feature which scores the highest (lowest). More complex searches include "floating" methods [91] which dynamically adjust the size of the selected feature set, adding features when they improve the scoring criteria and removing those features which do not decrease the criteria. There exist optimal search strategies based upon Branch & Bound methods [99] which can exclude groups of features from consideration if they can never improve in performance. However such complex search algorithms are unnecessary in certain situations, notably in the case of Bayesian Networks where the Markov Blanket can be recovered using a greedy search (see Section 3.6). For the remainder of this thesis we will use greedy searches to test our scoring criteria, and leave the investigation of more complex search methods to future work.

The choice of stopping criterion is also an important question in filter methods, as there is no error measure to monitor the performance. In general either a fixed number of features is selected or the search continues until the score measure for all remaining unselected features drops below a threshold. Again as we are interested in the scoring criterion itself we will leave the investigation of stopping criteria to future work, and simply select a fixed number of features.

One benefit of filter methods is due to the use of abstract measures of correlation between variables, they return a feature set which should perform well across a wide range of classification algorithms, assuming the filter does not have drastically different assumptions to the classifier (a topic we investigate in Chapter

5). Filter methods are usually the fastest of the three kinds of feature selection technique mentioned here as they do not require the training of a classification algorithm to score the features.

3.1.2 Wrappers

In contrast to filters, wrapper approaches (*e.g.* Kohavi & John [62]) use the performance of a classification algorithm on a particular testing dataset as the evaluation function. This means the feature set is closely tailored to the classification algorithm used, and may not perform well if used with a different classifier. The name comes from the feature selection process being "wrapped" around a particular classification algorithm.

To evaluate the utility of a particular feature, it is included in the current selected feature set and the performance of the feature set as a whole is tested on the training data. This is a time intensive process as it involves training the classifier, and then testing on all the datapoints. However it does fully capture all the interactions between the features (that the classifier can use), and is thus unlikely to select redundant features.

In general the classification algorithm used in the wrapper is the same as the final classification algorithm which will form the final system, and so the main issue with wrapper methods is the choice of search method and stopping criterion. Much of what was mentioned in the previous section on filter methods is valid for the choice of search method and stopping criterion with wrappers.

3.1.3 Embedded methods

Embedded methods are a disparate group of feature selection algorithms which are similar to wrappers in that they use a classification algorithm in the feature selection. The feature selection process is "embedded" into the construction of the classifier, as the classifier learns the appropriate weights for a given feature, and potentially removes it from consideration. The term embedded methods thus covers a wide range of different feature selection techniques, making it difficult to analyse them as a group beyond their dependency on a particular classification algorithm. Common examples of this approach are the Recursive Feature Elimination algorithm for SVMs (SVM-RFE) [51] which repeatedly trains an SVM, at each stage removing features which are given a low weight by the SVM; and

the LASSO regression algorithm [104] which drives the weights of irrelevant features to zero in the process of constructing a linear model. We will look at Lasso in more detail when we discuss feature selection algorithms which include prior knowledge in Section 3.3. Like wrapper algorithms, embedded methods produce feature sets which are closely tied to the classification algorithm used. Again this may cause the feature sets to perform poorly when used with other classification algorithms, or if the feature set is used for further analysis of the underlying problem.

We have now reviewed the three main approaches to feature selection. Now we will explore the literature surrounding information theoretic filter algorithms, which are the topic of this thesis.

3.2 Information theoretic feature selection

An information theoretic filter algorithm is one that uses a measure drawn from Information Theory (such as the mutual information we described in Chapter 2) as the evaluation criterion. Evaluation criteria are designed to measure how useful a feature or feature subset is when used to construct a classifier. We will use J to denote an evaluation criterion which measures the performance of a particular feature or set of features in the context of the currently selected set. The most common heuristic evaluation criteria in information theoretic feature selection is simply selecting the feature with the highest mutual information to the class label Y, resulting in

$$J_{mim}(X_k) = I(X_k; Y). \tag{3.1}$$

We refer to this feature scoring criterion as 'MIM', standing for *Mutual Information Maximisation*. This heuristic, which considers a score for each feature independently of others, has been used many times in the literature, the first mention of such a scoring procedure is in Lewis (1962) [73] though it is not explicitly referred to as a mutual information. It reappears in more recent work under different guises, *e.g.* Lewis (1992) [72]. This criterion is very simple, and thus the choice of stopping condition in the search is more important than the search algorithm itself. This is because it is a univariate measure, and so each feature's score is independent of the other selected features. If we wish to select

k features using MIM we will pick the top k features, ranked according to their mutual information with the class. We could also select features until we had reached a predefined threshold of mutual information or another condition, but the choice of search would make little difference. We saw in Chapter 2 how the mutual information can be used to construct both an upper and lower bound on the Bayes error rate [39, 55], and these bounds form the justification for the use of this simple criterion. Unfortunately the independence assumed by measuring each feature's score without considering the currently selected features is a serious limitation of this approach. If all the features are independent then the assumption holds, and MIM will select a useful feature set. However the assumption of independent features is untrue in the vast majority of cases, and thus this approach is usually suboptimal.

We saw in the previous section that a useful and parsimonious set of features should not only be individually *relevant*, but also should not be *redundant* with respect to each other — selected features should not be highly correlated to other selected features. We note that while this statement is appealingly intuitive, it is *not strictly correct*, as we shall see in the next chapter. In spite of this, several criteria have been proposed that attempt to pursue this 'relevancy-redundancy' goal. For example, Battiti [6] presents the *Mutual Information Feature Selection* (MIFS) criterion:

$$J_{mifs}(X_k) = I(X_k;Y) - \beta \sum_{X_j \in S} I(X_k;X_j), \tag{3.2}$$

where S is the set of currently selected features. This includes the $I(X_k;Y)$ term to ensure feature *relevance*, but introduces a penalty to enforce low correlations with features already selected in S. MIFS was constructed (like many of the criteria in this chapter) to use a simple sequential forward search, greedily selecting the best feature in each iteration. The β in the MIFS criterion is a configurable parameter, which must be set experimentally. Using $\beta = 0$ is equivalent to $J_{mim}(X_k)$, selecting features independently, while a larger value will place more emphasis on reducing inter-feature dependencies. In experiments, Battiti found that $\beta = 1$ is often optimal, though with no strong theory to explain why. The MIFS criterion focuses on reducing *redundancy*; an alternative approach was proposed by Yang and Moody [110], and also later by Meyer *et al.* [80] using the

Joint Mutual Information (JMI), to focus on increasing *complementary* information between features. The JMI score for feature X_k is

$$J_{jmi}(X_k) = \sum_{X_j \in S} I(X_k X_j; Y). \tag{3.3}$$

This is the information between the target and a *joint* random variable $X_k X_j$, defined by pairing the candidate X_k with each feature previously selected. The idea is if the candidate feature is 'complementary' with existing features, we should include it.

The MIFS and JMI schemes were the first of many criteria that attempted to manage the relevance-redundancy trade-off with various heuristic terms, however it is clear they have very different motivations. The criteria identified in the literature 1992-2011 are listed in Table 3.1. One of the more popular criteria which trades off relevancy and redundancy is the Fast Correlation Based Filter (FCBF) of Yu & Liu [112]. This criterion selects a feature provided its individual relevancy $I(X_i; Y)$ is greater than the redundancy between X_i and any of the selected features $X_j \in S$, $I(X_i; X_j)$. The standard approach to creating filter criteria is to *hand-design* them, constructing a criterion from different terms where each term deals with a different part of the selection problem. It is common to see a relevancy term for an individual feature combined with some number of redundancy terms between that feature and the currently selected feature set. This has lead to many different criteria, each of which aims to manage the relevancy-redundancy trade-off in a different way. Several questions arise here: Which criterion should we believe? What do they assume about the data? Are there other useful criteria, as yet undiscovered? We explore these questions in Chapter 5 and the answers provide the basis for much of the work in this thesis.

There has been some previous work aiming to answer some of these questions; one of the first attempts to unify these varying criteria is due to Brown [12], which viewed them as approximations to the full mutual information $I(S; Y)$ between the set of selected features S and the label Y. This can be expanded into a series of terms based upon McGill's Interaction Information [78], and many of the criteria were found to follow a similar functional form which curtailed the expansion at a particular point. Balagani and Phoha [5] investigate the links between the mRMR, MIFS and CIFE criteria showing how each trades off different information theoretic terms to produce a scoring criteria and how these

Criterion	*Full name*	*Ref*
MIM	Mutual Information Maximisation	[72]
MIFS	Mutual Information Feature Selection	[6]
KS	Koller-Sahami metric	[63]
JMI	Joint Mutual Information	[110]
MIFS-U	MIFS-'Uniform'	[69]
IF	Informative Fragments	[109]
FCBF	Fast Correlation Based Filter	[112]
AMIFS	Adaptive MIFS	[103]
CMIM	Conditional Mutual Info Maximisation	[40]
mRMR	Min-Redundancy Max-Relevance	[86]
ICAP	Interaction Capping	[58]
CIFE	Conditional Infomax Feature Extraction	[74]
DISR	Double Input Symmetrical Relevance	[79]
MINRED	Minimum Redundancy	[34]
IGFS	Interaction Gain Feature Selection	[36]
SOA	Second Order Approximation	[48]
mIMR	Min-Interaction Max-Relevance	[11]
CMIFS	Conditional MIFS	[20]

Table 3.1: Various information-based criteria from the literature. In Chapter 5 we investigate the links between these criteria and incorporate them into a single theoretical framework.

terms affect the selected feature set. We present a different view of all these criteria in Chapter 5 where we investigate the links between them at a deeper level, namely what assumptions are they making about the underlying probability distribution p.

We now investigate an area with little relation to the information theoretic algorithms we have discussed, namely that of feature selection incorporating prior (domain) knowledge. In Chapter 6 we will see how to construct information theoretic algorithms which naturally incorporate such knowledge.

3.3 Feature selection with priors

We now turn to algorithms which allow the inclusion of prior knowledge into the feature selection process. This knowledge can take many forms, from information about the relevancy of specific features, or groups of features, to a preference for a certain size of feature set (or sparseness of the solution). The canonical algorithm which includes a sparsity prior is the LASSO [104] for regression using generalised

linear models. The LASSO performs an L_1 regularisation of the weight vector of the linear model, necessarily driving many of the weights to zero, leaving only the weights (and thus features) which are necessary for a good prediction. This can be expressed as follows,

$$E(\mathcal{D}, \mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2 + \lambda \sum_{j=1}^{d} |w_j|. \tag{3.4}$$

This is the error for a given training dataset $\mathcal{D}$ and weight vector $\mathbf{w}$, where λ is a parameter which controls the strength of the regularisation, and thus the amount of non-zero weights in $\mathbf{w}$. There have been many extensions to the basic framework, incorporating different kinds of knowledge in addition to a general sparsity prior. Helleputte and Dupont [54] present a good example of this recent work in informative priors for regularized linear models. They develop a prior for an approximate zero-norm minimization, constraining some of the dimensions according to knowledge gained from the biological literature.

Yu *et al.* [113] encode knowledge via constraints on a kernel canonical correlation analysis (KCCA) used to estimate the mutual information between a pair of features. They incorporated this modified mutual information estimate into the FCBF [112] algorithm, and use it to select features as inputs to regression. These constraints forced the KCCA to return a score above a certain value if their knowledge indicated a link between the features. However they do not investigate the effects of imposing incorrect constraints on their algorithm.

Krupka *et al.* [65] define *meta-features*, where each feature is qualified by additional information, and a mapping is learnt from meta-features to some measure of feature 'quality'. Knowledge can then be transferred between tasks by learning the feature-quality mapping for similar problems; however the challenge remains to define a good quality measure and reliably learn the mapping.

When we look at Bayesian Networks and structure learning in Section 3.6 we will find other algorithms which can incorporate prior knowledge into the feature selection process in terms of explicit prior structure, and more general network features.

3.4 Multi-class and cost-sensitive feature selection

Multi-class datasets pose a particular problem for feature selection algorithms, as features predictive of one class may not help predict others. In the binary case this is unlikely to lead to poor performance but in a multi-class problem this can lead to a feature set which has poor predictive performance for entire classes. This problem can be linked to the issue of cost-sensitive classification which we reviewed in the previous chapter, as with more classes there is more opportunity for them to have unbalanced misclassification costs. There may also be an unbalanced class distribution where some classes have a very small number of training examples, which can be interpreted as a cost-sensitive problem. In this section we review the literature in multi-class and cost-sensitive feature selection which will form the basis of the novel material in Chapter 7 where we derive a cost-sensitive feature selection criteria. A more extensive survey of empirical performance on multi-class datasets is found in Forman [42].

One work which highlights the main issue in multi-class feature selection is by Forman [43], which explores the problem of classes which have different predictive feature sets. The analysis shows that even when each class has the same number of examples, common filter feature selection algorithms like MIM and χ^2 ranking fail to select features which are predictive of all the classes. This leads to poor performance on certain classes with few predictive features and good performance on other classes which have strongly predictive features. The proposed solution to this problem is termed Spread-FX, which generates a feature ranking for each class using an input algorithm such as MIM, before selecting features using a scheduler from the different feature rankings. The per class feature ranking is generated by converting the multi-class problem into a one-versus-all problem, where the current class is the positive label, and all other classes are the negative label. The scheduling algorithm is then either an explicit round robin scheduler, where the top ranked feature is selected from each class label in turn, or a probabilistic scheduler where the next class is chosen by sampling from the distribution over classes. This technique is shown to improve performance against all the univariate ranking techniques in a wide variety of text-classification problems. An extension is proposed to cost-sensitive feature selection by altering the distribution sampled by the probabilistic scheduler to incorporate cost information. One

issue with this technique is that it is unclear how to adapt it to multivariate ranking algorithms like MIFS or JMI, where the score given to a particular feature is dependent upon the previously selected features.

The FCCF algorithm proposed by Chidlovskii and Lecerf [21] approaches the multi-class problem from a different perspective. It is based upon the FCBF algorithm discussed in Section 3.2, but modified so the exclusion heuristic takes into account the presence of multiple classes. In addition to the standard FCBF exclusion heuristic that the candidate feature X_i has shares more information with a selected feature than the class label, it must also have less class specific information than that selected feature. Therefore the feature X_i is excluded iff $\exists\ y \in Y, X_j \in S$ s.t. $SU(Y = y; X_j) \geq SU(Y = y; X_i)$ and $SU(X_i; X_j) \geq SU(Y; X_i)$, where $SU(X; Y)$ is the symmetric uncertainty between X and Y (see Section 2.3).

Chapelle and Keerthi [18] present a modification of L_1-SVM to extend it to the multi-class case. L_1-SVM is a regularised version of the standard binary SVM algorithm which like LASSO mentioned in the previous section performs an L_1 regularisation of the feature weight vector driving most of those weights to zero, resulting in a sparse selected feature set. As SVMs are binary classification algorithms the standard RFE and L_1 methods select independent feature subsets for each possible class. The proposed method shares the regularisation penalty across all the individual SVM optimisation functions, thus ensuring that each binary problem is properly penalised by the number of features in use.

The final algorithm we review is an explicit cost-sensitive feature selection algorithm, which aims to select features which minimise the misclassification cost. This approach is due to Robnik-Šikonja [95], and works with many univariate feature ranking procedures used in decision trees as splitting criteria. The proposed technique adjusts the probabilities of each split criteria, altering the probability for each class based upon the expected risk of misclassification as follows,

$$\epsilon_y = \frac{1}{1 - p(y)} \sum_{\hat{y} \neq y}^{|Y|} p(\hat{y}) C(y, \hat{y}) \tag{3.5}$$

$$p'(y) = \frac{p(y)\epsilon_y}{\sum_{\hat{y}}^{|Y|} p(\hat{y})\epsilon_{\hat{y}}}. \tag{3.6}$$

In the equation above $C(y, \hat{y})$ is the cost of misclassifying class y as $\hat{y}$, and $p(y)$ is the marginal probability of the label y. This approach can be seen as extending

the work of Elkan [38] to feature selection, as it effectively resamples the data according to its expected misclassification cost. The new probability values can then be incorporated into a function such as the mutual information to score the features.

We now move to a different but related section of the literature, that relating to Bayesian Networks and specifically the learning of network structure.

3.5 Bayesian Networks

A Bayesian Network is a model of a probability distribution which shows how the variables interact in a system. They are first defined by Pearl [84] as a method for encoding the interactions between variables, showing the independences in the system. The whole system is modelled as a *directed acyclic graph* (DAG), with the variables being nodes in the graph, and the arrows denoting the direction of influence. In classification problems we also include the class label as a node in the graph, in addition to all the features. Each node takes a state which is probabilistically dependent on its parent nodes, and only those nodes. The graph is acyclic (*i.e.* has no directed path from one node back to itself) to ensure no node ends up as its own ancestor, as this could cause nodes to oscillate between states. If there is no path between any two variables then the probability distributions of those variables are independent. Any node is made conditionally independent from the rest of the graph by its *Markov Blanket*, the set of all parents, children and spouses (other parents of the child nodes) of that particular node. Any set of nodes which removes the dependence between two other nodes is said to d-separate those two nodes. The Markov Blanket can be seen as d-separating the target node from the rest of the network. This is useful as it means that only the states of the nodes in the Markov Blanket are required to predict the state of the target node. A Bayesian Network classifier can be constructed by encoding a set of independence statements between the features and the class label, and then learning the probability distributions over the states of each node conditioned on its parents. The Naïve Bayes classifier is an example of a Bayesian Network classifier, where all the features are child nodes of the class label, and are thus class-conditionally independent of each other. Figure 3.1 shows a generic Bayesian Network, highlighting the Markov Blanket for the central node.

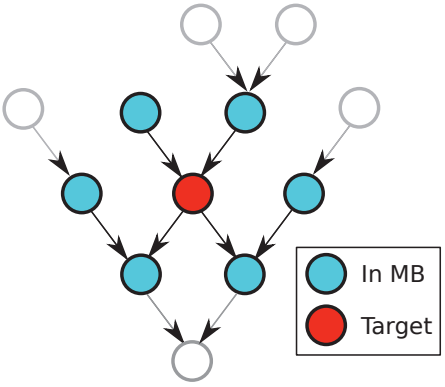


Figure 3.1: A Bayesian network, with the target node shaded in red, and the Markov Blanket of that node shaded in cyan.

We will formally define the properties of Bayesian Networks in terms of conditional independences using the notation $X \perp\!\!\!\perp Y|Z$ to mean X is conditionally independent of Y given Z. A Bayesian Network can be defined for any probability distribution where the following properties hold:

- **Symmetry:** $X \perp\!\!\!\perp Y|Z \Leftrightarrow Y \perp\!\!\!\perp X|Z$.
- **Decomposition:** $X \perp\!\!\!\perp (Y \cup W)|Z \Rightarrow X \perp\!\!\!\perp Y|Z \;\&\; X \perp\!\!\!\perp W|Z$.
- **Weak Union:** $X \perp\!\!\!\perp (Y \cup W)|Z \Rightarrow X \perp\!\!\!\perp Y|(Z \cup W)$.
- **Contraction:** $X \perp\!\!\!\perp Y|Z \;\&\; X \perp\!\!\!\perp W|(Z \cup Y) \Rightarrow X \perp\!\!\!\perp (Y \cup W)|Z$.
- **Intersection:** $X \perp\!\!\!\perp Y|(Z \cup W) \;\&\; X \perp\!\!\!\perp W|(Z \cup Y) \Rightarrow X \perp\!\!\!\perp (Y \cup W)|Z$.

One further important property of a Bayesian Network is *faithfulness*. A Bayesian Network is said to be *faithful* to a probability distribution if the network encodes all conditional independence statements which can be made about the distribution, and if the distribution has all conditional independence properties which can be inferred from the network. The set of probability distributions which are faithful to a Bayesian Network is smaller than the set of all probability distributions, and does not include distributions which have deterministic relationships between nodes [84]. This means a Bayesian Network can model a smaller class of problems than the general supervised learning approach. One important point is that a node may have multiple different Markov Blankets if the probability distribution is not faithful. An example of this problem is given in the TIED dataset constructed by Statnikov *et al.* [101].

3.6 Structure Learning

An important part of learning with Bayesian Networks is determining the graph structure which relates the nodes. This can either be done by hand, where domain experts construct the relationships between the nodes, or through statistical inference. The process is termed Structure Learning when the network is learned algorithmically from a particular dataset. There are two different approaches to structure learning, constraint-based or score and search. Constraint-based structure learning finds variables which are dependent upon each other and links the two nodes. Once all links have been found, they are oriented using a variety of different statistical tests, to produce the required DAG. Alternatively some constraint-based algorithms start from a fully connected graph and use independence tests to remove links between nodes which are conditionally independent. Score and search methods use a scoring metric for how well the current network structure fits the data, and then search in the space of possible structures for the structure which maximises the score measure. The scoring metric is invariant to certain valid permutations of the graph, therefore multiple graphs may have the same score and so another method is required to differentiate between them.

There are strong links between structure learning algorithms and feature selection algorithms. This is due to the properties of Markov Blankets. As a Markov Blanket is the set of nodes which make the target node independent from the rest of the graph, it is also the set of features required for optimal prediction of that target node [107]. Thus a structure learning algorithm can be thought of as a global feature selection algorithm, which learns the features required to predict each node in turn. In problems where the probability distribution $p(x, y)$ is not faithful to a Bayesian Network then there may be multiple possible structures, all of which are in some sense a valid representation of that distribution. In this case there are multiple Markov Blankets and thus many equally valid solutions to the feature selection problem.

Conditional independence testing algorithms can be further divided into those which do "local" learning, and those which do "global" learning [2]. Local learning algorithms are concerned with finding the Markov Blanket of a particular node, and thus only give the local structure around that node. Global learning algorithms aim to find the whole structure of the Bayesian Network, this structure can then be examined separately to find the Markov Blanket for any given node.

3.6.1 Conditional independence testing

As mentioned previously the Markov Blanket of a node is a solution to the feature selection problem when working with Bayesian Networks. The Markov Blanket discovery task is easier than the full structure learning task, as it does not require the orientation of the links between nodes, nor differentiating between the indirectly connected spouse nodes and the directly connected parent and child nodes. We first explore the local learning algorithms which use conditional independence testing to find Markov Blankets. These algorithms are in practice very similar to the filter feature selection algorithms we looked at in Section 3.2, and we investigate these links in Chapter 6. They are also known as constraint-based structure learning algorithms, and we will use the shorthand CB to refer to them as a group. We then look at methods for combining local structure into global structure, and other global structure learning methods.

Local structure learning

The first algorithm which attempted to learn the Markov Blanket of a node was strictly a feature selection approach, presented in Koller & Sahami [63]. It proceeded via backwards elimination from the full feature set, removing the feature which had the smallest interaction with the class label, given its (approximate) Markov Blanket. This approximate algorithm is closest to the CMIM algorithm we discuss as part of Chapter 5, in that each feature is scored by its minimal interaction when conditioned on the selected feature set. This algorithm does not return the Markov Blanket of the target node (usually the class label), but it was used as a baseline in the development of other structure learning algorithms.

The first true structure learning algorithm is the Grow-Shrink (GS) algorithm by Margaritis and Thrun [77]. This adopted the two stage algorithm which is common to many local learning algorithms, first growing the candidate Markov Blanket by adding new features until all remaining unselected features are conditionally independent of the target, then shrinking the candidate Markov Blanket to remove any false positives which may have been selected. This local algorithm for constructing Markov Blankets is then ran over each node of the network, and the resulting subgraphs are combined to construct a DAG for the entire network. The choice of conditional independence test used in the algorithm is left unspecified, as there are multiple ones which are suitable. The IAMB algorithm by Tsamardinos and Aliferis [107] is a refinement of the GS algorithm. It uses a

different ordering heuristic to choose in what order to select and remove features, compared to the GS algorithm. This heuristic simply selects the feature which has the largest conditional mutual information, and removes the feature which has the smallest conditional mutual information. They state that this heuristic improves the runtime of the algorithm by prioritising features which most improve the quality of the returned Markov Blanket. The algorithm for IAMB is given in Algorithm 2, though the general structure is true for most of the local structure learning algorithms we explore in this section. The $f(X; Y|\text{CMB})$ in Algorithm 2 represents the conditional independence test used, and is a parameter of the algorithm.

Algorithm 2 IAMB [107].

Phase 1 (forward)
CMB $= \emptyset$
while CMB has changed **do**
  Find $X \in \Omega \setminus \text{CMB}$ to maximise $f(X; Y|\text{CMB})$
  if $f(X; Y|\text{CMB}) > \epsilon$ **then**
    Add X to CMB
  end if
end while
Phase 2 (backward)
while CMB has changed **do**
  Find $X \in \text{CMB}$ to minimise $f(X; Y|\text{CMB} \setminus X)$
  if $f(X; Y|\text{CMB} \setminus X) < \epsilon$ **then**
    Remove X from CMB
  end if
end while

The authors of IAMB proceeded to publish several more data efficient variants of the IAMB algorithm, which require fewer samples to accurately estimate the necessary tests. The most common variants are the MMMB [106] and HITON [4] algorithms. MMMB first finds the set of parents and children of a target node, by finding the minimal set of nodes which makes each node most independent of the target. This is similar to the heuristic proposed by Koller & Sahami for Markov Blanket recovery in classification problems. Once the set of parents and children have been found these are added to the candidate Markov Blanket. Then the parents and children are found for each node in the candidate Markov Blanket, and these are tested to see if they are spouse nodes of the original target. This approach reduces the computation by only conditioning on the minimal set of

nodes (*i.e.* the set of parents and children of the target). The HITON algorithm is essentially similar to the MMMB algorithm, but is tailored for prediction tasks. It uses a final wrapper to prune the candidate Markov Blanket by removing features which do not affect classification performance.

One further local structure learning algorithm is the new variant of GS developed by Margaritis [76]. This extends the GS framework beyond the learning of Markov Blankets to the general case of learning Markov Boundaries. This is still a set of variables which make a particular node probabilistically independent from the rest, but it includes cases which cannot be expressed as Bayesian Networks, such as in the TIED dataset [101], where there are multiple different Markov Blankets (which is not possible in a true Bayesian Network). The algorithm is extended to test sets of variables for dependence in the inclusion phase. This makes the algorithm exponential rather than polynomial in the number of nodes, which precludes its usage in practice. Margaritis thus proposes a randomised version, which randomly samples sets of a fixed size, tests each set for dependence, and adds the set with the largest measured dependence (similar to the heuristic ordering added in the IAMB algorithm).

Global structure learning

One of the first global structure learning algorithms was based upon the conditional independence testing methodology, namely the PC algorithm by Spirtes *et al.* [100]. This first constructs an undirected graph where the absence of a link between two nodes indicates they are conditionally independent. After this construction process each link is oriented (if possible) by analysing the graph structure, as a Bayesian Network is an *acyclic* graph, so there are no directed paths starting at one node and returning to that node. The PC algorithm is not usually able to orient all the edges, and thus returns a partially directed graph where some edges are left undirected. These partially directed graphs are usually called "patterns" or "essential graphs".

The PC algorithm is unusually reliant upon the quality of the independence test used, as it uses the current graph state to construct the set of independence tests needed for the next node. This causes errors to cascade through the graph structure as one mistake produces an incorrect structure to base the next test on, which in turn causes more failures [27]. This problem is partially solved by the LGL family of algorithms developed by Aliferis *et al.* [2, 3] which learn the

local structure for each node independently before combining each local structure to learn the full graph. A local learning algorithm such as an IAMB variant is used to learn the set of parents and children for each node in turn. Those local structures are then used to produce an undirected graph for the whole structure (as it cannot differentiate between the parents and the children) before using another algorithm to orient the edges. In the paper they explore the use of the BDeu score to orient the edges, which is an example of the score and search methods we review in the next section.

3.6.2 Score and search methods

Score and search (S&S) methods for structure learning aim to maximise a function of the network structure with respect to a given dataset. This can be analysed in a similar way to a filter feature selection algorithm, as indicated by the name score and search. Each technique is made up of the scoring function (or criterion) and the search method used to maximise that scoring function.

Many of the techniques use similar search techniques based upon the concept of a neighbourhood in graph space. From a given graph structure G the neighbourhood of G, $\eta(G)$, is defined as all DAGs which can be constructed from G via addition, deletion or reversal of a single edge [82]. Within this neighbourhood view there are many different search strategies based upon hillclimbing [53], Simulated Annealing [61], and Markov-Chain Monte-Carlo (MCMC) [82] techniques. We will briefly outline a few scoring functions along with their associated search methods.

The most common approaches found in the S&S literature are based upon the Bayesian Dirichlet (BD) score [53]. This family of scoring functions make several assumptions about the underlying true network which they are trying to recover:

1. The data is drawn from a multinomial, with positive probability everywhere (*i.e.* there are no logical relationships between variables).

2. That the data generating parameters are both globally independent across the network, and locally independent with respect to the state of the parent set of a node.

3. That each node's parameters only depend upon the parent set of that node.

4. That each node's parameters form a Dirichlet distribution.

The most popular member of this family is the BDe (Bayesian Dirichlet equivalence) metric [53], which imposes an additional assumption, that equivalent network structures should have the same score. This effectively replaces the Dirichlet assumption, as the assumption of equivalence implies that all node parameters are Dirichlet distributed. The BDe score for any given graph G given a training dataset $\mathcal{D}$ is

$$p(\mathcal{D}, G) = p(G) \prod_{i}^{d} \prod_{j=1}^{\Pi_i} \frac{\Gamma(N'_{ij})}{\Gamma(N'_{ij} + N_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(N'_{ijk} + N_{ijk})}{\Gamma(N'_{ijk})}. \tag{3.7}$$

In the equation above N is the number of datapoints, N' is the equivalent sample size in the prior network (*i.e.* how strong the prior is), N_{ijk} is the number of examples where the ith node takes the kth state and the parent set of i takes the jth state, and Γ is the gamma function. It is also possible to add more specific domain knowledge about the possible structures by defining the prior $p(G)$. This measure is then paired with a neighbourhood search based upon hillclimbing or simulated annealing. The hillclimbing approach simply moves to the graph in the neighbourhood which most improves the BDe score, terminating when no graph in the neighbourhood improves the score. This search method is very dependent upon a good choice of the initial graph, which is usually constructed incorporating all the available domain knowledge. Simulated annealing provides a more general approach, where the next graph structure is allowed to have a lower BDe score with a given probability based upon the current temperature. This temperature is gradually lowered as the search progresses, allowing fewer and fewer moves which decrease the score. The search terminates when a particular temperature is reached and no more moves which increase the score are available. The BDeu score mentioned previously is simply the BDe score with a uniform distribution over possible structures [15].

Mukherjee and Speed [82] construct different kinds of structure priors for use with the BDe score. This allows the prior knowledge to constrain abstract graph features such as the number of parents of a node, or the connectivity between two groups of nodes. They couple the BDe score and the structure priors with an MCMC based search. The search aims to sample from the distribution $p(G|\mathcal{D})$, so the probability of various graph features can be calculated, along with the most probable graph (*i.e.* the MAP solution). The proposal distribution for the Metropolis-Hastings sampler used is based on the neighbourhood of the graph,

only allowing proposals which are within the neighbourhood of the current graph. This proposal distribution can optionally be modified to incorporate the prior distributions over graph features. This in turn means graphs which are *a priori* more likely to be proposed more often.

Grossman and Domingos [45] present a different take on the score and search paradigm, as they wish to learn the structure of a Bayesian Network to construct a classifier for a particular node. This can be seen as generalising the construction of a Naïve Bayes classifier (see Chapter 2) to arbitrary network structures around the class node Y. They do this by aiming to maximise the conditional log-likelihood of the structure, inferring the individual node parameters from their maximum likelihood estimates. This takes a discriminative approach to the learning of structure which is a perspective we will examine more closely in the next chapter. Each network structure is scored by the likelihood, $\mathcal{L}$, of Y given the inputs X as follows,

$$\mathcal{L}(G|\mathcal{D}) = \sum_{i=1}^{N} \log p(y^i|x_1^i, \ldots, x_d^i). \tag{3.8}$$

This scoring function is coupled with the simple hillclimbing search used in BDe, except it starts from the empty network which has no arcs. Unfortunately this scoring function requires the estimation of the complex distribution $p(y|\mathbf{x})$, which requires a relatively large amount of data to calculate when there are many nodes connected to Y. Carvalho *et al.* [16] present a new scoring function approximating the conditional log-likelihood which decomposes over the network structure, allowing it to be calculated on a per node basis (thus reducing the complexity of each estimated distribution). This function is an approximate factorised conditional log-likelihood, and can be expressed as the sum of information theoretic components plus a fixed constant which does not depend upon the network,

$$\hat{f}\mathcal{L}(G|\mathcal{D}) = \sum_{i=1}^{d} (\alpha+\beta) NI(X_i; \Pi(X_i)|Y) + \beta\lambda NI(\{Y; X_i; \Pi(X_i)\}) + \text{const.} \tag{3.9}$$

In the above notation $I(\{\ldots\})$ denotes the interaction information [78], α, β and λ are constants which do not depend on the network structure, and $\Pi(X_i)$ denotes the parent set of X_i. This is a decomposable measure, which means each node contributes independently to the overall score for a particular graph G. This score in particular links the conditional likelihood, information theory and structure learning in a way which parallels the results presented in Chapters

4 & 6, though our results provide a more general framework, and are applicable to the general feature selection problem.

One final relevant score and search approach is that of de Campos [28]. This paper describes a scoring function which is based upon measures of conditional independence as calculated by the mutual information. Each node is scored by the mutual information with it's current parent set, penalised by a function of the χ value expected if the parents are independent of the node. This leads to a scoring function which is not a probability or log-probability unlike the other measures we have discussed and is expressed as,

$$f(G, \mathcal{D}) = \sum_{i=1}^{d} \left(2NI(X_i; \Pi(X_i)) - \max_{\sigma_i} \sum_{j=1}^{|\Pi(X_i)|} \chi_{\alpha, l_{i,\sigma_i}} \right). \tag{3.10}$$

In the above equation α is the confidence level of the χ^2 test, $|\Pi(X_i)|$ is the number of parents of X_i, σ_i are the possible permutations of the parent set, and l_{i,σ_i} is the degrees of freedom, based upon the number of possible states for each permutation. Again this scoring function can be decomposed over the nodes, and can be interpreted under the Minimum Description Length (MDL) framework [94] as the decrease in description length between the candidate graph G and the empty graph.

The twin approaches of conditional independence testing and score & search initially appear to be very different, as the CB methods add links based upon the value of an independence test, and S&S measures the change in global score as the links are added, removed or inverted. In fact in the global case instances of these two approaches are equivalent. Cowell [25] showed that for a given node ordering with complete data, independence testing based upon the KL-Divergence is identical to scoring networks by their log-likelihood. In Chapter 6 we present a similar result for local structure learning with mutual information, showing that this is exactly equivalent to hill-climbing the joint likelihood of the local structure (which is a greedy search on the neighbourhood of the local structure graph).

3.7 Chapter Summary

In this chapter we reviewed the literature surrounding feature selection and Bayesian Networks which provide the landscape for the contributions of this thesis. In summary,

- We looked at feature selection, and the three main paradigms: filters, which select features based upon a statistical measure of correlation; wrappers, which select features based upon the performance of a classification algorithm; and embedded methods, a wide group of algorithms which select features as part of the classification process.

- We reviewed the literature on information theoretic filter algorithms, where the relevancy and redundancy of a feature is scored using concepts such as the mutual information.

- We looked at feature selection algorithms which can incorporate prior (domain) knowledge about the sparseness of the solution, or the relevancy of particular features.

- We reviewed a selection of feature selection algorithms designed specifically for multi-class environments, and looked at how they try to ensure they have predictive features for all the classes.

- We looked at how Bayesian Network classifiers can be constructed to solve classification problems, whilst giving more information about the structure of the problem. We also saw how learning the structure of a Bayesian Network is equivalent to the feature selection problem.

- Finally we reviewed literature on structure learning in Bayesian Networks, investigating the two main paradigms: constraint based methods, and score & search methods. We saw how several of the constraint based methods used mutual information measures to rank features and how these approaches are similar to the information theoretic filter literature.

In the next chapter we present the central result of this thesis, a derivation of mutual information based feature selection criteria from a clearly defined loss function, namely the joint likelihood of a discriminative model. We derive update rules for this loss function which allow us to iteratively maximise the

joint likelihood by selecting the feature which maximises the conditional mutual information. In Chapter 5 we use this probabilistic framework to understand the different approximations and assumptions made by the information theoretic heuristics we have reviewed in this chapter. In Chapter 6 we link our probabilistic framework to the problem of Markov Blanket discovery, showing in the process that some common local structure learning algorithms are actually maximising the joint likelihood under a flat prior over network structure.

Chapter 4

Deriving a selection criterion

In Chapter 3 we briefly outlined the three main classes of feature selection algorithms: filters, wrappers, and embedded methods. We saw how many of the filter techniques are heuristic, combining different kinds of correlation terms without any understanding of the objective function they were optimising. We now recast the feature selection problem as a constrained optimisation problem in a high dimensional space, so our task is to find a n-dimensional bit vector $\boldsymbol{\theta}$ with at most k bits set, representing our selected features. We should then choose $\boldsymbol{\theta}$ to optimise some evaluation criterion. There has been much attention given to this problem of search in high dimensional spaces (see Reunanen [93] for a review of search strategies in feature selection), and a good search technique is an integral part of any feature selection algorithm. There has been a similarly large amount of attention given to the construction of evaluation criteria, but many of these criteria are based upon heuristics, with little investigation into the underlying metrics which they are attempting to optimise. We will focus on the derivation of these evaluation criteria, and leave the question of constructing a search algorithm which best optimises our criteria for future work. In particular we will *derive* the optimal evaluation criterion for a particular loss function which we wish to optimise.

4.1 Minimising a Loss Function

We now formally develop feature selection as the optimisation of a discriminative model likelihood, following Lasserre *et al.* [70], and Minka [81] in the construction of such a model. This derivation of feature selection forms the basis of the rest of

this thesis. In Chapter 5 we will investigate the links between our formal framework based upon the likelihood and the literature of feature selection heuristics based upon mutual information. In Chapter 6 we will look at what benefits our likelihood framework gives when we wish to extend these criteria to incorporate prior information. In Chapter 7 we will use a similar derivation to construct *cost-sensitive* feature selection criteria.

4.1.1 Defining the feature selection problem

We assume an underlying i.i.d. process $p : X \to Y$, from which we have a sample of N observations. Each observation is a pair $(\mathbf{x}, y)$, consisting of a d-dimensional feature vector $\mathbf{x} = [x_1, ..., x_d]^T$, and a target class y, drawn from the underlying random variables $X = \{X_1, ..., X_d\}$ and Y. We further assume that $p(y|\mathbf{x})$ is defined by a *subset*, X^*, of the features X, while the remaining features are redundant or irrelevant. Our modeling task is therefore two-fold: firstly to identify the features that play a functional role, and secondly to use these features to perform predictions.

We adopt a d-dimensional binary vector $\boldsymbol{\theta}$, specifying the selected features: a 1 indicates the feature is selected, and a 0 indicates it is discarded. We use $\neg\boldsymbol{\theta}$ for the negation of $\boldsymbol{\theta}$, *i.e.* the unselected features. We then define $X_{\boldsymbol{\theta}}$ as the set of selected features, and $X_{\neg\boldsymbol{\theta}}$ as the set complement of $X_{\boldsymbol{\theta}}$, the set of unselected features. Therefore $X = X_{\boldsymbol{\theta}} \cup X_{\neg\boldsymbol{\theta}}$, as $X_{\boldsymbol{\theta}}$ and $X_{\neg\boldsymbol{\theta}}$ form a partition. We use $\mathbf{x}_{\boldsymbol{\theta}}$ for an observation of the selected features $X_{\boldsymbol{\theta}}$, and similarly for $\mathbf{x}_{\neg\boldsymbol{\theta}}$. We define $p(y|\mathbf{x}, \boldsymbol{\theta})$ as $p(y|\mathbf{x}_{\boldsymbol{\theta}})$, and use the latter when specifically talking about feature selection. As mentioned, we assume the process p is defined by a subset of the features, so for some unknown optimal vector θ^*, we have that $p(y|\mathbf{x}) = p(y|\mathbf{x}_{\theta^*})$. We then formally define X^* as the minimal feature set s.t. $\forall\, \mathbf{x}, y\ p(y|\mathbf{x}_{\boldsymbol{\theta}^*}) = p(y|\mathbf{x})$ and use $\boldsymbol{\theta}^*$ as the vector indicating this feature set. The feature selection problem is to identify this vector. We define τ as the other model parameters involved in the generation of class labels, and λ as the generative parameters which create the observations $\mathbf{x}$. Each of these model parameters, $\lambda, \tau, \boldsymbol{\theta}$, has an associated prior probability distribution, $p(\lambda), p(\tau, \boldsymbol{\theta})$, which represents our belief *a priori* in each particular value of the parameters. Note that τ and $\boldsymbol{\theta}$ are jointly distributed, as the feature set influences the classification model parameters.

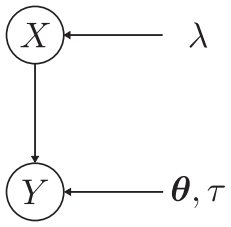


Figure 4.1: The graphical model for the likelihood specified in Equation (4.1).

4.1.2 A discriminative model for feature selection

We approximate the true distribution p with a hypothetical model q, with separate parameters for the feature selection, $\boldsymbol{\theta}$, and for classification, τ. Following Minka [81] and Lasserre *et al.* [70], in the construction of a discriminative model, our joint likelihood is

$$\mathcal{L}(\mathcal{D}, \boldsymbol{\theta}, \tau, \lambda) = p(\boldsymbol{\theta}, \tau)p(\lambda) \prod_{i=1}^{N} q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)q(\mathbf{x}^i|\lambda). \tag{4.1}$$

This is the joint likelihood for the graphical model specified in Figure 4.1. In discriminative models we wish to maximise our classification performance, therefore we maximize $\mathcal{L}$ with respect to $\boldsymbol{\theta}$ (our feature selection parameters) and τ (our model parameters). We therefore ignore the generative parameters λ as they do not directly influence the classification performance. Excluding the generative terms gives

$$\mathcal{L}(\mathcal{D}, \boldsymbol{\theta}, \tau, \lambda) \propto p(\boldsymbol{\theta}, \tau) \prod_{i=1}^{N} q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau). \tag{4.2}$$

We wish to find the Maximum a Posteriori (MAP) solution, the mode of the distribution $\mathcal{L}$, with respect to the parameters $\{\boldsymbol{\theta}, \tau\}$. This means we will find a single feature set which maximises our likelihood. We leave a fully Bayesian treatment of the feature selection problem, where we calculate a probability distribution over possible feature sets, to future work.

We choose to work with the scaled negative log-likelihood, $-\ell$, converting our maximization problem into a minimization problem, without changing the position of the optima. This gives

$$-\ell = -\frac{1}{N}\left(\sum_{i=1}^{N} \log q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau) + \log p(\boldsymbol{\theta}, \tau) \right) \tag{4.3}$$

which is the function we will minimize with respect to $\{\boldsymbol{\theta}, \tau\}$; the scaling term is to simplify exposition later.

We wish to decompose this log-likelihood to extract terms directly related to feature selection and to classification performance. This will allow us to express the feature selection problem directly and to find what functions maximise the likelihood of our model. We first compare our predictive model against the true distribution of $p(y^i|\mathbf{x}^i)$, and so we introduce the ratio $\frac{p(y^i|\mathbf{x}^i)}{p(y^i|\mathbf{x}^i)}$ into the logarithm. This is the probability of the correct class given all the data, without any feature selection. As this ratio is unity it does not change the value of the log-likelihood, nor the positions of its optima. We can then expand the resulting logarithm to give several terms,

$$-\ell = -\frac{1}{N}\left(\sum_{i=1}^{N} \log \frac{q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)}{p(y^i|\mathbf{x}^i)} + \sum_{i=1}^{N} \log p(y^i|\mathbf{x}^i) + \log p(\boldsymbol{\theta}, \tau)\right). \tag{4.4}$$

These terms are: the log-likelihood ratio between the true model and our predictive model, the log-likelihood of the true model, and the prior term. The first term is small when our predictive model is a good approximation to the true distribution. We can see that the middle term is a finite sample approximation to the conditional entropy $H(Y|X)$ as follows,

$$H(Y|X) = -\sum_{\mathbf{x}\in X, y\in Y} p(\mathbf{x}, y) \log p(y|\mathbf{x}) \approx -\frac{1}{N}\sum_{i=1}^{N} \log p(y^i|\mathbf{x}^i). \tag{4.5}$$

This represents the total amount of uncertainty there is about the class label given the data. The conditional entropy is large when the features we have do not constrain the class label well, *i.e.* it is hard to accurately predict the label from the features. The conditional entropy is the log-likelihood of the true model when taking the limit of data points, and thus provides a lower bound on our performance, as our model cannot perform better than the data allows.

We are concerned with separating out the influence of feature selection and classification in our model, and thus introduce an extra ratio $\frac{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}$ into the first term. This is the probability of the correct class given the features we have selected with $\boldsymbol{\theta}$, and thus represents how useful a set of features we have selected.

We can then further expand the first logarithm as follows,

$$-\ell = -\frac{1}{N}\Bigg(\sum_{i=1}^{N} \log \frac{q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)}{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})} + \sum_{i=1}^{N} \log \frac{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}{p(y^i|\mathbf{x}^i)} + \sum_{i=1}^{N} \log p(y^i|\mathbf{x}^i) + \log p(\boldsymbol{\theta}, \tau) \Bigg). \tag{4.6}$$

We then bring the minus sign inside the brackets, and flip the ratios inside the logarithms, which gives

$$-\ell = \frac{1}{N}\Bigg(\sum_{i=1}^{N} \log \frac{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}{q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)} + \sum_{i=1}^{N} \log \frac{p(y^i|\mathbf{x}^i)}{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})} - \sum_{i=1}^{N} \log p(y^i|\mathbf{x}^i) - \log p(\boldsymbol{\theta}, \tau) \Bigg). \tag{4.7}$$

As before the last two terms are the log likelihood of the true model and the prior term. We have now separated out the first log likelihood ratio into two terms. The first term is the log ratio between our predictive model and the true distribution of the labels given our selected subset of features. This represents how well our model fits the data given the current set of features. When the ratio is 1, the log ratio is 0 and our model has the best possible fit given the features selected. The second term is the log ratio between the true distribution given the selected features, and the true distribution of the labels given all the data. This measures the quality of the selected feature set $\boldsymbol{\theta}$, based on how close the conditional distribution of y is to the one conditioned on all the data. We can see that this term is a finite sample approximation to the expected KL-Divergence between $p(y|\mathbf{x})$ and $p(y|\mathbf{x}, \boldsymbol{\theta})$ as follows

$$\mathbb{E}_{\mathbf{x},y}\{p(y|\mathbf{x})||p(y|\mathbf{x}, \boldsymbol{\theta})\} = \sum_{\mathbf{x}\in X, y\in Y} p(\mathbf{x}, y) \log \frac{p(y|\mathbf{x})}{p(y|\mathbf{x}, \boldsymbol{\theta})} \approx \frac{1}{N} \sum_{i=1}^{N} \log \frac{p(y^i|\mathbf{x}^i)}{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}. \tag{4.8}$$

This KL-Divergence has appeared before in the feature selection literature. Koller and Sahami [63] introduce this divergence as a sensible objective for a feature selection algorithm to minimise. With our expansion we show it to be a direct consequence of optimising a discriminative model likelihood, though their approach ignores the prior over the features. As $\mathbf{x} = \{\mathbf{x}_{\boldsymbol{\theta}}, \mathbf{x}_{\neg\boldsymbol{\theta}}\}$, we can further

develop this term:

$$\begin{aligned}
\Delta_{KS} &= \mathbb{E}_{\mathbf{x},y}\{p(y|\mathbf{x}_{\boldsymbol{\theta}}, \mathbf{x}_{\neg\boldsymbol{\theta}})||p(y|\mathbf{x}_{\boldsymbol{\theta}})\} \\
&= \sum_{\mathbf{x}} p(\mathbf{x}) \sum_{y} p(y|\mathbf{x}) \log \frac{p(y|\mathbf{x}_{\boldsymbol{\theta}}, \mathbf{x}_{\neg\boldsymbol{\theta}})}{p(y|\mathbf{x}_{\boldsymbol{\theta}})} \\
&= \sum_{\mathbf{x},y} p(\mathbf{x}, y) \log \frac{p(y|\mathbf{x}_{\boldsymbol{\theta}}, \mathbf{x}_{\neg\boldsymbol{\theta}})}{p(y|\mathbf{x}_{\boldsymbol{\theta}})} \frac{p(\mathbf{x}_{\neg\boldsymbol{\theta}}|\mathbf{x}_{\boldsymbol{\theta}})}{p(\mathbf{x}_{\neg\boldsymbol{\theta}}|\mathbf{x}_{\boldsymbol{\theta}})} \\
&= \sum_{\mathbf{x},y} p(\mathbf{x}, y) \log \frac{p(\mathbf{x}_{\neg\boldsymbol{\theta}}, y|\mathbf{x}_{\boldsymbol{\theta}})}{p(\mathbf{x}_{\neg\boldsymbol{\theta}}|\mathbf{x}_{\boldsymbol{\theta}})p(y|\mathbf{x}_{\boldsymbol{\theta}})} \\
&= I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}). \qquad (4.9)
\end{aligned}$$

This is the conditional mutual information between the class label and the remaining features, given the selected features. We can now write the negative log-likelihood as the sum of information theoretic quantities plus the prior over $\{\boldsymbol{\theta}, \tau\}$,

$$-\ell \approx \mathbb{E}_{\mathbf{x},y}\left\{ \log \frac{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}{q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)} \right\} + I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}) + H(Y|X) - \frac{1}{N} \log p(\boldsymbol{\theta}, \tau). \quad (4.10)$$

Assuming for the moment that we have the optimal feature set or a superset thereof (*i.e.* $X^* \subseteq X_{\boldsymbol{\theta}}$) then $p(y|\mathbf{x}, \boldsymbol{\theta}) = p(y|\mathbf{x})$. Then as the expectation in the first term is over $p(y, \mathbf{x})$, the first term can be seen as a finite sample approximation to the expected KL-Divergence over $p(\mathbf{x})$ representing how well the predictive model fits the true distribution, given a superset of the optimal feature set.

The first term is a measure of the difference between the predictive model q, and the true distribution p given the selected features. When a superset of the optimal feature set has been found, it becomes the KL-Divergence between p and q. The second term is $I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}})$, the conditional mutual information between the class label and the unselected features, given the selected features. The size of this term depends solely on the choice of features, and will decrease as the selected feature set $X_{\boldsymbol{\theta}}$ explains more about Y, until eventually becoming zero when the remaining features $X_{\neg\boldsymbol{\theta}}$ contain no additional information about Y in the context of $X_{\boldsymbol{\theta}}$. Note that due to the chain rule, $I(AB; Y) = I(A; Y) + I(B; Y|A)$, and $X = X_{\boldsymbol{\theta}} \cup X_{\neg\boldsymbol{\theta}}$,

$$I(X; Y) = I(X_{\boldsymbol{\theta}}; Y) + I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}). \quad (4.11)$$

Since $I(X; Y)$ is constant, minimizing $I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}})$ is equivalent to maximizing

$I(X_{\boldsymbol{\theta}}; Y)$, which is the goal of many mutual information based filter algorithms. The third term in Eq (4.10) is $H(Y|X)$, the conditional entropy of the labels given *all features*; this is an irreducible constant, dependent only on the dataset $\mathcal{D}$. As mentioned previously this term represents the quality of the data, and how predictive X is of Y. When this value is small the data constrains the choice of Y, and thus it has a low Bayes rate, whereas when this value is large the data does not constrain the choice of Y, and the Bayes rate is higher.

This expansion makes explicit the effect of the feature selection parameters $\boldsymbol{\theta}$, separating them from the effect of the parameters τ in the model that *uses* those features. If we somehow had the optimal feature subset $\boldsymbol{\theta}^*$, which perfectly captured the underlying process p, then $I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}})$ would be zero. The remaining (reducible) error is then down to the KL divergence $p||q$, expressing how well the predictive model q can *make use* of the provided features. Of course, different models q will have different predictive ability: a good feature subset will not necessarily be put to good use if the model is too simple to express the underlying function. This perspective was also considered by Tsamardinos and Aliferis [107], and earlier by Kohavi and John [62] — the above results place these in the context of a precise objective function, the joint likelihood of a discriminative model.

We now make an assumption made *implicitly* by all filter methods, that model fitting can be separated from the feature selection process. For completeness we formalise this assumption as:

Definition 8. Filter assumption
Given an objective function for a classifier, we can address the problems of optimizing the feature set and optimizing the classifier in two stages: first picking good features, then building the classifier to use them.

In our framework we make this assumption explicit by specifying that the prior $p(\boldsymbol{\theta}, \tau)$ factorizes into $p(\boldsymbol{\theta})p(\tau)$, thus decoupling the model fitting from the feature selection. We note that τ is independent of the second term in our expansion, and by factorising the prior we can select features before fitting the model. This assumes that our model q will fit the distribution $p(y|\mathbf{x}, \boldsymbol{\theta})$ and that it can exploit all information given in the feature set. We therefore can optimise the feature selection first, as with enough data our model will fit the true distribution $p(y|\mathbf{x}, \boldsymbol{\theta})$ optimally, and the first ratio in Equation (4.10) will become zero. This

is a valid assumption if our model q is a consistent estimator of p, as with increasing N it will more closely approximate the true distribution. In essence this assumption means the classification model is sufficiently complex to adapt to any feature set, without making additional limiting assumptions about the distribution. Whereas the filter criteria literature makes the filter assumption implicitly, the formalism we have presented has made it explicit. In filters, to maximize the likelihood of the feature set we are only concerned with how $p(y|\mathbf{x}, \boldsymbol{\theta})$ approximates $p(y|\mathbf{x}, \boldsymbol{\theta}^*)$, so we can now specify the optimization problem that defines the feature selection task for the model in Equation (4.1) as,

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \left(I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}) - \frac{1}{N} \log p(\boldsymbol{\theta}) \right). \tag{4.12}$$

This optimisation problem relies upon the prior to ensure there is a unique global optimum, as with a flat prior any superset of an optimal feature set is also optimal. In the next section we will tighten our definition of the feature selection task to remove this problem.

We note that in contrast to filter algorithms, wrapper and embedded approaches optimise jointly over the first two terms in Equation (4.10), by fitting the classification model together with the feature selection.

We now turn to the problem of how to optimise the parameter $\boldsymbol{\theta}$, *i.e.* how do we choose a feature. We show how the commonly used simple greedy searches are iterative maximisers of the likelihood, and under what conditions such a search returns the optimal solution.

4.1.3 Optimizing the feature selection parameters

Under the filter assumption in Definition 8, Equation (4.12) specifies the optimal feature set, in the sense of maximising the joint likelihood. However there may of course be multiple global optima giving multiple optimal feature sets, in addition to the trivial optima of selecting all features. In fact, due to the nature of the mutual information, any feature set which contains the optimal feature set will be a global optima of the likelihood. As we wish to perform feature selection, we express a preference for the smallest such feature set which maximises the likelihood.

With this in mind, we can introduce a minimality constraint on the size of

the feature set, and define our problem:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}'} \left\{ |\boldsymbol{\theta}'| : \boldsymbol{\theta}' = \arg\min_{\boldsymbol{\theta}} \left(I(X_{\neg\boldsymbol{\theta}}; Y | X_{\boldsymbol{\theta}}) - \frac{1}{N} \log p(\boldsymbol{\theta}) \right) \right\}. \tag{4.13}$$

This is the smallest feature set $X_{\boldsymbol{\theta}}$, such that the mutual information $I(X_{\neg\boldsymbol{\theta}}; Y | X_{\boldsymbol{\theta}})$ plus the prior is minimal, and thus the joint likelihood is maximal. It should be remembered that the likelihood is only our proxy for classification error, and the minimal feature set in terms of classification could be smaller than that which optimises likelihood.

A common heuristic approach is a sequential search considering features one-by-one for addition/removal; this is used for example in Markov Blanket learning algorithms such as IAMB [108] (we will return to the IAMB algorithm in Chapter 6). We will now demonstrate that this sequential search heuristic is in fact equivalent to a greedy iterative optimisation of Equation (4.13). First we derive the appropriate update rules for a iterative optimisation of Equation (4.13) and then in Section 5.1 we show how different assumptions coupled with these greedy update rules generates many of the different criteria in the literature.

We first introduce extra notation, $\boldsymbol{\theta}^t$ and $\boldsymbol{\theta}^{t+1}$, denoting the selected feature set at timesteps t and $t+1$. We use J^t to denote our objective function (Equation 4.12) at the timestep t. We define a simple greedy sequential search, so only one feature is added/removed at each timestep, so there is exactly one bit different between $\boldsymbol{\theta}^t$ and $\boldsymbol{\theta}^{t+1}$. The flipped bit we denote as θ_k.

We define a greedy forward step as the selection of the feature, X_k, which most improves our selected feature set $\boldsymbol{\theta}^t$. Therefore:

$$\begin{aligned} X_k^* &= \arg\max_{X_k \in X_{\neg\boldsymbol{\theta}^t}} \left(J_t - J_{t+1} \right) \\ X_{\boldsymbol{\theta}^{t+1}} &\leftarrow X_{\boldsymbol{\theta}^t} \cup X_k^* \\ X_{\neg\boldsymbol{\theta}^{t+1}} &\leftarrow X_{\neg\boldsymbol{\theta}^t} \setminus X_k^* \end{aligned}$$

We now derive the update for a forward search which optimises the likelihood.

Theorem 1. *The forward step that optimizes Eq (4.12) at timestep $t+1$ from timestep t is to add the feature,*

$$X_k^* = \arg\max_{X_k \in X_{\neg\boldsymbol{\theta}^t}} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t}) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \tag{4.14}$$

Proof. We wish to minimize J_{t+1} from J_t. This is equivalent to maximizing the difference $(J_t - J_{t+1})$ by selecting the feature X_k. The objective at an arbitrary timestep t is:

$$J_t = I(X_{\neg\boldsymbol{\theta}^t}; Y | X_{\boldsymbol{\theta}^t}) - \frac{1}{N} \log p(\boldsymbol{\theta}^t). \tag{4.15}$$

and at timestep $t+1$ is:

$$J_{t+1} = I(X_{\neg\boldsymbol{\theta}^{t+1}}; Y | X_{\boldsymbol{\theta}^{t+1}}) - \frac{1}{N} \log p(\boldsymbol{\theta}^{t+1}) \tag{4.16}$$

We wish to add the feature X_k that minimizes J_{t+1}, and thus maximizes the difference $J_t - J_{t+1}$,

$$J_t - J_{t+1} = I(X_{\neg\boldsymbol{\theta}^t}; Y | X_{\boldsymbol{\theta}^t}) - \frac{1}{N} \log p(\boldsymbol{\theta}^t) - I(X_{\neg\boldsymbol{\theta}^{t+1}}; Y | X_{\boldsymbol{\theta}^{t+1}}) + \frac{1}{N} \log p(\boldsymbol{\theta}^{t+1}). \tag{4.17}$$

After applying the chain rule of mutual information we arrive at:

$$\begin{aligned} X_k^* &= \underset{X_k \in X_{\neg\boldsymbol{\theta}^t}}{\arg\max} \left(J_t - J_{t+1} \right) \\ &= \underset{X_k \in X_{\neg\boldsymbol{\theta}^t}}{\arg\max} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t}) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \end{aligned}$$

Thus the feature which minimises J_{t+1} from J_t is the feature

$$X_k^* = \underset{X_k \in X_{\neg\boldsymbol{\theta}^t}}{\arg\max} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t}) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \tag{4.18}$$

□

A subtle (but important) implementation point for this selection heuristic is that it should *not* add another feature if

$$\forall X_k,\ I(X_k; Y | X_{\boldsymbol{\theta}}) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \leq 0. \tag{4.19}$$

This ensures we will not unnecessarily increase the size of the feature set.

We define a greedy backwards step along similar lines. We remove the feature

X_k which minimises the difference between J^t and J^{t+1}. Therefore:

$$\begin{aligned} X_k^* &= \arg\min_{X_k \in X_{\neg\boldsymbol{\theta}^t}} \left(J_t - J_{t+1}\right) \\ X_{\boldsymbol{\theta}^{t+1}} &\leftarrow X_{\boldsymbol{\theta}^t} \setminus X_k^* \\ X_{\neg\boldsymbol{\theta}^{t+1}} &\leftarrow X_{\neg\boldsymbol{\theta}^t} \cup X_k^* \end{aligned}$$

We now derive the update for a backward search which optimises the likelihood.

Theorem 2. *The backward step that optimizes (4.12) at timestep $t+1$ from timestep t is to remove the feature,*

$$X_k^* = \arg\min_{X_k \in X_{\boldsymbol{\theta}^t}} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t} \setminus X_k) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \tag{4.20}$$

Proof. We wish to keep $J_{t+1} \approx J_t$. This is equivalent to minimising the difference ($J_t - J_{t+1}$, by removing the feature X_k. As before our objective at an arbitrary timestep t is:

$$J_t = I(X_{\neg\boldsymbol{\theta}^t}; Y | X_{\boldsymbol{\theta}^t}) - \frac{1}{N} \log p(\boldsymbol{\theta}^t). \tag{4.21}$$

and at timestep $t+1$ is:

$$J_{t+1} = I(X_{\neg\boldsymbol{\theta}^{t+1}}; Y | X_{\boldsymbol{\theta}^{t+1}}) - \frac{1}{N} \log p(\boldsymbol{\theta}^{t+1}) \tag{4.22}$$

We wish to remove the feature X_k that maximises J_{t+1}, and thus minimises the difference $J_t - J_{t+1}$,

$$\begin{aligned} X_k^* &= \arg\min_{X_k \in X_{\boldsymbol{\theta}^t}} \left(J_t - J_{t+1} \right) \\ &= \arg\min_{X_k \in X_{\boldsymbol{\theta}^t}} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t} \setminus X_k) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \end{aligned}$$

Thus the feature which minimises J_{t+1} from J_t is the feature

$$X_k^* = \arg\min_{X_k \in X_{\boldsymbol{\theta}^t}} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t} \setminus X_k) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \tag{4.23}$$

□

To strictly achieve our optimization goal, a backward step should *only* remove a

feature if

$$I(X_k; Y|\{X_{\boldsymbol{\theta}^t} \backslash X_k\}) + \frac{1}{N} \log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \leq 0. \tag{4.24}$$

With an uninformative prior $p(\boldsymbol{\theta}) \propto 1$, the prior ratio in both of the updates cancels, and we recover the maximum likelihood estimate of the optimal feature set, with the forward iterative minimization update becoming

$$X_k^* = \underset{X_k \in X_{\neg \boldsymbol{\theta}^t}}{\arg\max}\, I(X_k; Y|X_{\boldsymbol{\theta}^t}). \tag{4.25}$$

The prior ratio similarly disappears from the backward iterative update, resulting in

$$X_k^* = \underset{X_k \in X_{\boldsymbol{\theta}^t}}{\arg\min}\, I(X_k; Y|X_{\boldsymbol{\theta}^t} \setminus X_k). \tag{4.26}$$

These two updates look very familiar in the context of the different criteria we reviewed in the previous chapter. The next chapter explores the links between optimising the model likelihood and the information theoretic feature selection literature, showing many common techniques to be approximate maximisers of the model likelihood. We return to the full model including priors over the feature selection parameters in Chapter 6.

4.2 Chapter Summary

In this chapter we approached the problem of feature selection from a theoretical perspective. We asked two questions: what do we want from a feature selection algorithm, and how do we measure the performance? We answered these questions by turning to the statistical concept of likelihood, deciding that maximising the joint likelihood of a discriminative model would be the target of our system, rather than trying to minimise the error rate, or maximise the information held in our feature set.

We showed that choosing to maximise the likelihood implies a particular feature selection criterion, namely the conditional mutual information between the unselected features and the class, conditioned on the selected features. Maximising this quantity maximises the joint likelihood of our model. This term is penalised by a prior term which allows the incorporation of domain knowledge into the feature selection process, a topic we return to in Chapter 6. We then constructed hillclimbers on the likelihood, which iteratively maximise it by adding

or removing features. We now take the insights from our probabilistic model and apply them to the literature surrounding information theoretic feature selection, linking our iterative maximisers of the likelihood to feature selection criteria found in the literature.

Chapter 5

Unifying information theoretic filters

In the previous chapter we derived an information theoretic feature selection criterion directly from our choice of loss function (the joint likelihood). In this chapter we investigate how our derived criterion links to the existing literature on information theoretic feature selection which we looked at in Chapter 3. These algorithms, referred to collectively as information theoretic filters, have proven popular over the past 20 years as the mutual information provides a strong link to the Bayes error of a classification problem. A feature set which has high mutual information with the class label, is a feature set with a low conditional entropy $H(Y|X)$, which forms an upper bound on the Bayes error. Therefore maximising the mutual information, minimises the conditional entropy, which in turn minimises an upper bound on the Bayes error (see Section 2.3.2). In light of the derivation from the previous chapter we can now see that by using the mutual information they are in fact optimising a discriminative model likelihood. We use this viewpoint to unify these information theoretic criteria, and expose the *implicit* assumptions they make about the underlying data. We show how Equation (4.25) can be seen as a root criterion from which all others are derived by making different assumptions about the underlying distribution p.

5.1 Retrofitting Successful Heuristics

In the previous chapter, starting from a clearly defined discriminative model, we derived a greedy optimization process which maximises the joint likelihood of

that model by assessing features based on a simple scoring criterion on the utility of including a feature $X_k \in X_{\neg\boldsymbol{\theta}}$. We now consider how we can relate various criteria which have appeared in the literature to our framework. None of these criteria include the prior term, so we assume a flat prior with $p(\boldsymbol{\theta}) \propto 1$, which gives the maximum likelihood updates in Equations (4.25) and (4.26). We will consider the use of priors with these criteria in next Chapter. From the previous chapter we note that the ML scoring criterion for a feature X_k is,

$$J_{cmi}(X_k) = I(X_k; Y|S), \tag{5.1}$$

where *cmi* stands for conditional mutual information, and for notational brevity we now use $S = X_{\boldsymbol{\theta}}$ for the currently selected set. We wish to investigate how Equation (5.1) relates to existing heuristics in the literature, such as the MIFS criterion we discussed in Chapter 3? Repeating the definition of the MIFS criterion for clarity,

$$J_{mifs}(X_k) = I(X_k; Y) - \beta \sum_{X_j \in S} I(X_k; X_j). \tag{5.2}$$

We can see that we first need to rearrange Equation (5.1) into the form of a simple relevancy term between X_k and Y, plus some additional terms, before we can compare it to MIFS. Using the identity $I(A; B|C) - I(A; B) = I(A; C|B) - I(A; C)$ (a variant of the chain rule of mutual information), we can re-express Equation (5.1) as,

$$J_{cmi}(X_k) = I(X_k; Y|S) = I(X_k; Y) - I(X_k; S) + I(X_k; S|Y). \tag{5.3}$$

It is interesting to see terms in this expression corresponding to the concepts of "relevancy" and "redundancy", i.e. $I(X_k; Y)$ and $I(X_k; S)$. The score will be increased if the relevancy of X_k is large and the redundancy with existing features is small. This is in accordance with a common view in the feature selection literature, observing that we wish to avoid redundant variables. However, we can also see an important additional term $I(X_k; S|Y)$, which is not traditionally accounted for in the feature selection literature — we call this the *conditional redundancy* (this notion was first explored by Brown [12]). This term has the opposite sign to the redundancy $I(X_k; S)$, hence J_{cmi} will be increased when this is large, i.e. a strong class-conditional dependence of X_k with the existing set S. Thus, we come to the important conclusion that *the inclusion of correlated*

features can be useful, provided the correlation *within classes* is stronger than the overall correlation. We note that this is a similar observation to that of Guyon [50], that "correlation does not imply redundancy" — Equation (5.3) embodies this statement in information theoretic terms.

We present a graphical demonstration of these properties in Figure 5.1 (based upon an example from Guyon [50]). We plot the two features X_1 and X_2 against each other, and denote the class by either a red circle or a blue star. Here we can see how the class conditional information is useful, by rewriting $I(X_1; X_2|Y)$ as follows:

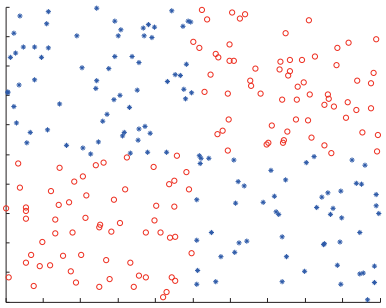
$$I(X_1; X_2|Y) = \sum_{y \in Y} p(y) I(X_1; X_2|Y = y). \tag{5.4}$$

Individually the features are irrelevant, as $I(X_1; Y) \approx I(X_2; Y) \approx 0$, as the feature has equal numbers of positive and negative classes for each value. The redundancy term, $I(X_1; X_2)$ is similarly small as for each value of X_1 there are both large and small values of X_2. However when we break down the class-conditional term as in Equation (5.4), we can see that $I(X_1; X_2|Y) \approx 1$. These values are approximate as this is calculated on a continuous random variable rather than the discrete random variables considered throughout the rest of this thesis. We would say that X_1 and X_2 are complementary variables, as they combine to improve performance beyond the sum of their parts.

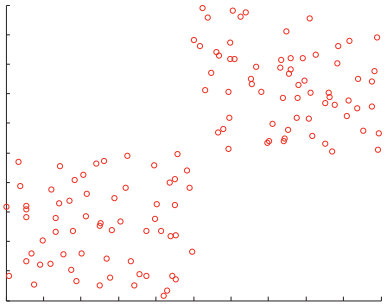
The sum of the last two terms in Equation (5.3) represents the three-way interaction between the existing feature set S, the target Y, and the candidate feature X_k being considered for inclusion in S. This is known as the *Interaction Information* [78], $I(\{X, Y, Z\})$, which measures dependencies within a set of variables. To further understand this, we can note the following property:

$$\begin{aligned} I(X_k S; Y) &= I(S; Y) + I(X_k; Y|S) \\ &= I(S; Y) + I(X_k; Y) - I(X_k; S) + I(X_k; S|Y). \end{aligned} \tag{5.5}$$

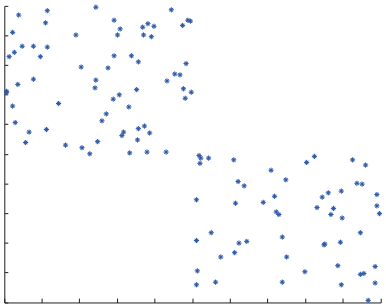
We see that if $I(X_k; S) > I(X_k; S|Y)$, then the total utility when including X_k, that is $I(X_k S; Y)$, is *less* than the sum of the individual relevancies $I(S; Y) + I(X_k; Y)$. This can be interpreted as X_k having unnecessary duplicated information, which means the total information is less than the sum of the parts, hence we call this a *negative* interaction. In the opposite case, when $I(X_k; S) < I(X_k; S|Y)$, then X_k and S combine well and provide more information *together* than by the



(a) Scatter plot of X_1 v X_2, individually $I(X_1;Y) \approx I(X_2;Y) \approx 0$, yet $I(X_1X_2;Y) = 1$



(b) Scatter plot of X_1 v X_2 when $Y = 1$, $I(X_1;X_2|y=1) \approx 1$



(c) Scatter plot of X_1 v X_2 when $Y = 2$, $I(X_1;X_2|y=2) \approx 1$

Figure 5.1: Figure 5.1a shows the scatter plot between X_1 and X_2. Figure 5.1b shows the scatter plot between X_1 and X_2 when $Y = 1$. Figure 5.1c shows the scatter plot between X_1 and X_2 when $Y = 2$.

sum of their parts, $I(S;Y)$, and $I(X_k;Y)$, hence we call this a *positive* interaction.

The important point to take away from this expression is that the terms are in a *trade-off* — we do not require a feature with low redundancy for its own sake, but instead require a feature that best trades off the three terms so as to maximise the score overall. Much like the bias-variance dilemma [35], attempting to decrease one term is likely to increase another.

We will investigate what assumptions about the underlying distribution $p(\mathbf{x}, y)$ are sufficient to derive MIFS (Equation 5.2) from the optimal maximum likelihood criterion (Equation 5.1). We begin by writing the latter two terms of Equation (5.3) as entropies:

$$\begin{aligned} J_{cmi}(X_k) = & I(X_k;Y) \\ & - H(S) + H(S|X_k) \\ & + H(S|Y) - H(S|X_kY). \end{aligned} \tag{5.6}$$

To further develop this, we require an assumption.

Assumption 1: *For all unselected features* $X_k \in X_{\neg\boldsymbol{\theta}}$,

$$p(\mathbf{x}_{\boldsymbol{\theta}}|x_k) = \prod_{j\in S} p(x_j|x_k) \tag{5.7}$$

$$p(\mathbf{x}_{\boldsymbol{\theta}}|x_k y) = \prod_{j\in S} p(x_j|x_k y). \tag{5.8}$$

This states that the selected features $X_{\boldsymbol{\theta}}$ *are independent and class-conditionally independent given the unselected feature* X_k *under consideration.*

Using this, Equation (5.6) becomes,

$$\begin{aligned} J'_{cmi}(X_k) = I(X_k;Y) & \\ & - H(S) + \sum_{j\in S} H(X_j|X_k) \\ & + H(S|Y) - \sum_{j\in S} H(X_j|X_k Y). \end{aligned} \tag{5.9}$$

where the prime on J indicates we are making assumptions on the distribution. Now, if we introduce $\sum_{j\in S} H(X_j) - \sum_{j\in S} H(X_j)$, and $\sum_{j\in S} H(X_j|Y) - \sum_{j\in S} H(X_j|Y)$, we recover mutual information terms, between the candidate feature and each member of the set S, plus some additional terms,

$$\begin{aligned} J'_{cmi}(X_k) = I(X_k;Y) & \\ & - \sum_{j\in S} I(X_j;X_k) + \sum_{j\in S} H(X_j) - H(S) \\ & + \sum_{j\in S} I(X_j;X_k|Y) + \sum_{j\in S} H(X_j|Y) - H(S|Y). \end{aligned} \tag{5.10}$$

Several of the terms in (5.10) are constant with respect to X_k — therefore removing them will have *no effect on the choice of feature* as our goal is to find the highest scoring feature not the score itself. Removing these terms, we have an equivalent criterion,

$$J'_{cmi}(X_k) = I(X_k;Y) - \sum_{j\in S} I(X_j;X_k) + \sum_{j\in S} I(X_j;X_k|Y). \tag{5.11}$$

This has in fact already appeared in the literature as a filter criterion, originally proposed by Lin *et al.* [74], as Conditional Infomax Feature Extraction (CIFE), though it has been repeatedly rediscovered by other authors [36, 48]. It is particularly interesting as it represents a sort of 'root' criterion, from which several others can be derived. For example, the link to MIFS can be seen with one further assumption, that the features are pairwise class-conditionally independent.

Assumption 2: *For all features i, j,*

$$p(x_i x_j|y) = p(x_i|y)p(x_j|y). \tag{5.12}$$

This states that the features are pairwise class-conditionally independent.

With this assumption, the term $\sum I(X_j; X_k|Y)$ will be zero, and Equation (5.11) becomes Equation (5.2), the MIFS criterion, with $\beta = 1$. The β parameter in MIFS can be interpreted as encoding a strength of belief in another assumption, that of unconditional independence.

Assumption 3: *For all features i, j,*

$$p(x_i x_j) = p(x_i)p(x_j). \tag{5.13}$$

This states that the features are pairwise independent.

A β close to zero implies very strong belief in the independence statement, indicating that any measured association $I(X_j; X_k)$ is in fact spurious, possibly due to noise in the data. A β value closer to 1 implies a lesser belief, that any measured dependency $I(X_j; X_k)$ should be incorporated into the feature score exactly as observed. Since the MIM criterion is produced by setting $\beta = 0$, we can see that MIM also adopts Assumption 3. The same line of reasoning can be applied to a very similar (and very popular) criterion proposed by Peng *et al.* [86], the *Minimum-Redundancy Maximum-Relevance* criterion,

$$J_{mrmr}(X_k) = I(X_k; Y) - \frac{1}{|S|} \sum_{j \in S} I(X_k; X_j). \tag{5.14}$$

Since mRMR omits the conditional redundancy term entirely, it is implicitly using Assumption 2. The β coefficient has been set inversely proportional to the size of the current feature set. If we have a large set S, then β will be extremely small. The interpretation is then that as the set S grows, mRMR adopts a stronger belief in Assumption 3. In the original paper, [86, section 2.3], it is claimed that mRMR is a first order approximation to Equation (5.1). By making explicit the intrinsic assumptions of the criterion we have clearly illustrated that this claim is incorrect as it does not include a conditional redundancy term, and in fact the mRMR criterion does not allow for *any* positive interactions between features.

The relation of the MIFS/mRMR to Equation (5.11) is relatively straightforward. It is more challenging to consider how closely other criteria might be re-expressed in this form. Yang and Moody [110] propose using *Joint Mutual Information* (JMI),

$$J_{jmi}(X_k) = \sum_{j \in S} I(X_k X_j; Y). \tag{5.15}$$

Using some relatively simple manipulations (see Brown [12]) this can be re-written as,

$$J_{jmi}(X_k) = I(X_k; Y) - \frac{1}{|S|} \sum_{j \in S} \Big[I(X_k; X_j) - I(X_k; X_j | Y) \Big].$$

The criterion (5.16) returns *exactly* the same set of features as the JMI criterion (5.15); however in this form, we can see the relation to our proposed framework. The JMI criterion, like mRMR, has a stronger belief in the pairwise independence assumptions as the feature set S grows. Similarities can of course be observed between JMI, MIFS and mRMR — the differences being the scaling factor and the conditional term — and their subsequent relation to Equation (5.11). It is in fact possible to identify numerous criteria from the literature that can all be re-written into a common form, corresponding to different assumptions made upon Equation (5.11). A *space* of potential criteria can be imagined, where we parametrise criterion (5.11) as:

$$J'_{cmi} = I(X_k; Y) - \beta \sum_{j \in S} I(X_j; X_k) + \gamma \sum_{j \in S} I(X_j; X_k | Y). \tag{5.16}$$

Figure 5.2 shows how the criteria we have discussed so far can all be fitted inside this unit square corresponding to β/γ parameters. MIFS sits on the left

hand axis of the square — with $\gamma = 0$ and $\beta \in [0, 1]$. The MIM criterion, Equation (3.1), which simply assesses each feature individually without any regard of others, sits at the bottom left, with $\gamma = 0, \beta = 0$. The top right of the square corresponds to $\gamma = 1, \beta = 1$, which is the CIFE criterion [74], also suggested by El Akadi *et al.* [36] and Guo and Nixon [48]. A very similar criterion, using an assumption to approximate the terms, was proposed by Cheng *et al.* [20].

The JMI and mRMR criteria are different from CIFE and MIFS in that they *move linearly* within the space as the feature set S grows. As the size of the set S increases they move closer towards the origin and the MIM criterion. The particularly interesting point about this property is that the *relative magnitude* of the relevancy term to the redundancy terms stays approximately constant as S grows, whereas with MIFS, the redundancy term will in general be $|S|$ times bigger than the relevancy term. We explore the practical consequences of this in Section 5.2 where we see it plays an important role in explaining the experimental results. Any criterion expressible in the unit square has made independence Assumption 1. In addition, any criteria that sit at points other than $\beta = 1, \gamma = 1$ have adopted varying degrees of belief in Assumptions 2 and 3.

A further interesting point about this square is simply that it is sparsely populated, an obvious unexplored region is the bottom right, the corner corresponding to $\beta = 0, \gamma = 1$; though there is no clear intuitive justification for this point, for completeness in the experimental section we will evaluate it, as the *conditional redundancy* or 'condred' criterion.

A paper by Brown [12] explores this unit square, though from a different perspective gained by expanding the multivariate mutual information. In fact much of this thesis arises from extensive consideration of the results in that paper, though the approach presented here is quite different. Our probabilistic perspective, deriving our selection criteria from the joint likelihood of a specific model allows the precise specification of the underlying assumptions required to produce different criteria from Equation (5.16). Further (unpublished) work by Brown [13] has shown that the space of criteria with fixed β and γ is not in general competitive with the criteria which move through the space, such as mRMR or JMI.

All the criteria in Figure 5.2 are *linear*, as they take linear combinations of the relevance/redundancy terms. One interesting perspective is to look at the criteria not as points but as paths through this space, mRMR is a line along the

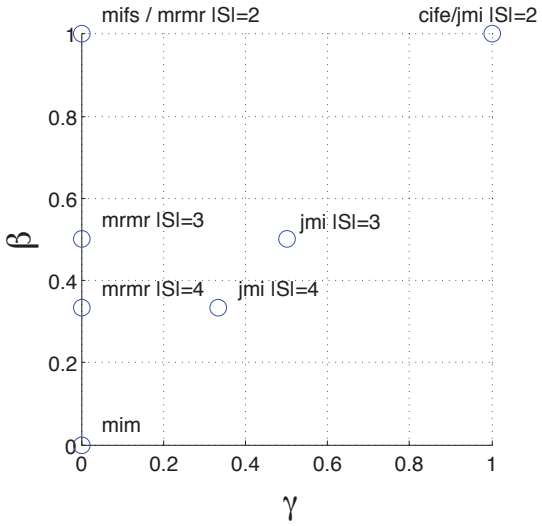


Figure 5.2: The full space of *linear* filter criteria, describing several examples from Table 3.1. Note that *all* criteria in this space adopt Assumption 1. Additionally, the γ and β axes represent the criteria belief in Assumptions 2 and 3, respectively. The left hand axis is where the mRMR and MIFS algorithms sit. The bottom left corner, MIM, is the assumption of completely independent features, using just marginal mutual information. Note that some criteria are equivalent at particular sizes of the current feature set $|S|$.

β axis, and JMI is a line along $\beta = \gamma$. Once we have understood this property it is natural to ask can there be other paths through this space. Indeed there exist other criteria which follow a similar form to these linear criteria, except they include other operations like minimizations, making them take a *non-linear* path.

Fleuret [40] proposed the *Conditional Mutual Information Maximization* criterion,

$$J_{cmim}(X_k) = \min_{X_j \in S} \Big[I(X_k; Y | X_j) \Big]. \tag{5.17}$$

This can be re-written,

$$J_{cmim}(X_k) = I(X_k; Y) - \max_{X_j \in S} \Big[I(X_k; X_j) - I(X_k; X_j | Y) \Big]. \tag{5.18}$$

Again these manipulations are found in Brown [12]. Due to the *max* operator, the probabilistic interpretation is less straightforward. It is clear however that CMIM adopts Assumption 1, since it evaluates only pairwise feature statistics. Vidal-Naquet and Ullman [109] propose another criterion used in Computer Vision,

which we refer to as *Informative Fragments*,

$$J_{if}(X_k) = \min_{X_j \in S}\Big[I(X_k X_j; Y) - I(X_j; Y)\Big]. \tag{5.19}$$

The authors motivate this criterion by noting that it measures the gain of combining a new feature X_k with each existing feature X_j, over simply using X_j by itself. The X_j with the least 'gain' from being paired with X_k is taken as the score for X_k. Interestingly, using the chain rule $I(X_k X_j; Y) = I(X_j; Y) + I(X_k; Y|X_j)$, therefore IF is equivalent to CMIM, i.e. $J_{if}(X_k) = J_{cmim}(X_k)$, making the same assumptions. In a similar vein, Jakulin [58] proposed the ICAP criterion,

$$J_{icap}(X_k) = I(X_k; Y) - \sum_{X_j \in S} \max\Big[0, \{I(X_k; X_j) - I(X_k; X_j|Y)\}\Big]. \tag{5.20}$$

Again, this adopts Assumption 1, using the same redundancy and conditional redundancy terms, yet the exact probabilistic interpretation is unclear. This criteria is designed to penalise criteria which interact negatively, but does not select those which interact positively. It is designed for use with classifiers which make similar assumptions of class conditional independence, such as the Naïve Bayes classifier.

An interesting class of criteria use a normalisation term on the mutual information to offset the inherent bias toward high arity features [34]. An example of this is *Double Input Symmetrical Relevance* [79], a modification of the JMI criterion:

$$J_{disr}(X_k) = \sum_{X_j \in S} \frac{I(X_k X_j; Y)}{H(X_k X_j Y)}. \tag{5.21}$$

The inclusion of this normalisation term breaks the strong theoretical link to a likelihood function, but again for completeness we will include this in our empirical investigations. While the criteria in the unit square can have their probabilistic assumptions made explicit, the non-linearity in the CMIM, ICAP and DISR criteria make such an interpretation far more difficult.

5.1.1 Bounding the criteria

There is one more important factor to note about many of these filter criteria, and that is their relative size compared to the optimal criterion of Equation (5.1). Using the properties of the mutual information we reviewed in Section 2.3 we can

upper bound each mutual information term by various different entropies (all Shannon mutual information terms are lower bound by zero). In particular we can bound J^* as follows,

$$0 \leq J^*(X_k) = I(X_k; Y|S) \leq H(X_k|S) \leq H(X_k). \tag{5.22}$$

If we consider the CIFE criterion (repeated for clarity),

$$J_{cife}(X_k) = I(X_k; Y) - \sum_{X_j \in S} I(X_k; X_j) + \sum_{X_j \in S} I(X_k; X_j|Y), \tag{5.23}$$

we can bound the individual terms separately,

$$\begin{aligned} I(X_k; Y) &\leq H(X_k) \\ \sum_{X_j \in S} I(X_k; X_j) &\leq |S| \cdot H(X_k) \\ \sum_{X_j \in S} I(X_k; X_j|Y) &\leq |S| \cdot H(X_k|Y) \leq |S| \cdot H(X_k). \end{aligned} \tag{5.24}$$

However the entire CIFE criterion is not so well behaved, as it is neither bounded above by $H(X_k)$ nor bounded below by 0. This is because the redundancy and conditional redundancy terms are bound by a function of $|S|$, and so grow in size compared to the relevancy term. This issue is also apparent in the MIFS and ICAP criteria, and we will see how it explains many of the differences in experimental performance.

If we consider the JMI criterion, we can see that the averaging of the redundancy and conditional redundancy terms removes this problem, stopping those terms from growing as a function of $|S|$. However the JMI criterion poses another problem, as it has multiple variants. We presented two versions of this criterion in Equations (5.15) and (5.16) and stated that they rank features identically. However we might expect that these different versions would interact in different ways with the prior term which exists in the derivation. We will return to this issue when we address informative priors in Chapter 6.

5.1.2 Summary of theoretical findings

In this section we have shown that numerous criteria published over the past two decades of research can be "retro-fitted" into the framework we have proposed

— the criteria are approximations to Equation (5.1), each making different assumptions on the underlying distributions. Since in the previous section we saw that accepting the top ranked feature according to Equation (5.1) provides the maximum possible increase in the likelihood, we see now that the criteria are *approximate* maximisers of the likelihood under an uninformative prior over the choice of features. Whether or not they indeed provide the maximum increase at each step will depend on how well the implicit assumptions on the data distribution match the true distribution. Also, it should be remembered that even if we used the optimal stepwise criterion, it is not guaranteed to find the global optimum of the likelihood, since (a) it is a greedy search, and (b) finite data will mean distributions cannot be accurately modelled. There are a subset of problems where this greedy search is optimal, namely in Markov Blanket discovery algorithms, which we return to in Chapter 6. In this case, we have reached the limit of what a theoretical analysis can tell us about these criteria, and we must close the remaining 'gaps' in our understanding with an experimental study.

5.2 Experimental Study

In this section we empirically evaluate a selection of the criteria in the literature against one another. Note that we are not pursuing an exhaustive analysis, attempting to identify the 'winning' criterion that provides best performance overall[1] — rather, we primarily observe how the theoretical properties of criteria relate to the similarity of the returned feature sets. While these properties are interesting, we of course must acknowledge that classification performance is the ultimate evaluation of a criterion — hence we also include here classification results on UCI datasets and in Section 5.3 on the well-known benchmark NIPS Feature Selection Challenge.

In the following sections, we ask the questions: "how stable is a criterion to small changes in the training data set?", "how similar are the criteria to each other?", "how do the different criteria behave in small-sample situations?", and finally, "what is the relationship between stability and accuracy?".

To address these questions, we use the 15 datasets detailed in Table 5.1. These are chosen to have a wide variety of example-feature ratios, and a range of multi-class problems. The features within each dataset have a variety of characteristics

[1] In any case, the No Free Lunch Theorem applies [107].

— some binary/discrete, and some continuous. Continuous features were discretised, using an equal-width strategy into 5 bins, while features already with a categorical range were left untouched. The 'ratio' statistic quoted in the final column is an indicator of the difficulty of the feature selection for each dataset. This uses the number of datapoints (N), the median arity of the features (m), and the number of classes (c) — the ratio quoted in the table for each dataset is $\frac{N}{mc}$ — hence a smaller value indicates a more challenging feature selection problem.

A key feature of this work is to understand the statistical assumptions on the data imposed by the feature selection criteria — if our classification model were to make even more assumptions, this is likely to obscure the experimental observations relating performance to theoretical properties. For this reason, in the experiments in this chapter we use a simple nearest neighbour classifier ($k = 3$), this is chosen as it makes few (if any) assumptions about the data, and we avoid the need for parameter tuning. We apply the filter criteria using a simple forward selection to select a fixed number of features, before being used with the classifier. The number of features selected varies between the experiments, but is detailed for each experiment. We will consider the 9 criteria previously studied in our theoretical analysis for all the experiments. One important criterion which we cannot use in this study is a direct implementation of Equation (5.1), which we showed to be the optimal criterion for iteratively maximising the likelihood. This criterion requires the estimation of an $|S|$ dimensional probability distribution, which is in general intractable for small and medium sized datasets, and thus we will not use it for this section of the empirical study. However in Section 5.3 we will look at two larger datasets, and there we will benchmark the performance of Equation (5.1), referring to it as the CMI criterion.

5.2.1 How stable are the criteria to small changes in the data?

The set of features selected by any procedure will of course depend on the data provided. It is a plausible complaint if the set of returned features varies wildly with only slight variations in the supplied data. In general we do not wish the feature set to have high variance, *i.e.* small changes in the data should have consequently small changes in the selected feature set. This is an issue reminiscent of the *bias-variance dilemma*, where the sensitivity of a classifier to its initial

Data	*Features*	*Examples*	*Classes*	Ratio
breast	30	569	2	57
congress	16	435	2	72
heart	13	270	2	34
ionosphere	34	351	2	35
krvskp	36	3196	2	799
landsat	36	6435	6	214
lungcancer	56	32	3	4
parkinsons	22	195	2	20
semeion	256	1593	10	80
sonar	60	208	2	21
soybeansmall	35	47	4	6
spect	22	267	2	67
splice	60	3175	3	265
waveform	40	5000	3	333
wine	13	178	3	12

Table 5.1: Datasets used in experiments. The final column indicates the difficulty of the data in feature selection, a smaller value indicating a more challenging problem.

conditions causes high variance responses. However, while the bias-variance decomposition is well-defined and understood, the corresponding issue for feature selection, the "stability", has only recently been studied. The stability of a feature selection criterion requires a measure to quantify the similarity between two selected feature sets. This was first discussed by Kalousis *et al.* [59], who investigated several measures, with the final recommendation being the Tanimoto distance between sets. Such set-intersection measures seem appropriate, but have limitations; for example, if two criteria selected identical feature sets of size 10, we might be less surprised if we knew the overall pool of features was of size 12, than if it was size 12,000. Kuncheva [67] presents a *consistency index* which takes this into account, based on the hypergeometric distribution with a correction for the probability of selecting the same feature set at random.

Definition 9. *The consistency for two subsets $A, B \subset X$, such that $|A| = |B| = k$, and $r = |A \cap B|$, where $0 < k < |X| = d$, is*

$$C(A, B) = \frac{rd - k^2}{k(d - k)}. \tag{5.25}$$

The consistency takes values in the range $[-1, +1]$, with a positive value indicating similar sets, a zero value indicating a purely random relation, and a negative value indicating a strong anti-correlation between the features sets.

One problem with the consistency index is that it does not take feature *redundancy* into account. That is, two procedures could select features which have different indices, so are identified as "different", but in fact are so highly correlated that they are effectively identical. A method to deal with this situation was proposed by Yu *et al.* [111]. This method constructs a weighted complete bipartite graph, where the two node sets correspond to two different feature sets, and weights are assigned to the arcs are the normalized mutual information between the features at the nodes, also sometimes referred to as the symmetrical uncertainty. The weight between node i in set A, and node j in set B, is

$$w(A(i), B(j)) = \frac{I(X_{A(i)}; X_{B(j)})}{H(X_{A(i)}) + H(X_{B(j)})}. \tag{5.26}$$

The Hungarian algorithm is then applied to identify the maximum weighted matching between the two node sets, and the overall similarity between sets A and B is the final matching cost. This is the *information consistency* of the two sets. For more details, we refer the reader to Yu *et al.* [111].

An ideal consistency metric would include both of these properties, a correction for random selection and an ability to detect when similar features have been selected. However we leave the construction of such a metric for future research.

We now compare these two measures on the criteria from the previous sections. For each dataset, we take a bootstrap sample and select a set of features using each feature selection criterion. The (information) stability of a single criterion is quantified as the average pairwise (information) consistency across 50 bootstraps from the training data.

Figure 5.3 shows Kuncheva's stability measure on average over 15 datasets, selecting feature sets of size 10; note that the criteria have been displayed ordered left-to-right by their median value of stability over the 15 datasets. The marginal mutual information, MIM, is as expected the most stable, given that it has the lowest dimensional distribution to estimate. The next most stable is JMI which includes the relevancy/redundancy terms, but *averages* over the current feature set; this averaging process might therefore be interpreted empirically as a form of 'smoothing', enabling the criteria overall to be resistant to poor estimation of

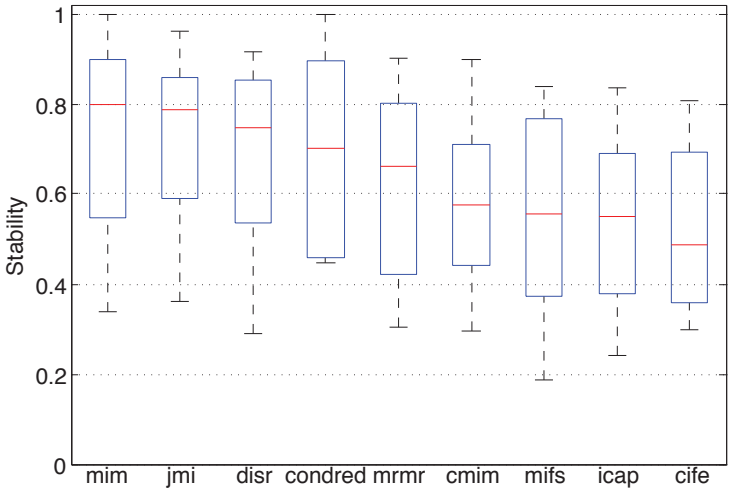


Figure 5.3: Kuncheva's Stability Index [67] across 15 datasets. The box indicates the upper/lower quartiles, the horizontal line within each shows the median value, while the dotted crossbars indicate the maximum/minimum values. For convenience of interpretation, criteria on the x-axis are ordered by their median value.

probability distributions. It can be noted that the far right of Figure 5.3 consists of the MIFS, ICAP and CIFE criteria, all of which do not attempt to average the redundancy terms.

Figure 5.4 shows the same datasets, but instead the *information stability* is computed; as mentioned, this should take into account the fact that some features are highly correlated. Interestingly, the two box-plots show broadly similar results. MIM is the most stable, and CIFE is the least stable, though here we see that JMI, DISR, and mRMR are actually more stable than Kuncheva's stability index can reflect.

5.2.2 How similar are the criteria?

Two criteria can be directly compared with the same methodology: by measuring the consistency and information consistency between selected feature subsets on a common set of data. We calculate the mean consistencies between two feature sets of size 10, repeatedly selected over 50 bootstraps from the original data. This is then arranged in a similarity matrix, and we use classical multi-dimensional scaling [26] to visualise this as a 2D map, shown in Figures 5.5a and 5.5b. Note

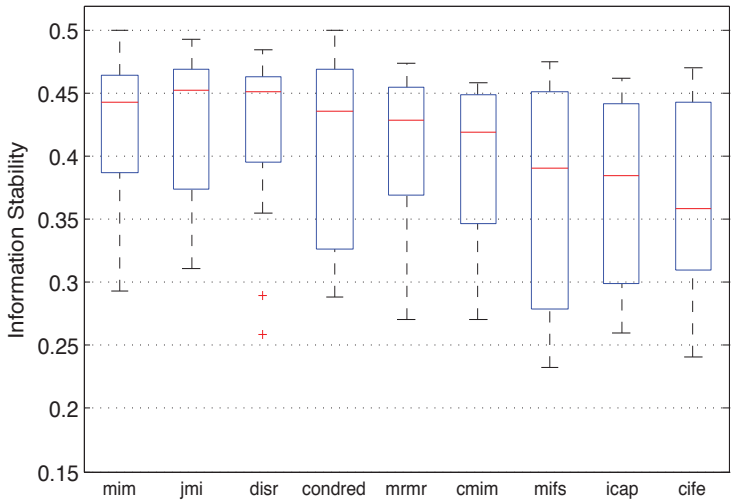
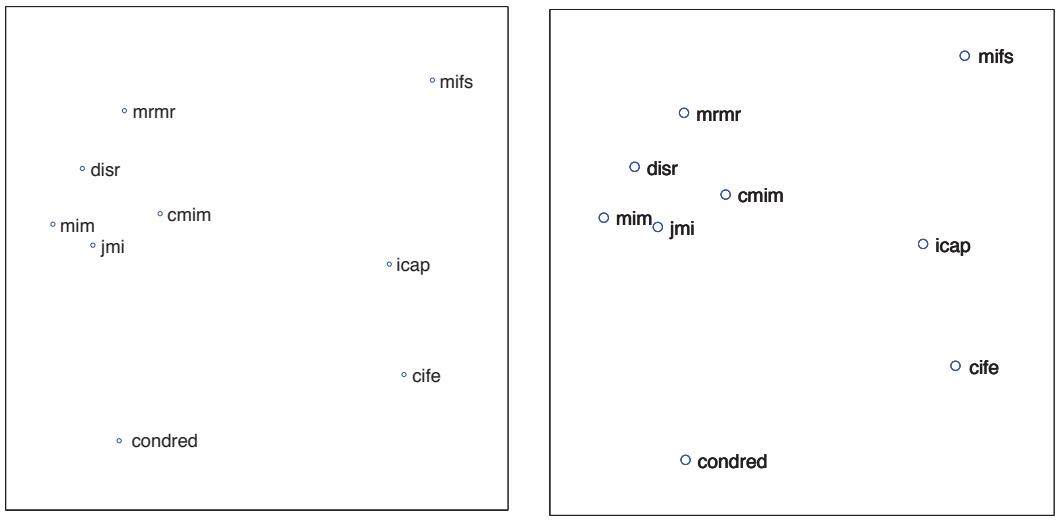


Figure 5.4: Yu *et al.*'s Information Stability Index [111] across 15 datasets. For comparison, criteria on the x-axis are ordered identically to Figure 5.3. A similar general picture emerges to that using Kuncheva's measure, though the information stability index is able to take feature redundancy into account, showing that some criteria are slightly more stable than expected.

again that while the indices may return different absolute values (one is a normalized mean of a hypergeometric distribution and the other is a pairwise sum of mutual information terms) they show very similar relative 'distances' between criteria.

Both diagrams show a cluster of several criteria, and 4 clear outliers: MIFS, CIFE, ICAP and CondRed. The 5 criteria clustering in the upper left of the space appear to return relatively similar feature sets. The 4 outliers appear to return quite significantly different feature sets, both from the clustered set, and from each other. A common characteristic of these 4 outliers is that they do not scale the redundancy or conditional redundancy information terms. In these criteria, the upper bound on the redundancy term $\sum_{j \in S} I(X_k; X_j)$ grows linearly with the number of selected features, whilst the upper bound on the relevancy term $I(X_k; Y)$ remains constant. When this happens the relevancy term is overwhelmed by the redundancy term and thus the criterion selects features with minimal redundancy, rather than trading off between the two terms. This leads to strongly divergent feature sets being selected, which is reflected in the stability of the criteria. Each of the outliers are different from each other as they have different combinations of redundancy and conditional redundancy. We will



(a) Kuncheva's Consistency Index. (b) Yu *et al.*'s Information Stability Index.

Figure 5.5: Relations between feature sets generated by different criteria, on average over 15 datasets. 2D visualisation generated by classical multi-dimensional scaling.

see this "balance" between relevancy and redundancy emerge as an important property in the experiments over the next few sections.

5.2.3 How do criteria behave in small-sample situations?

To assess how criteria behave in data poor situations, we vary the number of datapoints supplied to perform the feature selection. The procedure was to randomly select 140 datapoints, then use the remaining data as a hold-out set. From this 140, the number provided to each criterion was increased in steps of 10, from a minimal set of size 20. To allow a reasonable testing set size, we limited this assessment to only datasets with at least 200 datapoints total; this gives us 11 datasets from the 15, omitting *lungcancer*, *parkinsons*, *soybeansmall*, and *wine*. For each dataset we select 10 features and apply the 3-NN classifier, recording the rank-order of the criteria in terms of their generalisation error. This process was repeated and averaged over 50 trials, giving the results in Figure 5.6.

To aid interpretation we label MIM with a simple point marker, MIFS, CIFE, CondRed, and ICAP with a circle, and the remaining criteria (DISR, JMI, mRMR and CMIM) with a star. The criteria labelled with a star balance the relative magnitude of the relevancy and redundancy terms, those with a circle do not

attempt to balance them, and MIM contains no redundancy term. There is a clear separation between those criteria with a star outperforming those with a circle, and MIM varying in performance between the two groups as we allow more training datapoints.

Notice that the highest ranked criteria coincide with those in the cluster at the top left of Figures 5.5a and 5.5b. We suggest that the relative difference in performance is due to the same reason noted in Section 5.2.2, that the redundancy term grows with the size of the selected feature set. In this case, the redundancy term eventually grows to outweigh the relevancy by a large degree, and the new features are selected solely on the basis of redundancy, ignoring the relevance, thus leading to poor classification performance.

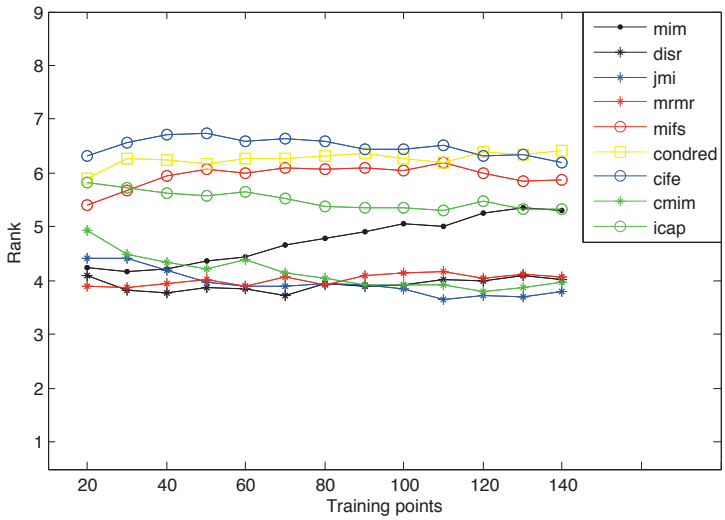


Figure 5.6: Average ranks of criteria in terms of test error, selecting 10 features, across 11 datasets. Note the clear dominance of criteria which do not allow the redundancy term to overwhelm the relevancy term (stars) over those that allow redundancy to grow with the size of the feature set (circles).

Extreme small-sample experiments

In the previous sections we discussed two theoretical properties of information-based feature selection criteria: whether it balances the relative magnitude of relevancy against redundancy, and whether it includes a class-conditional redundancy term. Empirically on the UCI datasets, we see that the balancing is far more important than the inclusion of the conditional redundancy term — for example, mRMR succeeds in many cases, while MIFS performs poorly. Now, we

Data	*Features*	*Examples*	*Classes*
Colon	2000	62	2
Leukemia	7070	72	2
Lung	325	73	7
Lymph	4026	96	9
NCI9	9712	60	9

Table 5.2: Datasets from Peng *et al.* [86], used in small-sample experiments.

consider whether the same property may hold in extreme small-sample situations, when the number of examples is so low that reliable estimation of distributions becomes extremely difficult. We use data sourced from Peng *et al.* [86], detailed in Table 5.2.

Results are shown in Figure 5.7, selecting 50 features from each dataset and plotting leave-one-out classification error. It should of course be remembered that on such small datasets, making just one additional datapoint error can result in seemingly large changes in accuracy. For example, the difference between the best and worst criteria on Leukemia was just 3 datapoints. In contrast to the UCI results, the picture is less clear. On Colon, the criteria all perform similarly; this is the least complex of all the datasets, having the smallest number of classes with a (relatively) small number of features. As we move through the datasets with increasing numbers of features/classes, we see that MIFS, CondRed, CIFE and ICAP start to break away, performing poorly compared to the others. Again, we note that these do not attempt to balance relevancy/redundancy. This difference is clearest on the NCI9 data, the most complex with 9 classes and 9712 features. However, as we may expect with such high dimensional and challenging problems, there are some exceptions — the Colon data as mentioned, and also the Lung data where ICAP/MIFS perform well.

5.2.4 What is the relationship between stability and accuracy?

An important question is whether we can find a good balance between the stability of a criterion and the classification accuracy. This was considered by Gulgezen *et al.* [47], who studied the stability/accuracy trade-off for the mRMR criterion. In the following, we consider this trade-off in the context of *Pareto-optimality*, across the 9 criteria, and the 15 datasets from Table 5.1. Experimental protocol

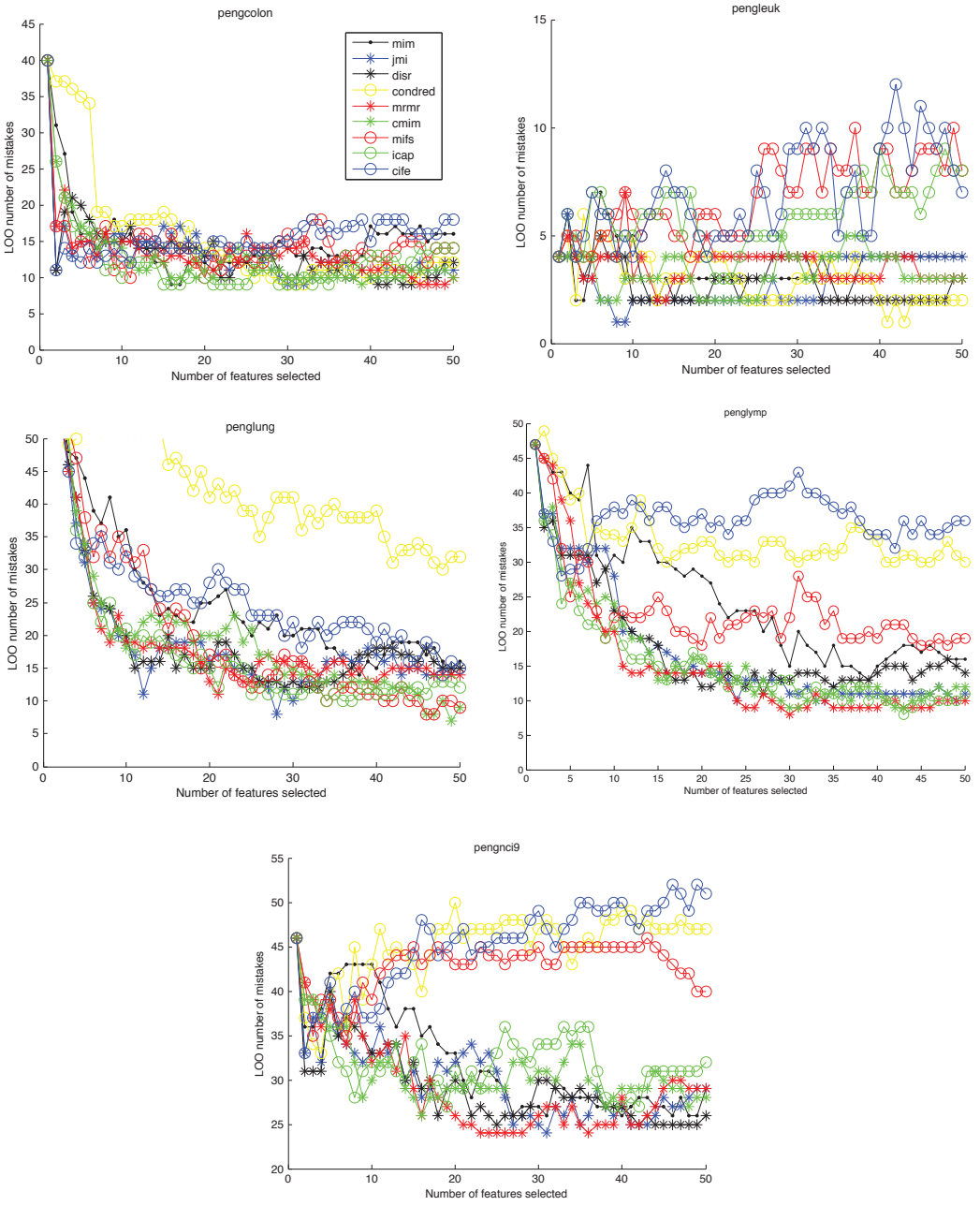


Figure 5.7: LOO results on Peng's datasets: Colon, Lymphoma, Leukemia, Lung, NCI9.

was to take 50 bootstraps from the dataset, each time calculating the out-of-bag error using the 3-NN. The stability measure was Kuncheva's stability index calculated from the 50 feature sets, and the accuracy was the mean out-of-bag accuracy across the 50 bootstraps. The experiments were also repeated using the Information Stability measure, revealing almost identical results. Results using Kuncheva's stability index are shown in Figure 5.8.

The *Pareto-optimal set* is defined as the set of criteria for which no other criterion has both a higher accuracy and a higher stability, hence the members of the Pareto-optimal set are said to be *non-dominated* [41]. Thus in each of the graphs in Figure 5.8, criteria that appear further to the top-right of the space *dominate* those toward the bottom left — in such a situation there is no reason to choose those at the bottom left, since they are dominated on both objectives by other criteria.

A summary (for both stability and information stability) is provided in the first two columns of Table 5.3, showing the *non-dominated rank* of the different criteria. This is computed per dataset as the number of other criteria which dominate a given criterion, in the Pareto-optimal sense, then averaged over the 15 datasets. We can see that these rankings are similar to the results earlier, with MIFS, ICAP, CIFE and CondRed performing poorly. We note that JMI, (which both balances the relevancy and redundancy terms and includes the conditional redundancy) outperforms all other criteria.

We present the average accuracy ranks across the 50 bootstraps in the third column of Table 5.3. These are similar to the results from Figure 5.6 but use a bootstrap of the full dataset, rather than a small sample from it. Following Demšar [29] we analysed these ranks using a Friedman test to determine which criteria are statistically significantly different from each other. We then used a Nemenyi post-hoc test to determine which criteria differed, with statistical significances at 90%, 95%, and 99% confidences. These give a partial ordering for the criteria which we present in Figure 5.9, showing a *Significant Dominance Partial Order* diagram. Note that this style of diagram encapsulates the same information as a Critical Difference diagram [29], but allows us to display multiple levels of statistical significance. A bold line connecting two criteria signifies a difference at the 99% confidence level, a dashed line at the 95% level, and a dotted line at the 90% level. Absence of a link signifies that we do not have the statistical power to determine the difference one way or another. Reading Figure

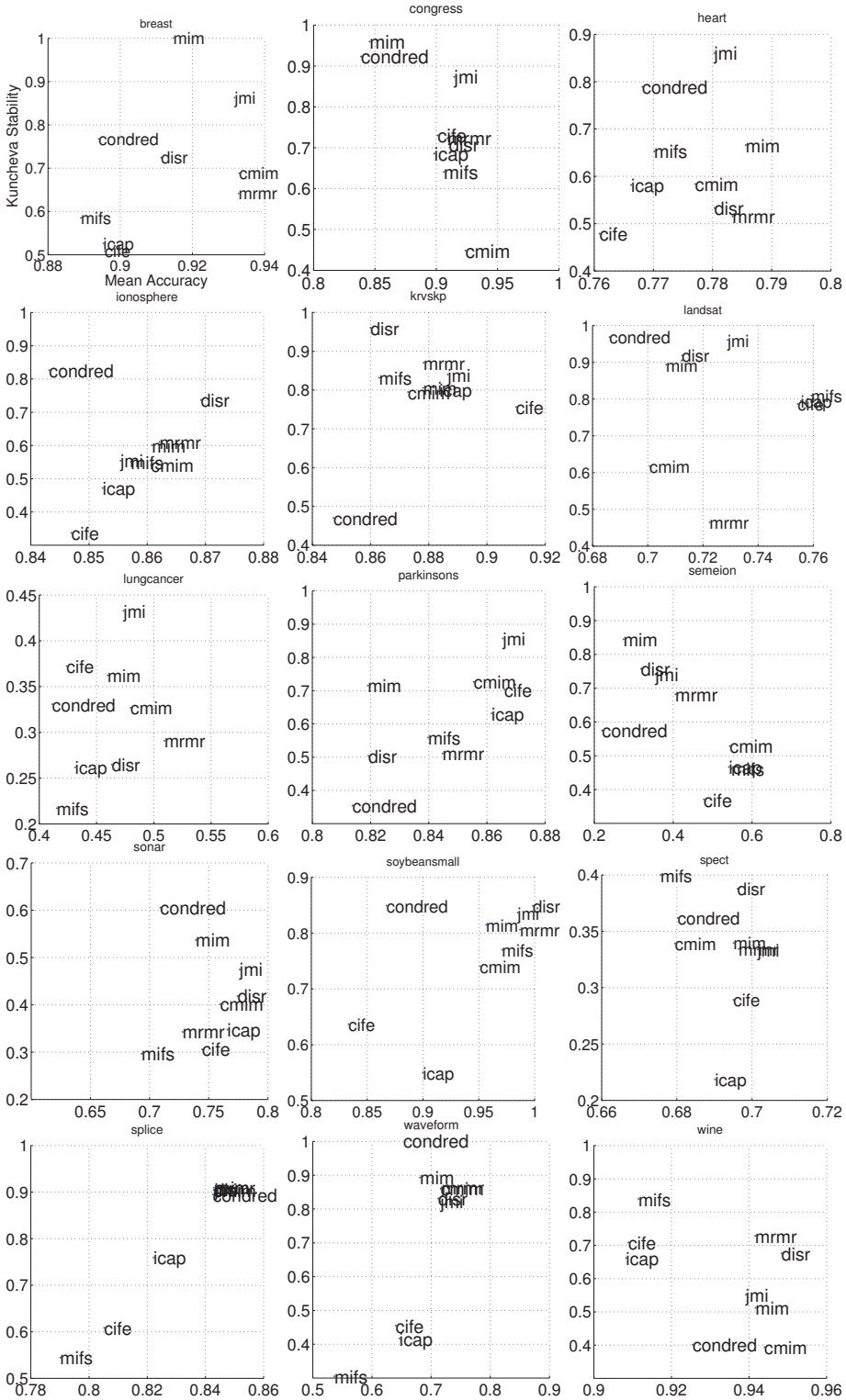


Figure 5.8: Stability (y-axes) versus Accuracy (x-axes) over 50 bootstraps for the final quarter of the UCI datasets. The pareto-optimal rankings are summarised in Table 5.3.

Accuracy/Stability(Yu)	Accuracy/Stability(Kuncheva)	Accuracy
JMI (1.6)	JMI (1.5)	JMI (2.6)
DISR (2.3)	DISR (2.2)	mRMR (3.6)
MIM (2.4)	MIM (2.3)	DISR (3.7)
mRMR (2.5)	mRMR (2.5)	CMIM (4.5)
CMIM (3.3)	CONDRED (3.2)	ICAP (5.3)
ICAP (3.6)	CMIM (3.4)	MIM (5.4)
CONDRED (3.7)	ICAP (4.3)	CIFE (5.9)
CIFE (4.3)	CIFE (4.8)	MIFS (6.5)
MIFS (4.5)	MIFS (4.9)	CONDRED (7.4)

Table 5.3: **Column 1:** Non-dominated Rank of different criteria for the trade-off of accuracy/stability. Criteria with a higher rank (closer to 1.0) provide a better trade-off than those with a lower rank. **Column 2:** As column 1 but using Kuncheva's Stability Index. **Column 3:** Average ranks for accuracy alone.

5.9, we see that with 99% confidence JMI is significantly superior to CondRed, and MIFS, but not statistically significantly different from the other criteria. As we lower our confidence level, more differences appear, for example mRMR and MIFS are only significantly different at the 90% confidence level.

5.2.5 Summary of empirical findings

From experiments in this section, we conclude that the balance of relevancy and redundancy terms is extremely important, while the inclusion of a class conditional term seems to matter less. We find that some criteria are inherently more *stable* than others, and that the trade-off between accuracy (using a simple k-NN classifier) and stability of the feature sets differs between criteria. The best overall trade-off for accuracy/stability was found in the JMI and mRMR criteria. In the following section we check these findings in the context of two problems posed for the NIPS Feature Selection Challenge.

5.3 Performance on the NIPS Feature Selection Challenge

In this section we investigate performance of the criteria on datasets taken from the NIPS Feature Selection Challenge [49]. We present results using GISETTE (a handwriting recognition task), and MADELON (an artificially generated dataset).

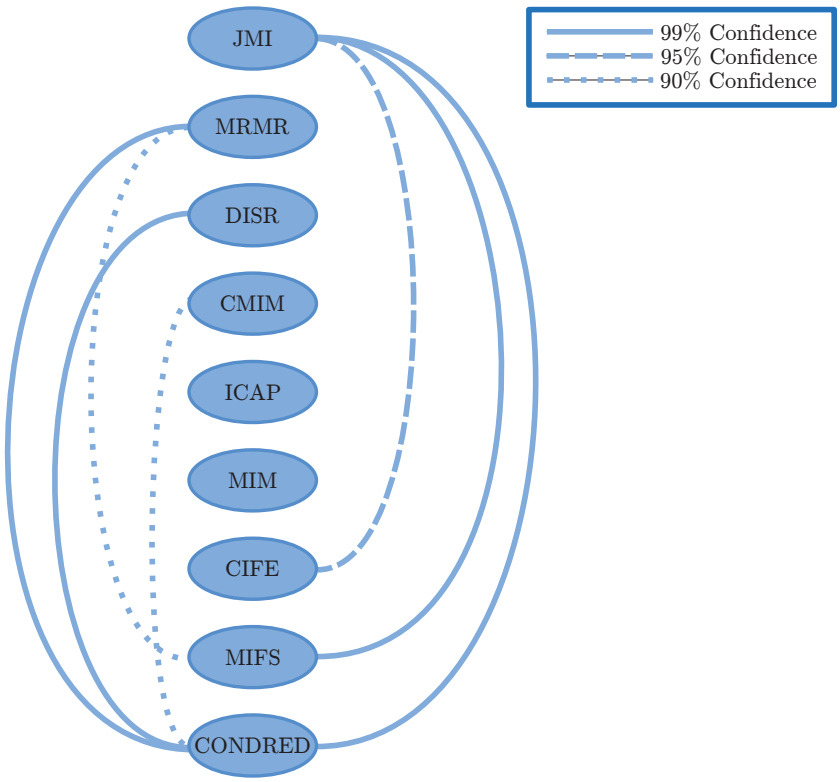


Figure 5.9: Significant dominance partial-order diagram. Criteria are placed top to bottom in the diagram by their rank taken from column 3 of Table 5.3. A link joining two criteria means a statistically significant difference is observed with a Nemenyi post-hoc test at the specified confidence level. For example JMI is significantly superior to MIFS ($\beta = 1$) at the 99% confidence level. Note that the absence of a link does not signify the lack of a statistically significant difference, but that the Nemenyi test does not have sufficient power (in terms of number of datasets) to determine the outcome [29]. It is interesting to note that the four bottom ranked criteria correspond to the corners of the unit square in Figure 5.2; while the top three (JMI/mRMR/DISR) are all very similar, scaling the redundancy terms by the size of the feature set. The middle ranks belong to CMIM/ICAP, which are similar in that they use the min/max strategy instead of a linear combination of terms.

Data	*Features*	*Examples (Tr/Val)*	*Classes*
GISETTE	5000	6000/1000	2
MADELON	500	2000/600	2

Table 5.4: Datasets from the NIPS challenge, used in experiments.

To apply the mutual information criteria, we estimate the necessary distributions using histogram estimators: features were discretised independently into 10 equal width bins, with bin boundaries determined from training data. After the feature selection process the original (undiscretised) datasets were used to classify the validation data. Each criterion was used to generate a ranking for the top 200 features in each dataset. We show results using the full top 200 for GISETTE, but only the top 20 for MADELON as after this point all criteria demonstrated severe overfitting. We use the Balanced Error Rate, for fair comparison with previously published work on the NIPS datasets. We accept that this does not necessarily share the same optima as the classification error (nor the same maxima of the joint likelihood). We investigate cost-sensitive versions of the model likelihood in Chapter 7, where we derive criteria which could be tailored to the Balanced Error Rate (on the training data).

Validation data results are presented in Figure 5.10 (GISETTE) and Figure 5.11 (MADELON). The minimum of the validation error was used to select the best performing feature set size, the training data alone used to classify the testing data, and finally test labels were submitted to the challenge website. Test results are provided in Table 5.5 for GISETTE, and Table 5.6 for MADELON[2].

Unlike in Section 5.2, the datasets we use from the NIPS Feature Selection Challenge have many more datapoints (GISETTE has 6000 training examples, MADELON has 2000) and thus we can present results using a direct implementation of Equation (5.1) as a criterion. We refer to this criterion as CMI, as it is using the conditional mutual information to score features. Unfortunately there are still estimation errors in this calculation when selecting a large number of features, even given the large number of datapoints and so the criterion fails to select features after a certain point, as each feature appears equally irrelevant. In GISETTE, CMI selected 13 features, and so the top 10 features were used and one result is shown. In MADELON, CMI selected 7 features and so 7 results are shown.

[2]We do not provide classification confidences as we used a nearest neighbour classifier and thus the AUC is equal to 1− BER.

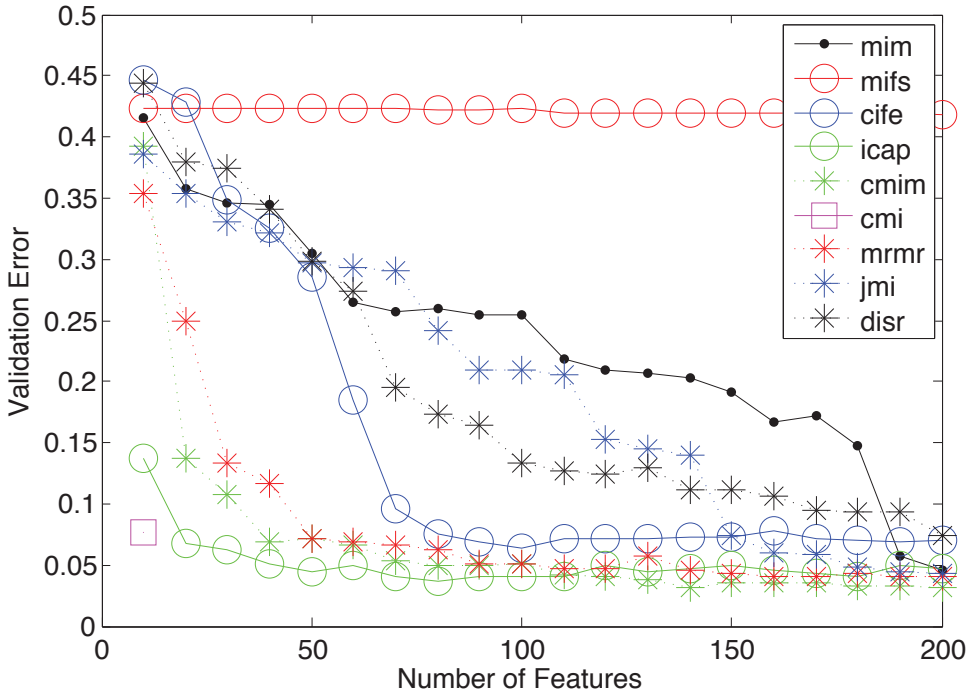


Figure 5.10: Validation Error curve using GISETTE.

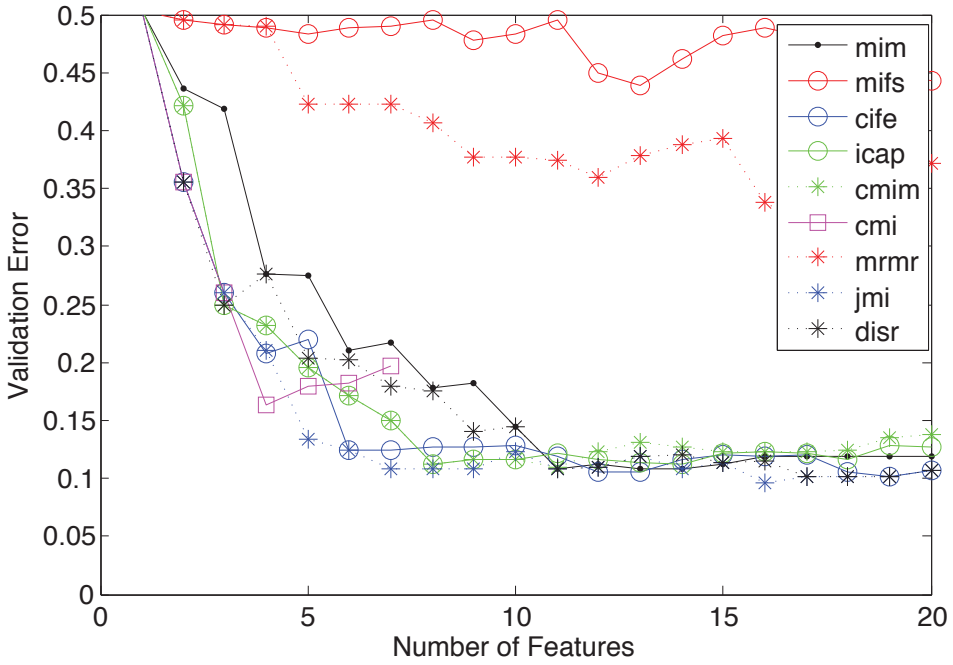


Figure 5.11: Validation Error curve using MADELON.

5.3.1 GISETTE testing data results

In Table 5.5 there are several distinctions between the criteria, the most striking of which is the failure of MIFS to select an informative feature set. The importance of balancing the magnitude of the relevancy and the redundancy can be seen whilst looking at the other criteria in this test. Those criteria which balance the magnitudes, (CMIM, JMI, & mRMR) perform better than those which do not (ICAP,CIFE). The DISR criterion forms an outlier here as it performs poorly when compared to JMI. The only difference between these two criteria is the normalization in DISR — as such, this is likely the cause of the observed poor performance, due to the introduction of more variance by estimating the normalization term $H(X_k, X_j, Y)$.

We can also see how important the low dimensional approximation is, as even with 6000 training examples CMI cannot estimate the required joint distribution to avoid selecting probes, despite being a direct iterative maximisation of the joint likelihood, under a flat prior, in the limit of datapoints.

Criterion	*BER*	*AUC*	*Features (%)*	*Probes (%)*
MIM	4.18	95.82	4.00	0.00
MIFS	42.00	58.00	4.00	58.50
CIFE	6.85	93.15	2.00	0.00
ICAP	4.17	95.83	1.60	0.00
CMIM	**2.86**	**97.14**	**2.80**	**0.00**
CMI	8.06	91.94	0.20	20.00
mRMR	2.94	97.06	3.20	0.00
JMI	3.51	96.49	4.00	0.00
DISR	8.03	91.97	4.00	0.00
Winning Challenge Entry	**1.35**	**98.71**	**18.3**	**0.0**

Table 5.5: NIPS FS Challenge Results: GISETTE.

5.3.2 MADELON testing data results

The MADELON results (Table 5.6) show a particularly interesting point — the top performers (in terms of BER) are JMI and CIFE. Both these criteria include the class-conditional redundancy term, but CIFE does not balance the influence of relevancy against redundancy. In this case, it appears the 'balancing' issue, so important in our previous experiments, appears unimportant — instead, the presence of the conditional redundancy term is the differentiating factor between

Criterion	*BER*	*AUC*	*Features (%)*	*Probes (%)*
MIM	10.78	89.22	2.20	0.00
MIFS	46.06	53.94	2.60	92.31
CIFE	**9.50**	**90.50**	**3.80**	**0.00**
ICAP	11.11	88.89	1.60	0.00
CMIM	11.83	88.17	2.20	0.00
CMI	21.39	78.61	0.80	0.00
mRMR	35.83	64.17	3.40	82.35
JMI	**9.50**	**90.50**	**3.20**	**0.00**
DISR	9.56	90.44	3.40	0.00
Winning Challenge Entry	**7.11**	**96.95**	**1.6**	**0.0**

Table 5.6: NIPS FS Challenge Results: MADELON.

criteria (note the poor performance of MIFS/mRMR). This is perhaps not surprising given the nature of the MADELON data, constructed precisely to require features to be evaluated jointly.

It is interesting to note that the challenge organisers benchmarked a 3-NN using the optimal feature set, achieving a 10% test error [49]. Many of the criteria managed to select feature sets which achieved a similar error rate using a 3-NN, and it is likely that a more sophisticated classifier is required to further improve performance.

Our experimental results have shown another difference between the criteria, which was less apparent from our theoretical study. The criteria which implemented scaling, or some other method of balancing the size of the relevancy and redundancy terms have outperformed all others. The criteria which do not, like CIFE and MIFS, perform poorly across many datasets. We now integrate our theoretical view of feature relevancy and redundancy into that of Kohavi and John's notions of Strong and Weak Relevance from their landmark 1997 paper [62].

5.4 An Information Theoretic View of Strong and Weak Relevance

We reviewed the definitions of relevance and irrelevance given by Kohavi and John [62] in Section 3.1. These definitions are statements about the conditional probability distributions of the variables involved. We can re-state the definitions

of Kohavi and John (hereafter KJ) in terms of mutual information, and see how they can fit into our likelihood maximisation framework. In the notation below, notation X_i indicates the ith feature in the overall set X, and notation $X_{\setminus i}$ indicates the set $\{X \setminus X_i\}$, all features *except* the ith. The definitions of strong and weak relevance are taken from KJ's paper, but the corollaries are novel restatements in information theoretic terms. We also extend the notion of weak relevance by separating it into two disjoint definitions.

Definition 10. Strongly Relevant Feature [62]
Feature X_i is strongly relevant *to Y iff there exists an assignment of values x_i, y, $x_{\setminus i}$ for which $p(X_i = x_i, X_{\setminus i} = x_{\setminus i}) > 0$ and $p(Y = y|X_i = x_i, X_{\setminus i} = x_{\setminus i}) \neq p(Y = y|X_{\setminus i} = x_{\setminus i})$.*

Corollary 1. *A feature X_i is* strongly relevant *iff $I(X_i; Y|X_{\setminus i}) > 0$.*

Proof. The KL divergence $D_{KL}(p(y|x,z) \;||\; p(y|z)) > 0$ iff $p(y|x,z) \neq p(y|z)$ for some assignment of values x, y, z. A simple re-application of the manipulations leading to Equation (4.9) demonstrates that the expected KL-divergence $E_{xz}\{p(y|x,z)||p(y|z)\}$ is equal to the mutual information $I(X;Y|Z)$. In the definition of strong relevance, if there exists a single assignment of values x_i, y, $x_{\setminus i}$ that satisfies the inequality, then $E_x\{p(y|x_i x_{\setminus i})||p(y|x_{\setminus i})\} > 0$ and therefore $I(X_i; Y|X_{\setminus i}) > 0$. □

Given the framework we have presented, we can note that this strong relevance comes from a combination of *three terms*,

$$I(X_i; Y|X_{\setminus i}) = I(X_i; Y) - I(X_i; X_{\setminus i}) + I(X_i; X_{\setminus i}|Y). \tag{5.27}$$

This view of strong relevance demonstrates explicitly that a feature may be individually irrelevant (i.e. $p(y|x_i) = p(y)$ and thus $I(X_i; Y) = 0$), but still strongly relevant if $I(X_i; X_{\setminus i}|Y) - I(X_i; X_{\setminus i}) > 0$.

Definition 11. Weakly Relevant Feature [62]
Feature X_i is weakly relevant *to Y iff it is not strongly relevant and there exists a subset $Z \subset X_{\setminus i}$, and an assignment of values x_i, y, z for which $p(X_i = x_i, Z = z) > 0$ such that $p(Y = y|X_i = x_i, Z = z) \neq p(Y = y|Z = z)$.*

Corollary 2. *A feature X_i is weakly relevant to Y iff it is not strongly relevant and $I(X_i; Y|Z) > 0$ for some $Z \subset X_{\setminus i}$.*

Proof. This follows immediately from the proof for the strong relevance above. □

The notion of weak relevance can however be refined further, if we constrain the subset Z such that it must contain all the strongly relevant features.

Definition 12. Weak Redundancy
Feature X_i *is* weakly redundant *if it is weakly relevant and* $\exists Z \subset X_{\setminus i}$ *such that* $I(X_i; Y|\{Z, SR\}) > 0$ *where* SR *is the set of strongly relevant features.*

Definition 13. Strong Redundancy
Feature X_i *is* strongly redundant *if it is weakly relevant and* $\forall Z \subset X_{\setminus i}\ I(X_i; Y|\{Z, SR\}) = 0$ *where* SR *is the set of strongly relevant features.*

The optimal subset (*i.e.* contains the necessary and sufficient features) is therefore all the strongly relevant and some weakly redundant features. The optimal subset does not contain any of the strongly redundant or irrelevant features. From this perspective the weakly redundant features are those which share the same data, some of them are necessary to capture all the available information but to select all of them would include redundant features. Note that this coincides with the definition of a *Surely Sufficient Feature Subset* [50, pg 19].

Another way of seeing this is, of the weakly relevant features, there are those which *duplicate* information in SR (the strongly redundant set), and those which *complement* information in SR (the weakly redundant set).

It is interesting, and somewhat non-intuitive, that there can be cases where there are *no* strongly relevant features, but *all* are weakly relevant. This will occur for example in a dataset where all features have exact duplicates: we have $2M$ features and $\forall i,\ X_{M+i} = X_i$. In this case, for any X_k (such that $k < M$) we will have $I(X_k; Y|X_{\setminus i}) = 0$ since its duplicate feature X_{M+k} will carry the same information. In this case, for any feature X_k (such that $k < M$) that is strongly relevant in the dataset $\{X_1, ..., X_M\}$, it is *weakly* relevant in the dataset $\{X_1, ..., X_{2M}\}$.

This issue can be dealt with by refining our definition of relevance with respect to a subset of the full feature space. A particular subset about which we have some information is the currently selected set S. We can relate our framework to KJ's definitions in this context. Following KJ's formulations,

Definition 14. Relevance with respect to the current set S**.**
Feature X_i *is* relevant *to* Y *with respect to* S *iff there exists an assignment of*

values x_i, y, s for which $p(X_i = x_i, S = s) > 0$ and $p(Y = y|X_i = x_i, S = s) \neq p(Y = y|S = s)$.

Corollary 3. *Feature X_i is* relevant *to Y with respect to S, iff $I(X_i; Y|S) > 0$.*

A feature that is relevant with respect to S is either strongly or weakly relevant (in the KJ sense) but it is not possible to determine in which class it lies, as we have not conditioned on $X_{\setminus i}$. Notice that the definition coincides exactly with the forward selection heuristic (Equation 4.14) when using an uninformative prior, which we have shown is a hill-climber on the joint likelihood of our discriminative model. As a result, we see *that hill-climbing on the joint likelihood corresponds to adding the* most *relevant feature with respect to the current set S*. Again we re-emphasize, that the resultant gain in the likelihood comes from a combination of *three sources*:

$$I(X_i; Y|S) = I(X_i; Y) - I(X_i; S) + I(X_i; S|Y). \tag{5.28}$$

It could easily be the case that $I(X_i; Y) = 0$, that is a feature is entirely irrelevant when considered on its own — but the sum of the two redundancy terms results in a positive value for $I(X_i; Y|S)$. We see that if a criterion does not attempt to model both of the redundancy terms, even if only using low dimensional approximations, it runs the risk of evaluating the relevance of X_i incorrectly.

Definition 15. Irrelevance with respect to the current set S.
Feature X_i is irrelevant *to Y with respect to S iff $\forall$ x_i, y, s for which $p(X_i = x_i, S = s) > 0$ and $p(Y = y|X_i = x_i, S = s) = p(Y = y|S = s)$.*

Corollary 4. *Feature X_i is* irrelevant *to Y with respect to S, iff $I(X_i; Y|S) = 0$.*

In a forward step, if a feature X_i is irrelevant with respect to S, adding it alone to S *will not increase the joint likelihood.* However, there may be further additions to S in the future, giving us a selected set S'; we may then find that X_i is then *relevant* with respect to S'. This is because the relevance measure is composed of the three terms mentioned previously, and the conditional redundancy depends upon the features which have already been selected. As we noted when talking about strong relevancy even if $I(X_i; Y) = 0$ the feature can still be strongly relevant. In a backward step we check whether a feature is irrelevant with respect to $\{S \setminus X_i\}$, using the test $I(X_i; Y|\{S \setminus X_i\}) = 0$. In this case, removing this feature *will not decrease the joint likelihood.*

5.5 Chapter Summary

In this chapter we have unified 20 years of literature on the construction of mutual information based feature selection criteria. We took the view of feature selection as likelihood maximisation from the previous chapter and showed how the various different mutual information criteria can be seen as approximate maximisers of this likelihood with an uninformative prior. Each of the criteria we discussed makes an of approximation to the true update rule, by assuming the underlying data distribution has various properties such as feature independence, or pairwise independence. By using our probabilistic formulation we can make these assumptions explicit. The most important theoretical difference between the criteria was how many of the information theory terms they included. Many criteria included both the relevancy and redundancy term, but fewer included the conditional redundancy term which accounts for how two features can combine to become more informative than their separate components. We then performed an empirical investigation into nine of these criteria, comparing their performance over a variety of metrics. We investigated their stability with respect to changes in the datasets, how the criteria perform with small sample sizes, and what the trade off is between accuracy and stability. We also benchmarked them on the NIPS feature selection challenge datasets to provide comparable results with the literature. In this comparison we saw how balancing the size of the relevancy and redundancy terms is the most important factor in determining empirical performance. Finally we related our likelihood based view of mutual information to the commonly referenced work of Kohavi and John, in the process splitting their notion of weak relevance into two categories.

Chapter 6

Priors for filter feature selection

In the previous chapter we showed how many common information theoretic feature selection criteria are approximate optimisers of the joint likelihood of a specific probabilistic model. We explored the theoretical implications of this result, analysing how different criteria assumed different factorisations (or independences) in the underlying probabilistic model. In this chapter we focus on what additional benefits we can extract from this novel perspective on feature selection. Specifically the joint likelihood of a model includes a prior distribution over the features which encodes how likely any feature is to be selected *a priori* (before we have examined any data). In the previous chapter we assumed this prior was flat or uninformative, now we investigate different kinds of *informative* priors, and how they influence the feature selection process. We develop greedy updates which maximise our joint likelihood under both sparsity and domain knowledge priors. We show that an algorithm for structure learning in Bayesian Networks called IAMB is an exact maximiser of the joint likelihood, under a specific sparsity prior. We then show how to include domain knowledge into IAMB.We present experimental results investigating the influence of domain knowledge on the performance of the modified criteria.

6.1 Maximising the Joint Likelihood

In Chapter 4 we specified our model as a function of $\boldsymbol{\theta}, \tau$ and λ,

$$\mathcal{L}(\mathcal{D}, \boldsymbol{\theta}, \tau, \lambda) = p(\boldsymbol{\theta}, \tau)p(\lambda) \prod_{i=1}^{N} q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)q(\mathbf{x}^i|\lambda). \tag{6.1}$$

We saw how to expand this likelihood into the sum of several terms,

$$-\ell \approx \mathbb{E}_{\mathbf{x},y}\left\{ \log \frac{p(y^i|\mathbf{x}^i,\boldsymbol{\theta})}{q(y^i|\mathbf{x}^i,\boldsymbol{\theta},\tau)} \right\} + I(X_{\neg\boldsymbol{\theta}};Y|X_{\boldsymbol{\theta}}) + H(Y|X) - \frac{1}{N}\log p(\boldsymbol{\theta},\tau). \quad (6.2)$$

Then we can maximise this model with respect to $\boldsymbol{\theta}$ by finding $\boldsymbol{\theta}^*$,

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \left(I(X_{\neg\boldsymbol{\theta}};Y|X_{\boldsymbol{\theta}}) - \frac{1}{N}\log p(\boldsymbol{\theta}) \right). \quad (6.3)$$

Finally we saw that we can greedily maximise the likelihood by selecting features one by one according to this *optimal* criterion,

$$X_k^* = \arg\max_{X_k \in X_{\neg\boldsymbol{\theta}^t}} \left(I(X_k;Y|X_{\boldsymbol{\theta}^t}) + \frac{1}{N}\log \frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} \right). \quad (6.4)$$

In the previous chapter we took this framework and looked at how the process of optimising Equation (6.4) under a flat prior relates to the literature. This framework explains many common information theoretic feature selection criteria by showing they derive from making different assumptions about the various probability distributions involved.

We now investigate combining these information theoretic filters with domain knowledge, in the form of informative prior distributions for $\boldsymbol{\theta}$ as opposed to the flat priors studied previously. We focus on fully factorised priors, where each feature is considered independently of the others, though the general framework presented in Chapter 4 can include more structured information.

In Section 3.6 we looked at structure learning algorithms for Bayesian Networks, focusing particularly on IAMB [107] and its derivatives. If we now look at IAMB from the perspective of the previous chapter we can see how it appears to directly optimise the joint likelihood. Features are selected greedily if they have a positive conditional mutual information, given all other selected features. Then IAMB has a backwards pruning step which removes features which have been made redundant. These two stages appear to be direct implementations of Equations (4.14) and (4.20), and the algorithm terminates when all remaining unselected features have zero information. In practice when working with real data it is likely that the estimate of the mutual information will differ from the true value, and it is rare that these calculated values will be exactly zero. Therefore IAMB uses a threshold value above zero to decide if the true mutual information

is non-zero. We will see how this threshold value can be interpreted as a sparsity prior controlling the number of selected features. We begin by constructing factorised priors to encode sparsity and domain knowledge.

6.2 Constructing a prior

We will construct priors assuming independence between all the features. As we saw in the previous chapter this assumption corresponds to the MIM algorithm, though we do not investigate the use of weaker assumptions in prior construction. We will use a Bernoulli distribution over the selection probability of each feature, and then show how to use this prior to impose sparsity or include domain knowledge.

6.2.1 A factored prior

As mentioned above we treat each feature independently, and assume each $p(\theta_i)$ is a Bernoulli random variable. Therefore the prior over $p(\boldsymbol{\theta})$ is

$$p(\boldsymbol{\theta}) = \prod_i^d p(\theta_i) = \prod_i^d \beta_i^{\theta_i}(1-\beta_i)^{1-\theta_i}. \tag{6.5}$$

We further define the success probability, β_i, of the Bernoulli as a logistic function,

$$\beta_i = \frac{e^{\alpha w_i}}{1+e^{\alpha w_i}} = \frac{1}{1+e^{-\alpha w_i}}. \tag{6.6}$$

We define $\alpha > 0$ as a scaling factor and w_i as a per-feature weight with $w_i = 0$ denoting no preference, $w_i < 0$ indicating we believe $X_i \notin X^*$, and $w_i > 0$ indicating we believe $X_i \in X^*$. We then define $\mathbf{w}$ as the vector of w_i elements. Therefore the prior for $p(\boldsymbol{\theta})$ is,

$$p(\boldsymbol{\theta}) = \prod_i^d \left(\frac{e^{\alpha w_i}}{1+e^{\alpha w_i}}\right)^{\theta_i} \left(1 - \frac{e^{\alpha w_i}}{1+e^{\alpha w_i}}\right)^{(1-\theta_i)}. \tag{6.7}$$

We can rewrite this prior into a more common form using the fact that θ_i is

binary, as follows,

$$\begin{aligned}
p(\boldsymbol{\theta}) &= \prod_i^d (\frac{e^{\alpha w_i}}{1+e^{\alpha w_i}})^{\theta_i} (1 - \frac{e^{\alpha w_i}}{1+e^{\alpha w_i}})^{(1-\theta_i)} \\
&= \prod_i^d (\frac{e^{\alpha w_i}}{1+e^{\alpha w_i}})^{\theta_i} (\frac{1}{1+e^{\alpha w_i}})^{(1-\theta_i)} \\
&= \prod_i^d \frac{1}{1+e^{\alpha w_i}} (e^{\alpha w_i})^{\theta_i} 1^{(1-\theta_i)} \\
&= \prod_i^d \frac{e^{\alpha w_i \theta_i}}{1+e^{\alpha w_i}} \\
&= \frac{\prod_i^d e^{\alpha w_i \theta_i}}{\prod_i^d (1+e^{\alpha w_i})} \\
&= \frac{e^{\alpha \sum_i^d w_i \theta_i}}{\prod_i^d (1+e^{\alpha w_i})} \\
&= \frac{e^{\alpha \mathbf{w}^T \boldsymbol{\theta}}}{\prod_i^d (1+e^{\alpha w_i})}
\end{aligned} \tag{6.8}$$

As $\prod_i^d (1+e^{\alpha w_i})$ is constant with respect to $\boldsymbol{\theta}$ this is equivalent to specifying $p(\boldsymbol{\theta})$ as

$$p(\boldsymbol{\theta}) \propto e^{\alpha \mathbf{w}^T \boldsymbol{\theta}}. \tag{6.9}$$

As the prior terms in our greedy maximisation of the likelihood are ratios, then we do not need the normalisation constant or any other constant factors for this prior. We note that this formulation is of a similar exponential form to the priors specified by Mukherjee and Speed [82], and we could extend our framework to incorporate many of their graph structure priors.

6.2.2 Update rules

When using this factored prior we can rewrite the update rules in Equations (4.14) and (4.20). The ratio term simplifies as each update only includes or excludes a single feature, and most of the terms in the prior are constant and cancel. Therefore the prior ratio when selecting an additional feature is,

$$\frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^t)} = e^{\alpha w_k} \tag{6.10}$$

where w_k denotes the weight of the candidate feature. The prior ratio when removing a feature is

$$\frac{p(\boldsymbol{\theta}^{t+1})}{p(\boldsymbol{\theta}^{t})} = e^{-\alpha w_k}. \tag{6.11}$$

The full update rule when selecting a new feature (*i.e.* a forward step) is:

$$X_k^* = \underset{X_k \in X_{\neg \boldsymbol{\theta}^t}}{\arg\max} \left(I(X_k; Y | X_{\boldsymbol{\theta}^t}) + \frac{\alpha w_k}{N} \right) \tag{6.12}$$

with a similar update for the backward step. These updates form a greedy maximisation of the joint likelihood given in Equation (6.1), where the α and w_k control the strength and class of knowledge respectively.

6.2.3 Encoding sparsity or domain knowledge

We now turn to how exactly to encode knowledge into our prior. When using the factorised prior described in Equation (6.9) we can specify priors for sparsity or domain knowledge.

We encode sparsity by setting all $w_i = -1$, and using the α parameter to decide how much sparsity we wish to impose. Increasing α in this case lowers the success probability of the Bernoulli distribution for each feature, and it is this probability that encodes how sparse a solution we impose. A lower success probability makes each feature less likely to be selected, and thus a smaller number of features are selected overall. The sparsity term effectively forms a fixed penalty on the usefulness of each feature. We will denote sparsity priors using the notation $p_s(\boldsymbol{\theta})$ and α_s. We therefore define a sparsity prior as

$$p_s(\boldsymbol{\theta}) \propto e^{-\alpha_s |\boldsymbol{\theta}|}. \tag{6.13}$$

We use $|\boldsymbol{\theta}|$ to represent the number of selected features in $\boldsymbol{\theta}$. This derives directly from setting all the $w_i = -1$ in Equation (6.9).

By allowing the w_i values to range freely we can encode varying levels of information into the prior, as these again change the success probability of the Bernoulli, thus encoding how useful *a priori* we think a given feature is. A positive w_i denotes that the feature is useful and the domain knowledge suggests it should be selected, and a negative w_i denotes the feature has no value and should not be selected. When $w_i = 0$ we have no extra information to include

about that particular feature and thus give it an equal probability of selection and remaining unselected. We will denote such knowledge priors with $p_d(\boldsymbol{\theta})$ and α_d leading to an knowledge prior where

$$p_d(\boldsymbol{\theta}) \propto e^{\alpha_d \mathbf{w}^T \boldsymbol{\theta}}. \tag{6.14}$$

We have now described two kinds of priors which we can integrate into any criterion derived from our discriminative model assumption. To combine both sparsity and domain knowledge into the same prior we will define $p(\boldsymbol{\theta}) \propto p_s(\boldsymbol{\theta}) p_d(\boldsymbol{\theta})$. When using our greedy updates the normalisation constants again disappear as the prior is only considered in a ratio. If we use this prior then the sparsity and domain knowledge terms separate out in the forward update as follows

$$X_k^* = \underset{X_k \in X_{\neg \boldsymbol{\theta}^t}}{\arg\max} \left(I(X_k; Y | X_{\boldsymbol{\theta}}) + \frac{1}{N} \log \frac{p_s(\boldsymbol{\theta}^{t+1})}{p_s(\boldsymbol{\theta}^t)} + \frac{1}{N} \log \frac{p_d(\boldsymbol{\theta}^{t+1})}{p_d(\boldsymbol{\theta}^t)} \right). \tag{6.15}$$

Which then further simplify to

$$X_k^* = \underset{X_k \in X_{\neg \boldsymbol{\theta}^t}}{\arg\max} \left(I(X_k; Y | X_{\boldsymbol{\theta}}) - \frac{\alpha_s}{N} + \frac{\alpha_d w_k}{N} \right). \tag{6.16}$$

We now turn to the issue of integrating these priors into a feature selection algorithm. We choose to look at the IAMB algorithm [107], and show how it maximises the joint likelihood with a sparsity prior.

6.3 Incorporating a prior into IAMB

In Chapter 3 we looked at structure learning algorithms for Bayesian Networks. We saw how algorithms which recover the Markov Blanket solve a special case of the feature selection problem, and how the IAMB family of Markov Blanket discovery algorithms use a conditional independence test based on the mutual information. In this section we explore the links between IAMB and our discriminative model framework, showing how IAMB optimises the joint likelihood under a specific sparsity prior.

We repeat the IAMB algorithm [107] in Algorithm 3. The algorithm is parameterised by the choice of a conditional independence test, $f(X; Y|\text{CMB})$, which measures the association of a candidate feature X to the target Y in the context

of the currently estimated Markov Blanket. Tsamardinos & Aliferis recommend that instead of a test against zero, that a threshold value is used — when the measured association is above this threshold, the variables are considered dependent. IAMB has two phases, a greedy forward search of the feature space until all remaining features are independent of the class given the currently selected set, and a backward search to remove false positives. Equating the notation in Algorithm 3 with our own, we have $\Omega = X$, $CMB = X_{\boldsymbol{\theta}}$, and the independence test $f(X; Y|CMB) = I(X_k; Y|X_{\boldsymbol{\theta}})$.

Algorithm 3 IAMB [107].

Phase 1 (forward)
CMB $= \emptyset$
while CMB has changed **do**
  Find $X \in \Omega \setminus$ CMB to maximise $f(X; Y|\text{CMB})$
  if $f(X; Y|\text{CMB}) > \epsilon$ **then**
    Add X to CMB
  end if
end while
Phase 2 (backward)
while CMB has changed **do**
  Find $X \in$ CMB to minimise $f(X; Y|\text{CMB} \setminus X)$
  if $f(X; Y|\text{CMB} \setminus X) < \epsilon$ **then**
    Remove X from CMB
  end if
end while

Given our probabilistic perspective we can interpret the threshold ϵ in the IAMB algorithm as a sparsity prior, p_s, by rearranging the independence test in Algorithm 3,

$$\begin{aligned} I(X_k; Y|X_{\boldsymbol{\theta}}) &> \epsilon \\ I(X_k; Y|X_{\boldsymbol{\theta}}) - \epsilon &> 0 \\ I(X_k; Y|X_{\boldsymbol{\theta}}) + \frac{1}{N} \log \frac{p_s(\boldsymbol{\theta}^{t+1})}{p_s(\boldsymbol{\theta}^t)} &\implies -\epsilon = \frac{1}{N} \log \frac{p_s(\boldsymbol{\theta}^{t+1})}{p_s(\boldsymbol{\theta}^t)}. \\ -\epsilon &= -\frac{\alpha_s}{N} \\ \alpha_s &= \epsilon N \end{aligned} \tag{6.17}$$

We can then see that the threshold ϵ is a special case of the sparsity prior in Eq (6.13) with $\alpha_s = \epsilon N$, where the strength of the prior is dependent on the number

of samples N, and a parameter ϵ.

Theorem 3. *Tsamardinos and Aliferis [107] proved that IAMB returns the true Markov Blanket under the condition of a perfect independence test $f(X;Y|CMB)$. Given this condition is satisfied, then IAMB is an iterative maximization of the discriminative model in Equation (6.1), under a specific sparsity prior.*

Proof. A perfect independence test comes as a result of sufficient data to estimate all necessary distributions. In this situation, the first KL term in Equation (6.2) will be zero. In the previous chapter we derived iterative update steps for our model, in Equations (4.14) and (4.20) — if we use a sparsity prior of the form in Equation (6.13), these coincide exactly with the steps employed by IAMB, therefore it is an iterative maximization of the discriminative model specified in Equation (6.1). □

We can now extend IAMB by introducing informative priors into the Markov Blanket discovery process. First we define $p(\boldsymbol{\theta}) \propto p_s(\boldsymbol{\theta})p_d(\boldsymbol{\theta})$ where $p_s(\boldsymbol{\theta})$ is the sparsity prior (or threshold), and $p_d(\boldsymbol{\theta})$ is our knowledge prior specified in Equation (6.14). We can ignore the normalisation constant as we only consider the ratio of the prior terms. We then use

$$I(X_k;Y|X_{\boldsymbol{\theta}}) + \frac{1}{N}\log\frac{p_s(\boldsymbol{\theta}^{t+1})}{p_s(\boldsymbol{\theta}^t)} + \frac{1}{N}\log\frac{p_d(\boldsymbol{\theta}^{t+1})}{p_d(\boldsymbol{\theta}^t)} > 0 \tag{6.18}$$

as the independence test having expanded out the prior $p(\boldsymbol{\theta})$. Incorporating $p_d(\boldsymbol{\theta})$ into IAMB lowers the "threshold" for features we believe are in the Markov Blanket and increases it for those we believe are not. We call this modified version *IAMB-IP* (IAMB-Informative Prior).

In some cases the knowledge prior, p_d, may be larger than the sparsity prior, p_s, causing the algorithm to unconditionally include feature X_k without reference to the data. We wish to blend the domain knowledge into the statistical evidence from the data, and so a prior which is strong enough to include features without reference to the data is undesirable. We therefore recommend a bound on the strength of the domain knowledge prior, by fixing $\alpha_d \leq \alpha_s$. This bounds the domain knowledge prior from above and below to ensure it is not strong enough to blindly include a feature without *some* evidence from the data.

Table 6.1: Dataset properties. $\#\ |MB| \geq 2$ is the number of features (nodes) in the network with an MB of at least size 2. Mean $|MB|$ is the mean size of these blankets. Median arity indicates the number of possible values for a feature. A large MB and high feature arity indicates a more challenging problem with limited data; i.e. Alarm is (relatively) the simplest dataset, while Barley is the most challenging with both a large mean MB size and the highest feature arity.

Name	**Features**	$\#\|MB\| \geq 2$	**Mean** $\|MB\|$	**Median Arity**
Alarm	37	31	4	2
Barley	48	48	5.25	8
Hailfinder	56	43	4.30	4
Insurance	27	25	5.52	3

6.4 Empirical Evaluation

We compare our novel IAMB-IP against the original IAMB algorithm using a selection of problems on MB discovery in artificial Bayesian Networks; these provide a ground truth feature set to compare the selected feature sets against. The networks used are standard benchmarks for MB discovery: Alarm [7], Barley [64], Hailfinder [1] and Insurance [9], downloaded from the Bayesian Network Repository [37]. We sample 20,000 data points from each network for use in all the experiments. More details are given in Table 6.1.

As our datasets are Bayesian Networks from fields with which we have no experience, we simulate the process of prior elicitation by selecting certain features at random. Features can be either *upweighted*, *i.e.* we believe them to be in the MB, or *downweighted*, *i.e.* we believe they are not in the MB. Upweighting feature X_i corresponds to $w_i = 1$, while downweighting sets $w_i = -1$. With this process, we emulate two types of *correct* prior knowledge: A *true positive* (TP) — a feature $X_j \in$ MB that we *upweight*. A *true negative* (TN) — a feature $X_j \notin$ MB that we *downweight*. Real prior knowledge is unlikely to be completely correct, hence we must also test the resilience of IAMB-IP when presented with false information. A *false positive* (FP) — a feature $X_j \notin$ MB that we *upweight*. A *false negative* (FN) — a feature $X_j \in$ MB that we *downweight*. Note that these definitions are slightly different to those given for TP etc in the general classification problem in Chapter 2. We will use the term *correct priors* to denote priors which only contain True Positives and True Negatives (*e.g.* 2 TP, TPTN). We will use the term *misspecified priors* to denote priors which contain a mixture of true and false information (*e.g.* TPFN, TPFP). We expect that these misspecified priors

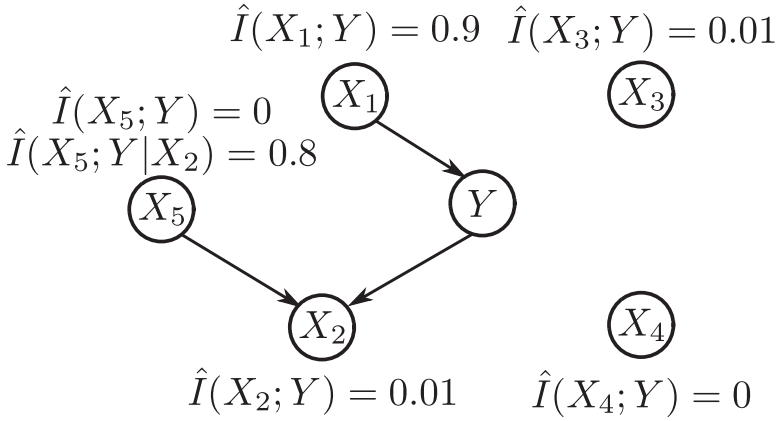


Figure 6.1: Toy problem, 5 feature nodes ($X_1 \ldots X_5$) and their estimated mutual information with the target node Y on a particular data sample. X_1, X_2, X_5 form the Markov Blanket of Y.

more accurately reflect the state of domain knowledge. In all experiments we only consider nodes with a Markov Blanket containing two or more features and we assess performance using the F-Measure (harmonic mean of precision & recall), comparing against the ground truth.

In Figure 6.1 we show a toy problem to illustrate the different effects prior knowledge can have on the Markov Blanket discovery process. Features X_1, X_2, X_5 are in the Markov Blanket of Y and features X_3 and X_4 are not. IAMB (with the default threshold) would select only X_1 as the MB, based upon the estimated mutual informations given. The performance of IAMB-IP will depend upon what knowledge is put into the prior. If we upweight X_1 it is a true positive, as it actually lies in the MB, similarly if we downweight X_3 it is a true negative. If we upweight X_4 it is a false positive, as it does not lie in the MB of Y, and similarly downweighting X_2 is a false negative as it does lie in the MB of Y. If we upweighted only X_1 IAMB-IP would perform similarly to IAMB, as X_1 has a strong measured association with Y, however upweighting X_2 would include that variable and then X_5, as X_2 only has a weak measured association with Y and so the prior will increase it. If X_4 is upweighted, (introducing a false positive into the prior) then it is unlikely to be included, as it has no measured association with Y, however X_3 would be included if it was upweighted. If we downweight X_2, (introducing a false negative) we can see this would remove both X_2 and X_5, as X_5 only becomes relevant when X_2 is included. We can see that false negatives in the prior are more problematic for IAMB-IP, as they can cause multiple variables to be incorrectly removed from the candidate MB.

Algorithm 4 Experimental Protocol

```
for each valid feature do
  for dataRepeats times do
    data ← selectFold()
    MB-I = IAMB(data,feature)
    Calculate MB-I F-measure
    for 40 repeats do
      Generate random prior
      MB-IP = IAMB-IP(data,feature,prior)
      Calculate MB-IP F-measure
    end for
    Calculate mean and std. err. for IAMB-IP
    Determine win/draw/loss
  end for
end for
Average wins/draws/losses over the features
```

We use the protocol in Algorithm 4 to test the relative performance for two groups of sample sizes: 10 to 100 samples in steps of 10 (small sample), and 200 to 1000 samples in steps of 100 (large sample). For the large sample we perform 10 trials over independent data samples, and for the smaller sizes we expect a greater variance and thus use 30 trials. The wins/draws/losses were assessed using a 95% confidence interval over the IAMB-IP results, compared to the IAMB result. The variance in IAMB-IP is due to the random selection of features which are included in the prior, which was repeated 40 times. We set $\alpha_d = \log 99$, except when this was above the bound $\alpha_d \leq \alpha_s$ where we set $\alpha_d = \alpha_s$. This is equivalent to setting individual priors $p(\theta_i = 1) = 0.99$ for upweighted features and $p(\theta_i = 1) = 0.01$ for downweighted features. We set α_s so $t = 0.02$ for both IAMB and IAMB-IP. We average these wins/draws/losses over *all valid features in a dataset*, where a valid feature is one with a Markov Blanket containing two or more features.

We first investigate the performance of IAMB-IP when using a correct prior. We tested priors that included 2 true positives, and 1 true positive and 1 true negative. The average results over the 4 datasets are in the first two columns of Figure 6.2. We can see that when incorporating correct priors IAMB-IP performs better than IAMB or equivalently to it in the vast majority of cases. The draws between IAMB and IAMB-IP are due to the overlap between the statistical information in the data and the information in the prior. When the prior upweights a feature with a strong signal from the data, then the behavior of IAMB-IP is the

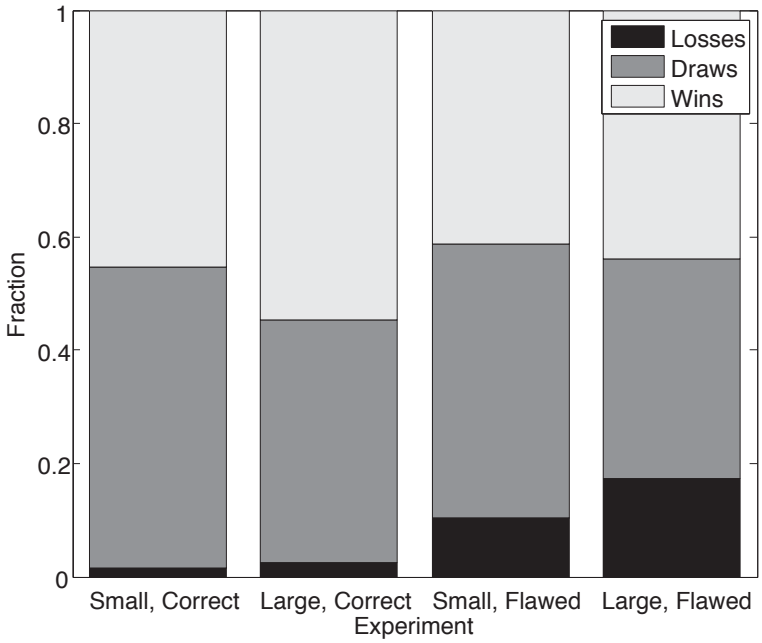


Figure 6.2: Average results: (a) Small sample, correct prior; (b) Large sample, correct prior; (c) Small sample, misspecified prior; (d) Large sample, misspecified prior.

same as IAMB. It is when the prior upweights a feature with a weak signal that the behavior of the two algorithms diverges, and similarly for features that are downweighted.

We now investigate the more interesting case of misspecified priors, where the prior contains some incorrect information. We tested priors using 1 true positive & 1 false negative, and 1 true positive & 1 false positive. These are presented in the last two columns of Figure 6.2. We can see that IAMB-IP performs equivalently or better than IAMB in four-fifths of the repeats, on average. We present results for Alarm in Table 6.2, for Barley in Table 6.3, for Hailfinder in Table 6.4 and for Insurance in Table 6.5. We can see that the algorithm is more sensitive to false negatives than false positives especially when there are small amounts of data, as the prior knowledge is more important in those situations, hence any flaws impact performance more. This is because false negatives may remove children from the MB, which in turn means no spouse nodes (the other parents of the common child node) will be included, which magnifies the effect of the false information.

In summary we can see that the addition of informative priors into IAMB to give IAMB-IP improves performance in many cases, even when half the prior

Table 6.2: Win/Draw/Loss results for ALARM network.

Size	**2 TP**	**TPTN**	**TPFN**	**TPFP**
10	12/18/0	12/17/0	12/16/2	12/17/1
20	12/18/0	12/18/0	11/17/2	12/18/1
30	13/17/0	11/19/0	11/16/2	11/18/1
40	12/17/0	12/17/0	10/17/3	11/17/2
50	13/17/1	12/17/1	11/15/4	12/16/2
60	13/17/1	12/17/1	10/15/5	11/16/3
70	13/17/0	12/17/1	11/14/5	12/15/4
80	12/17/1	13/16/1	10/14/6	12/14/4
90	13/16/1	14/15/1	10/13/7	12/13/6
100	16/13/1	16/13/1	13/12/6	14/11/4
Mean	**13/17/1**	**13/17/1**	**11/15/4**	**12/15/3**
200	5/4/0	5/4/0	4/4/2	4/3/3
300	6/3/0	6/3/0	4/3/3	4/3/4
400	6/4/0	6/4/0	4/4/3	4/3/4
500	5/4/0	6/4/0	4/4/3	4/3/3
600	4/6/0	4/5/0	3/5/2	3/4/3
700	4/6/0	5/5/0	3/5/2	3/4/3
800	4/6/0	4/6/0	3/5/2	3/4/3
900	3/7/0	3/7/0	2/6/2	2/5/2
1000	3/7/0	3/6/0	2/6/2	3/6/2
Mean	**5/5/0**	**5/5/0**	**3/4/2**	**3/4/3**

knowledge given is incorrect. This improvement can be seen in extremely small sample environments with as few as 10 datapoints and 56 features, and still provides a performance benefit with 1000 datapoints.

We have focused on adding true positives to the prior, and how they interact with the false information. In our datasets true positives are rarer than true negatives and thus more important, because the Markov Blankets are much smaller than the number of features. Therefore when we construct the prior at random, we are more likely to select true positives where the prior information is useful (*i.e.* there is not enough statistical information in the data to include the true positive) as there are fewer true positives to select from. When including true negatives the prior only improves performance if the true negative appears to be statistically dependent on the target (and then it is penalised by the prior and not included), if it does not appear dependent, then the prior information has no effect on its inclusion. Therefore when only including true negatives IAMB-IP performs similarly to IAMB.

Table 6.3: Win/Draw/Loss results for Barley network.

Size	**2 TP**	**TPTN**	**TPFN**	**TPFP**
10	10/20/0	10/20/0	11/19/1	10/19/1
20	21/9/0	21/9/0	21/8/0	21/7/2
30	20/10/0	20/10/0	20/8/2	20/8/3
40	15/15/0	14/16/0	15/14/2	14/15/1
50	10/20/0	9/21/0	9/19/2	9/20/1
60	12/18/0	12/18/0	11/17/2	11/18/1
70	17/13/0	16/14/0	16/13/1	16/13/1
80	20/10/0	20/10/0	20/9/1	20/8/2
90	21/9/0	21/8/0	21/8/1	21/7/2
100	22/8/0	22/8/0	21/7/1	22/6/2
Mean	**17/13/0**	**17/13/0**	**17/12/1**	**16/12/1**
200	7/3/0	6/3/0	6/3/1	7/2/1
300	9/1/0	8/2/0	8/1/0	8/2/1
400	8/2/0	8/2/0	8/2/0	8/1/1
500	8/2/0	7/3/0	7/2/1	7/2/1
600	7/3/0	7/3/0	6/3/1	6/3/1
700	6/4/0	5/5/0	5/4/1	5/4/1
800	5/5/0	5/5/0	5/5/1	4/5/1
900	5/5/0	4/6/0	4/5/1	4/5/1
1000	4/6/0	4/6/0	4/5/1	4/5/1
Mean	**7/3/0**	**6/4/0**	**6/3/1**	**6/3/1**

Table 6.4: Win/Draw/Loss results on Hailfinder

Size	**2 TP**	**TPTN**	**TPFN**	**TPFP**
10	16/14/0	15/15/0	15/12/3	15/14/1
20	13/17/0	13/17/0	12/15/3	12/17/1
30	12/18/0	12/18/0	11/15/4	11/18/1
40	10/19/0	11/19/0	10/16/3	10/19/1
50	14/16/0	14/16/0	12/14/4	12/16/1
60	12/18/0	12/18/0	11/14/5	11/17/1
70	10/20/0	10/20/0	9/16/5	9/20/1
80	11/19/0	10/20/0	10/16/4	10/19/1
90	12/17/0	12/18/0	11/15/4	12/17/1
100	15/15/0	15/14/1	13/12/5	14/14/1
Mean	**12/17/0**	**12/18/0**	**11/14/4**	**12/17/1**
200	6/4/0	6/4/0	5/4/2	5/4/1
300	6/4/0	6/4/0	5/4/2	6/4/1
400	6/4/0	6/4/0	5/4/2	5/4/1
500	6/4/0	5/4/0	4/4/2	5/4/1
600	6/4/0	5/5/0	4/4/2	4/4/1
700	5/5/0	5/5/0	4/4/2	4/5/1
800	4/6/0	4/6/0	4/4/2	4/5/1
900	4/6/0	3/6/0	3/5/2	4/6/0
1000	4/6/0	3/6/0	3/6/2	3/6/0
Mean	**5/5/0**	**5/5/0**	**4/4/2**	**4/5/1**

Table 6.5: Win/Draw/Loss results for Insurance.

Size	2 TP	TPTN	TPFN	TPFP
10	9/20/0	9/21/0	8/18/4	7/19/3
20	10/19/0	11/19/1	9/16/5	9/17/3
30	12/18/0	11/18/1	9/17/5	11/16/4
40	12/17/1	10/19/1	10/14/5	10/16/4
50	12/16/1	12/17/1	11/14/6	11/15/4
60	12/17/1	12/17/1	9/14/7	11/15/4
70	13/15/1	13/16/1	10/13/7	11/15/5
80	14/15/2	13/15/2	10/14/7	11/14/5
90	13/15/2	14/15/2	9/12/8	10/15/5
100	18/9/3	18/10/3	14/10/6	15/10/5
Mean	**13/16/1**	**12/17/1**	**10/14/6**	**11/15/4**
200	7/2/1	7/3/1	5/3/2	5/3/2
300	8/2/0	7/3/1	5/3/2	5/2/2
400	8/2/0	7/3/1	5/3/3	4/3/3
500	7/3/1	6/3/1	4/3/3	4/3/3
600	6/3/1	5/4/0	4/4/2	5/3/2
700	6/4/0	5/4/1	3/4/3	3/4/3
800	5/4/1	5/4/1	4/4/3	4/4/2
900	5/5/1	4/5/1	3/5/3	4/5/2
1000	4/5/1	4/5/1	3/5/2	3/5/2
Mean	**6/3/1**	**6/4/1**	**4/4/2**	**4/4/2**

6.5 Chapter Summary

In this chapter we explored one of the benefits of our likelihood based approach to feature selection, namely the inclusion of informative priors. We constructed simple factored priors which we used in two different ways, either to promote sparsity or to include domain knowledge. We incorporated these priors into the Markov Blanket discovery algorithm IAMB, blending the prior knowledge into the statistical information from the data.

We saw that analysing IAMB from the perspective of joint likelihood maximisation showed it to use a sparsity prior to control the number of features selected. Our extension of IAMB to include informative priors, called IAMB-IP, essentially adjusts the threshold in the IAMB algorithm based upon the supplied prior knowledge.

We tested IAMB-IP against IAMB, showing the new algorithm to be resistant to poor prior knowledge, as it improved performance against IAMB even when the prior contained 50% false information.

Chapter 7

Cost-sensitive feature selection

In the previous three chapters we looked at how feature selection using information theory maximises the joint likelihood of a discriminative model. This allows us to combine information theoretic measurements from the data, with prior knowledge from domain experts and therefore select features which best combines these two sources of information. In this chapter we apply the machinery from Chapter 4 to a different loss function, namely the weighted conditional likelihood [31]. In the binary classification problem this loss function is a bound on the empirical risk of the dataset, which measures how costly misclassification is for each example. We thus derive a *cost-sensitive* filter feature selection criteria, which coincides with Guiaşu's definition of weighted information theory [46]. We prove several novel results with respect to this variant of information theory, to allow its use as a feature selection criteria. We present experimental results showing that the cost-sensitive selection criteria can be combined with a *cost-insensitive* classifier to create an overall cost-sensitive system.

7.1 Deriving a Cost Sensitive Filter Method

In Chapter 2 we briefly looked at the weighted likelihood from Dmochowski *et al.* [31], detailing its properties. We now briefly revise those properties before moving on to novel material.

Dmochowski *et al.* [31] investigate using a weighted likelihood function to integrate misclassification costs into the (binary) classification process. Each example is assigned a weight based upon the tuple $\{\mathbf{x}, y\}$, and the likelihood of that example is raised to the power of the assigned weight. They prove that

the negative weighted log likelihood forms a tight, convex upper bound on the empirical loss, which is the expected conditional risk across a dataset. This property is used to argue that maximising the weighted likelihood is the preferred approach in the case where the classifier cannot perfectly fit the true model.

Unfortunately the weighted likelihood has only been shown to bound the risk in binary cost-sensitive problems. In multi-class cost-sensitive problems the likelihood does not accurately represent the misclassification probabilities of the other classes, as the sum of these values is equal to $1 - p(y^i|\mathbf{x}^i)$ and they may be unevenly weighted by the per example weight vector. Any weighted feature selection process is likely to work best in the multi-class case as then it is more probable that each label will have a different set of predictive features. Therefore we avoid this problem by adjusting the weight of each datapoint in the likelihood. We propose that if we use the sum of the per example weight vector,

$$w_s(y^i, \mathbf{x}^i) = \sum_{y \in Y, y \neq y^i} w(y^i, \mathbf{x}^i, y) \tag{7.1}$$

we will ensure the weighted likelihood still forms an upper bound on the empirical risk. This takes a pessimistic view of the classification problem, as a mis-prediction which has a high weight may have a very low probability, but the weighted likelihood will still be small. We note that this forms a looser upper bound on the empirical risk than in the binary case, but reduces to the same likelihood in binary problems. Cost-sensitive feature selection is an interesting case of the general cost-sensitive problem as when using a filter technique it is difficult to generate predicted labels with which to calculate the misclassification error. This generalisation of the weighted likelihood provides an objective function which allows the construction of cost-sensitive feature selection.

7.1.1 Notation

We use similar notation to Chapter 4 summarised here for clarity, with extensions to include misclassification costs. We assume an underlying i.i.d. process $p : X \to Y$, from which we have a sample of N observations. Each observation is a tuple $(\mathbf{x}, y, \mathbf{w})$, consisting of a d-dimensional feature vector $\mathbf{x} = [x_1, ..., x_d]^T$, a target class y, and an associated non-negative $|Y| - 1$ dimensional weight vector, $\mathbf{w}$, for that observation, with $\mathbf{x}$ and y drawn from the underlying random variables $X = \{X_1, ..., X_d\}$ and Y. Furthermore, we assume that $p(y|\mathbf{x})$ is defined

by a *subset* of the d features in $\mathbf{x}$, while the remaining features are irrelevant or redundant. We consider the weight for a particular example to be a function *only of the label* y. This important restriction is necessary (see Section 7.2) to ensure the weighted mutual information has a unique non-negative value. This is a slightly less general formulation for the weights than the standard definition given by Elkan [38], but is still flexible enough to include cost-matrices which do not depend upon $\mathbf{x}$.

We adopt a d-dimensional binary vector $\boldsymbol{\theta}$: a 1 indicating the feature is selected, a 0 indicating it is discarded. Notation $\mathbf{x}_{\boldsymbol{\theta}}$ indicates the vector of selected features, i.e. the full vector $\mathbf{x}$ projected onto the dimensions specified by θ. Notation $\mathbf{x}_{\neg\boldsymbol{\theta}}$ is the complement, i.e. the unselected features. The full feature vector can therefore be expressed as $\mathbf{x} = \{\mathbf{x}_{\boldsymbol{\theta}}, \mathbf{x}_{\neg\boldsymbol{\theta}}\}$. As mentioned, we assume the process p is defined by a subset of the features, so for some unknown optimal vector θ^*, we have that $p(y|\mathbf{x}) = p(y|\mathbf{x}_{\theta^*})$. In this chapter we consider the conditional likelihood of the labels given the data, rather than the full joint likelihood analysed in Chapter 4. This is due to the bound in Dmochowski *et al.* only being proved for the *weighted conditional likelihood*. The construction of a weighted discriminative model likelihood is left to future work. Therefore our model does not consider the generation of the datapoints, thus we only have two layers of parameters in our hypothetical model q, namely: θ representing which features are selected, and τ representing parameters used to predict y.

7.1.2 Deriving cost-sensitive criteria

In this section we take the weighted likelihood from Dmochowski *et al.* [31] and decompose it into a sum of terms, where each term relates to a different part of the classification process. This follows a similar process to the derivation in Chapter 4. If we further make the filter assumption (Definition 8) we derive a weighted feature selection criterion, which uses the weighted mutual information (see Section 7.2) to score features. As mentioned previously when working in the multi-class case, we use the sum of the per-example weight vector, $\mathbf{w}^i$ as the weight $w(y^i)$ in the likelihood.

We approximate the true distribution p with our model q, with separate parameters for the feature selection, $\boldsymbol{\theta}$, and for classification, τ. We define the

conditional likelihood as follows,

$$\mathcal{L}_w(\mathcal{D}, \boldsymbol{\theta}, \tau) = \prod_{i=1}^{N} q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)^{w(y^i)}. \tag{7.2}$$

We choose to work with the scaled negative log-likelihood, $-\ell_w$, converting our maximisation problem into a minimisation problem. This gives

$$-\ell_w = -\frac{1}{N}\sum_{i=1}^{N} w(y^i) \log q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau) \tag{7.3}$$

which is the function we will minimise with respect to $\{\boldsymbol{\theta}, \tau\}$ (this is the initial position of Dmochowski *et al.* as they only consider the log-likelihood). We first introduce the ratio $\frac{p(y|\mathbf{x})}{p(y|\mathbf{x})}$ into the logarithm, this is the probability of the correct class given all the features. We can then expand the logarithm into two terms,

$$-\ell = -\frac{1}{N}\Bigg(\sum_{i=1}^{N} w(y^i) \log \frac{q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)}{p(y^i|\mathbf{x}^i)} + \sum_{i=1}^{N} w(y^i) \log p(y^i|\mathbf{x}^i) \Bigg). \tag{7.4}$$

The first term is the weighted log-likelihood ratio between the true model and our predictive model, and the second term is the weighted log-likelihood of the true model. This latter term is a finite sample approximation to the *weighted* conditional entropy [46]. This represents both the amount of uncertainty in the data, and how costly that uncertainty is. It forms a bound on the maximum amount of performance we can extract from our dataset, in terms of the conditional risk.

We now wish to separate out feature selection from the classification process. We do this by introducing another ratio into the first logarithm, namely $\frac{p(y|\mathbf{x},\boldsymbol{\theta})}{p(y|\mathbf{x},\boldsymbol{\theta})}$. This is the probability of the correct class given the features selected by $\boldsymbol{\theta}$. We can then further expand the first logarithm as follows,

$$\begin{aligned} -\ell_w = -\frac{1}{N}\Bigg(&\sum_{i=1}^{N} w(y^i) \log \frac{q(y^i|\mathbf{x}^i, \boldsymbol{\theta}, \tau)}{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})} + \sum_{i=1}^{N} w(y^i) \log \frac{p(y^i|\mathbf{x}^i, \boldsymbol{\theta})}{p(y^i|\mathbf{x}^i)} \\ &+ \sum_{i=1}^{N} w(y^i) \log p(y^i|\mathbf{x}^i) \Bigg). \end{aligned} \tag{7.5}$$

Similarly to the previous expansion from Chapter 4, we have expanded the *weighted conditional likelihood* into a sum of *three* terms. In this case each term is

weighted by a per example cost. As our weights are functions of the class label y, the per-example weight $w(y^i)$ and the per-state weight $w(y)$ are identical. We can then treat each of the summations above as approximations to the expectation over each term, replacing the per-example weights with per-state weights. It is this step which removes some of the power of our weighted likelihood as compared to the weighted likelihood used in Dmochowski *et al.* , though we shall see it is necessary to ensure the information theoretic values remain non-negative.

Again by similar logic to Chapter 4, we can interpret the second term in Equation (7.5) as a finite sample approximation to the *weighted conditional mutual information* $I_w(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}})$,

$$\begin{aligned} I_w(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}) &= \sum_{\mathbf{x},y\in X,Y} w(y)p(\mathbf{x},y)\log\frac{p(\mathbf{x}_{\neg\boldsymbol{\theta}},y|\mathbf{x}_{\boldsymbol{\theta}})}{p(\mathbf{x}_{\neg\boldsymbol{\theta}}|\mathbf{x}_{\boldsymbol{\theta}})p(y|\mathbf{x}_{\boldsymbol{\theta}})} \\ &\approx -\frac{1}{N}\sum_{i=1}^{N} w(y^i)\log\frac{p(y^i|\mathbf{x}^i,\boldsymbol{\theta})}{p(y^i|\mathbf{x}^i)}. \end{aligned} \tag{7.6}$$

and the third term as a finite sample approximation to the weighted conditional entropy $H_w(Y|X)$,

$$H_w(Y|X) = -\sum_{\mathbf{x},y\in X,Y} w(y)p(\mathbf{x},y)\log p(y|\mathbf{x}) \approx -\frac{1}{N}\sum_{i=1}^{N} w(y^i)\log p(y^i|\mathbf{x}^i).$$

We can now write $-\ell_w$ as the sum of weighted information theoretic quantities,

$$-\ell_w \approx \mathbb{E}_{\mathbf{x},y}\left\{ w(y)\log\frac{p(y^i|\mathbf{x}^i,\boldsymbol{\theta})}{q(y^i|\mathbf{x}^i,\boldsymbol{\theta},\tau)}\right\} + I_w(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}) + H_w(Y|X). \tag{7.7}$$

We note that the optimal feature set $\boldsymbol{\theta}^*$ is the set which makes $I_w(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}}) = 0$. This can only occur when $p(\mathbf{x}_{\neg\boldsymbol{\theta}},y|\mathbf{x}_{\boldsymbol{\theta}}) = p(\mathbf{x}_{\neg\boldsymbol{\theta}}|\mathbf{x}_{\boldsymbol{\theta}})p(y|\mathbf{x}_{\boldsymbol{\theta}})$, as the addition of weights does not change position of the minima of the mutual information.

If we have discovered the optimal feature set or a superset thereof (i.e. $X^* \subseteq X_{\boldsymbol{\theta}}$) then $p(y|\mathbf{x},\boldsymbol{\theta}) = p(y|\mathbf{x})$. The expectation in the first term can also then be seen as a finite sample approximation to a weighted KL-Divergence (also known as the weighted relative entropy [102]). This divergence represents how well the predictive model fits the true distribution, given a superset of the optimal feature set and how important each prediction is.

We have now decomposed the weighted conditional likelihood ℓ_w into three

terms, which relate to the cost-weighted classification performance of an arbitrary probabilistic predictor, the quality of the chosen feature set, and the quality of the data respectively. An important point to note about this formulation of weighted feature selection is that the addition of weights does not change the optimal feature set, in the sense that the feature set $\boldsymbol{\theta}^*$ which makes $p(y|\mathbf{x}, \boldsymbol{\theta}^*) = p(y|\mathbf{x})$ is identical for all possible weightings. This is because the Markov Blanket for the class label does not change when using a different evaluation metric. Thus the use of the weighted mutual information as a selection criteria gives the *same* optimal set as the standard mutual information. However, in the case where we iteratively construct a feature set, the relative selection order *can be different* between the weighted and unweighted information. Also if we select features using an approximate criterion like those examined in Chapter 5 which cannot recover the Markov Blanket, we can expect that the weighted variant will return a different feature set. This is because while the minima of $I_w(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}})$ are identical to the minima of $I(X_{\neg\boldsymbol{\theta}}; Y|X_{\boldsymbol{\theta}})$, the same is not necessarily true for (for example) the JMI criterion. We will explore this effect in the experiments, and show how different the top 50 features are when chosen using a weighted mutual information versus the standard mutual information.

In the following section, we derive iterative update rules for the feature set, that guarantee an increase in weighted mutual information.

7.1.3 Iterative minimisation

We now derive iterative update rules which greedily maximise our formulation of the weighted likelihood. These derivations are similar to the derivations given in Chapter 4 but use the weighted mutual information. The literature surrounding the weighted mutual information has no proof for non-negativity or an equivalent definition for the chain rule of mutual information, which are necessary for the derivation of iterative update rules. We provide such proofs in the next section, and in this section assume the existence of such proofs.

By using the chain rule, we can separate out the most informative feature from $X_{\neg\boldsymbol{\theta}}$ and add it to $X_{\boldsymbol{\theta}}$. We add a superscript t to $\boldsymbol{\theta}$ to denote which time step the feature sets are from, and proceed to derive the forward update that maximises the weighted likelihood. The proof takes a similar form to the proof of Theorem 1 from Chapter 4.

Theorem 4. *The forward update which maximises the weighted likelihood is to select the feature* $X_j \in X_{\neg\boldsymbol{\theta}}$*,*

$$X_j = \arg\max_{X_j \in X_{\neg\boldsymbol{\theta}}} I_w(X_j; Y | X_{\boldsymbol{\theta}}). \tag{7.8}$$

Proof. The feature which maximises the weighted likelihood is the feature which minimises $I_w(X_{\neg\boldsymbol{\theta}^{t+1}}; Y | X_{\boldsymbol{\theta}^{t+1}})$ from $I_w(X_{\neg\boldsymbol{\theta}^t}; Y | X_{\boldsymbol{\theta}^t})$, where $X_{\boldsymbol{\theta}^{t+1}} = X_{\boldsymbol{\theta}^t} \cup X_j$ and $X_{\neg\boldsymbol{\theta}^{t+1}} = X_{\neg\boldsymbol{\theta}^t} \setminus X_j$ for some $X_j \in X_{\neg\boldsymbol{\theta}^t}$. We can express this as,

$$I_w(X_{\neg\boldsymbol{\theta}^{t+1}}; Y | X_{\boldsymbol{\theta}^{t+1}}) = I_w(X_{\neg\boldsymbol{\theta}^t}; Y | X_{\boldsymbol{\theta}^t}) - I_w(X_j; Y | X_{\boldsymbol{\theta}^t}). \tag{7.9}$$

Then we see that the feature X_j which minimises $I_w(X_{\neg\boldsymbol{\theta}^{t+1}}; Y | X_{\boldsymbol{\theta}^{t+1}})$ is,

$$X_j = \arg\max_{X_j \in X_{\neg\boldsymbol{\theta}^t}} I_w(X_j; Y | X_{\boldsymbol{\theta}^t}). \tag{7.10}$$

□

A similar update can be found for the backwards step, analogous to Theorem 2 from Chapter 4. Both these updates are similar to the updates derived in Chapter 4 (which might be expected due to the machinery involved in generating them) though they use the *weighted mutual information* developed by Guiaşu, rather than Shannon's formulation. In Section 7.3 we proceed to create a weighted variant of the JMI filter criterion [110], by substituting the weighted mutual information for the Shannon mutual information, and supplying appropriate cost vectors. First we must prove the non-negativity property and the chain rule used in the above theorem.

7.2 Weighted Information Theory

The weighted mutual information has appeared several times in the literature [46, 75, 96] but there has been little investigation of the theoretical properties of such a measure. As mentioned previously this literature lacks two important properties necessary for feature selection using the kind of iterative updates used throughout this thesis. We now review those important properties of the weighted mutual information, namely, *non-negativity* and the *chain rule*.

Table 7.1: An example of a negative wI, $wI(X;Y) = -0.0214$.

w	$y=1$	$y=2$
$x=1$	1	1
$x=2$	1	2

$p(x,y)$	$y=1$	$y=2$
$x=1$	0.3	0.3
$x=2$	0.3	0.1

Value	$p(x)$	$p(y)$
1	0.6	0.6
2	0.4	0.4

7.2.1 Non-negativity of the weighted mutual information

Non-negativity is an important property to ensure that adding a feature does not *reduce* our measure of the information held in $X_{\boldsymbol{\theta}}$. The non-negativity of Shannon's mutual information is a well-known axiom of information theory, as it is based upon the KL-Divergence, which can be proved to be non-negative via Jensen's inequality [24]. Unfortunately the weighted mutual information is a form of weighted relative entropy [102], which was shown by Kvålseth [68] to take negative values in certain situations. We first present a concrete example with a negative weighted mutual information before providing a variant of the measure which is proved to be non-negative for all valid inputs.

The definition of the weighted mutual information given by Guiaşu [46] (defined as the Q-MI by Luan *et al.* [75] and wI by Schaffernicht and Gross [96]) is as follows,

$$wI(X;Y) = \sum_{x \in X} \sum_{y \in Y} w(x,y) p(x,y) \log \frac{p(x,y)}{p(x)p(y)}. \tag{7.11}$$

Note that this weight depends on the value of both x and y; in this case, the information can be *negative*. Table 7.1 presents an example distribution for X and Y which gives a negative weighted mutual information; in this case $wI(X;Y) = -0.0214$.

Therefore, knowledge of the variable X *reduces* what we know about Y[1]. We can avoid this problem with our measure if we define the weights so that they are dependent upon a single variable *i.e.* $\forall x, y \; w(x,y) = w(y)$. This still gives valid weights under the conditions of weighted information theory, *i.e.* $p(y)w(y) = \sum_{x \in X} w(x,y)p(x,y)$, which is the necessary condition for the definition of a unique mutual information [46]. We restricted the weights in our weighted likelihood such that they only depend upon y, therefore this limitation does not affect our earlier derivation. We therefore define our weighted mutual information as a function

[1] An alternative explanation is that knowledge of X may cause us to make more costly predictions for Y.

only of the class labels, as follows,

$$I_w(X;Y) = \sum_{x \in X} \sum_{y \in Y} w(y) p(x,y) \log \frac{p(x,y)}{p(x)p(y)}. \tag{7.12}$$

Theorem 5. *The weighted mutual information, I_w, is non-negative if the weights are a function of a single random variable. Therefore $\forall X, Y, w \; I_w(X;Y) \geq 0$.*

Proof. We begin by relating the weighted mutual information to the (unweighted) KL-Divergence.

$$\begin{aligned}
I_w(X;Y) &= \sum_{x \in X} \sum_{y \in Y} w(y) p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \\
&= \sum_{y \in Y} w(y) \sum_{x \in X} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \\
&= \sum_{y \in Y} w(y) p(y) \sum_{x \in X} p(x|y) \log \frac{p(x|y)p(y)}{p(x)p(y)} \\
&= \sum_{y \in Y} w(y) p(y) \sum_{x \in X} p(x|y) \log \frac{p(x|y)}{p(x)} \\
&= \sum_{y \in Y} w(y) p(y) D_{KL}\{p(x|y)||p(x)\}.
\end{aligned} \tag{7.13}$$

As all the weights $w(y)$ are non-negative, $p(y)$ is non-negative, and the KL-Divergence is non-negative, then our new weighted mutual information, I_w, is non-negative. □

7.2.2 The chain rule of weighted mutual information

One further essential property of an information measure defines how variables interact. In the standard formulation of Shannon's Information Theory this is the chain rule of mutual information, $I(AB;Y) = I(A;Y) + I(B;Y|A)$, and separates out the information shared between a joint random variable and a target random variable into two components, the individual mutual information of the first variable and the target, plus the second variable and the target conditioned upon the first. We provide an equivalent rule for the weighted mutual information.

Theorem 6. *The weighted mutual information, I_w, between a joint random variable and a single random variable can be decomposed as follows,*

$$I_w(AB;Y) = I_w(A;Y) + I_w(B;Y|A). \tag{7.14}$$

Proof. Due to Theorem 5 we only define the chain rule such that Y is never conditioned upon, and we define $\forall x, z, y \; w(x, z, y) = w(y)$. We thus define the chain rule as follows,

$$\begin{aligned}
I_w(XZ;Y) &= \sum_{x\in X}\sum_{y\in Y}\sum_{z\in Z} w(y)p(x,y,z)\log\frac{p(x,y,z)}{p(x,z)p(y)} \\
&= \sum_{x\in X}\sum_{y\in Y}\sum_{z\in Z} w(y)p(x,y,z)\log\frac{p(x,y)p(z|y,x)}{p(z|x)p(x)p(y)} \\
&= \sum_{x\in X}\sum_{y\in Y} w(y)p(x,y)\log\frac{p(x,y)}{p(x)p(y)} \\
&\quad + \sum_{x\in X}\sum_{y\in Y}\sum_{z\in Z} w(y)p(x,y,z)\log\frac{p(z|y,x)}{p(z|x)} \\
&= I_w(X;Y) \\
&\quad + \sum_{x\in X}\sum_{y\in Y}\sum_{z\in Z} w(y)p(x,y,z)\log\frac{p(z,y|x)}{p(z|x)p(y|x)} \\
&= I_w(X;Y) + I_w(Z;Y|X).
\end{aligned}$$

□

This property is independent of the restriction on the weights defined in Theorem 5, though the non-negativity property is crucial to ensure the iterative updates maximise the weighted likelihood. We can now see due to the chain rule and the definition of $X = \{X_{\boldsymbol{\theta}}, X_{\neg\boldsymbol{\theta}}\}$ that,

$$I_w(X;Y) = I_w(X_{\boldsymbol{\theta}};Y) + I_w(X_{\neg\boldsymbol{\theta}};Y|X_{\boldsymbol{\theta}}). \tag{7.15}$$

Therefore, since $I_w(X;Y)$ is a constant with respect to $\boldsymbol{\theta}$, minimizing $I_w(X_{\neg\boldsymbol{\theta}};Y|X_{\boldsymbol{\theta}})$ is equivalent to maximising $I_w(X_{\boldsymbol{\theta}};Y)$.

We now turn to the task of constructing filter criteria which approximate the difficult to estimate update rules given in Section 7.1.3.

7.3 Constructing filter criteria

We note from our work in the previous section that we can only construct weighted mutual informations which include the variable Y which our weights are defined over. This limits the possible feature selection criteria, but fortunately many of the common ones can be re-expressed in the right form. We focus on adapting the JMI criterion [110], as this is the best performing criterion from our earlier empirical study (see Chapter 5). We also use a weighted variant of MIM, which ranks features according to their univariate *weighted* mutual information. We expect that the other criteria we investigated in that chapter could be adapted to work in this weighted likelihood framework, and the weighted mutual information, provided they can be expressed using mutual informations between Y and X. Unfortunately this restriction excludes popular criteria such as mRMR, as they cannot be written in the necessary form.

We define the weighted variant of the MIM criterion (referred to as wMIM) as follows:

$$J_{wmim}(X_k, w) = I_w(X_k; Y). \tag{7.16}$$

Similarly, we define the weighted variant of the JMI criterion (referred to as wJMI) as follows:

$$J_{wjmi}(X_k, S, w) = \sum_{X_j \in S} I_w(X_k X_j; Y). \tag{7.17}$$

We then combine these criteria with a greedy forward search, to produce a feature selection algorithm. As mentioned previously the use of weights does not change the minima of the likelihood with respect to $\boldsymbol{\theta}$, however when using an approximate optimiser such as wJMI the feature sets returned are different. This is due to the pairwise independence assumption made in the JMI criterion [14], which stops the criterion from determining when it has reached the optima. We shall see this effect in the empirical study, as the feature sets selected by JMI and wJMI (and by MIM and wMIM) diverge.

One important point to note is that as we only consider the rankings of individual features the magnitude of the weight vector is irrelevant. If we normalise the weight vector $\mathbf{w}$ so it sums to 1, this will return exactly the same feature set (using wJMI or wMIM) as if we multiplied each weight by a positive value.

7.4 Empirical study of Weighted Feature Selection

We compare our cost-sensitive feature selection algorithm against three different competitors. The first is simply using a normal *cost-insensitive* feature selection algorithm (in our case JMI), combined with a standard classifier (a linear SVM). The second is the 'standard' cost-sensitive methodology, where a normal feature selection algorithm is used with a cost-sensitive classifier, in our case a weighted SVM [17], which aims to minimise the mis-classification cost of the training data. The third approach is a form of oversampling of the costly class. As our likelihood takes the form of examples raised to the power of a weight, it can be see as replicating an example $w(y)$ times. We mirror this process to produce a new dataset using a deterministic oversampling process which repeats an example $w(y)$ times, where $w(y)$ is the (integer) cost for that example's label. We also present results comparing against the multi-class feature selection algorithm (Spread-FX) from Forman [43], using the random scheduler, modified to sample from the weight distribution rather than the uniform distribution.

We use a selection of multi-class datasets to evaluate our new approach: the well-known MNIST digit classification dataset, and 5 text-mining datasets taken from Han and Karypis [52]. These datasets provide a large number of both features and samples, and the features from the MNIST dataset [71] can be easily visualised to show the differences between our technique and the cost-insensitive baseline. As before we calculate all mutual informations on discretised versions of the datasets, with 10 bins, using a histogram estimator of the necessary probabilities. Our scoring metrics are the precision, recall and F-measure of the costly class, along with the accuracy across all classes.

Our aim is to test the ability of cost-sensitive feature selection to produce a cost-sensitive system when combined with a standard (cost-insensitive) classifier, analogously to how resampling the training data produces a cost-sensitive system when combined with a standard (cost-insensitive) classifier.

7.4.1 Handwritten Digits

We selected 500 instances at random from each class label in the MNIST data, to give a 5000 example dataset, to reduce the training times of our classification models. All results reported are 10-fold cross validation runs, selecting the top 50

features according to the various feature selection algorithms. We used a linear Support Vector Machine (SVM) as the classification model, using the LibSVM [17] implementation with default parameter settings.

In Figures 7.2 and 7.3 we present results from this dataset where the costly class is the digit "4". The average 4 in our dataset is presented in Figure 7.1. Figure 7.2a shows the different algorithms tested with $w(y =$"4"$) = 5$, so the digit "4" is five times more important than the other labels, which were given a weight of one. Each group of bars represents a different approach to the cost-sensitive problem: the first group is the standard cost-insensitive approach, where the JMI algorithm is used to select 50 features, and then an SVM is trained on those features. The second group is our approach, where we include the weight in the feature selection process with wJMI and use a standard SVM to fit the data. The third group uses JMI with a weighted SVM, and finally the fourth group oversample the costly class according to the weight. We can see that the introduction of weights does not alter the overall classification performance (the leftmost bar in each group is approximately the same), but the precision, recall and F-measure change when the weighted approaches are used. Our method improves both precision and recall over the baseline, whereas using a weighted classifier trades off precision for recall (*i.e.* it predicts many more false positives). Figure 7.3a shows how the F-Measure on class 4 changes for the three weighted methods using weights $w(y = 4) = \{1, 5, 10, 15, 20, 25, 50, 100\}$. In contrast to wJMI the weighted classifier degrades performance as it predicts many false positives. Figure 7.3b shows a precision/recall plot of the various approaches, with the cost-insensitive approach appearing as a filled black circle. The size of the marker represents the weight, from the range given above. We can see how the weighted feature selection improves both precision and recall for all settings of the weights whereas oversampling only improves recall, and the weighted classifier improves recall at the cost of precision.

Finally in Figure 7.2b we show the different features selected by the standard JMI algorithm, and the wJMI algorithm with $w(y = 4) = 100$. The light gray features are those which were selected by JMI and not by wJMI, the dark gray features are those selected by both algorithms, and the black features are those selected by wJMI alone. This shows how the wJMI algorithm selects features which are predictive of the presence or absence of a 4. The large black block at the top of the image represents the area which differentiates a 4 from a 9 in

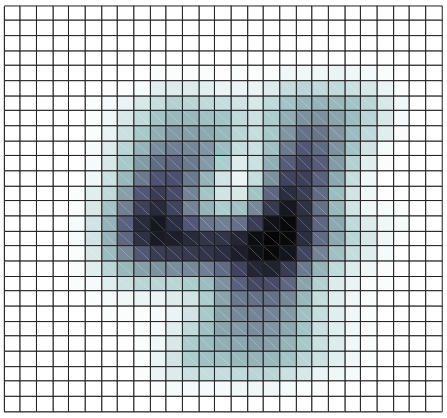
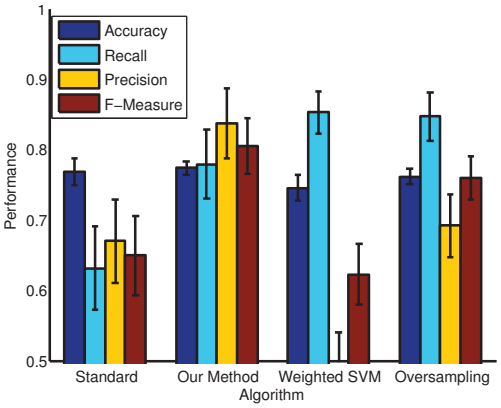
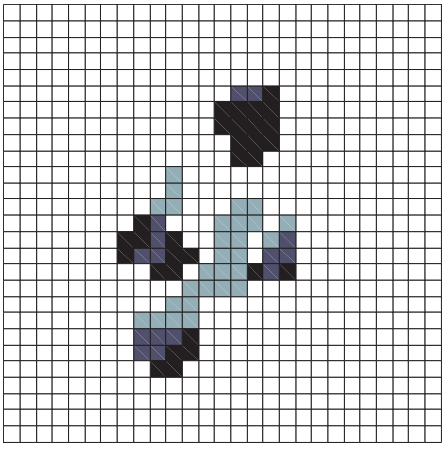


Figure 7.1: The average pixel values across all 4s in our sample of MNIST.



(a) Accuracy is across the whole dataset, with 95% Confidence across 10-fold CV, using (w)JMI.

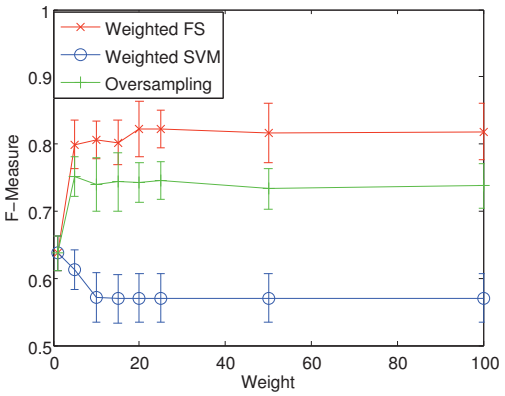


(b) Difference in selected features between JMI and wJMI, $w(y = 4) = 100$

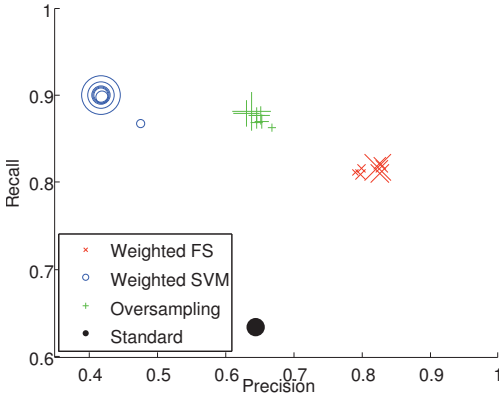
Figure 7.2: MNIST Results, with "4" as the costly digit.

the dataset, and the dark area in the bottom left differentiates a 4 from a 2, 5, 6, or 8 as those digits require pixels in that area. The other black features are to positively detect a 4. We can see that this weighted approach selects features which are predictive of the presence of a 4 and discriminate against false positives.

We present the average improvement in precision and recall across all digits in our MNIST dataset in Table 7.2, where each digit in turn was given a weight $w(y) = 10$. We can see that the weighted feature selection improves both precision and recall, resulting in an improved F-measure, whereas the other approaches have high recall, but low precision (*i.e.* predict many false positives), resulting in little improvement in the F-measure. We also present the improvement in precision and recall for the digit 4 in Table 7.3.



(a) F-Measure with 95% Confidence, across 10-fold CV.



(b) Precision/Recall plot, where the marker size indicates the weight w.

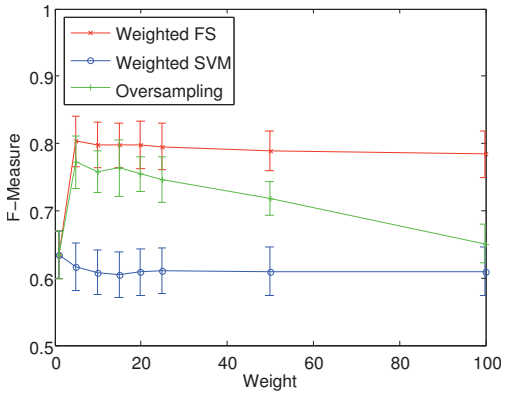
Figure 7.3: MNIST Results, with "4" as the costly digit, using $w(y = 4) = \{1, 5, 10, 15, 20, 25, 50, 100\}$ and (w)JMI. LEFT: Note that as costs for misclassifying "4" increase, the weighted FS method increases F-measure, while the weighted SVM suffers a decrease. RIGHT: The black dot is the cost-insensitive methodology. Note that the weighted SVM can increase recall above the 90% mark, but it does so by sacrificing precision. In contrast, the weighted FS method pushes the cluster of points up and to the right, increasing both recall and precision.

Table 7.2: MNIST results, averaged across all digits. Each value is the difference (x 100) in Precision, Recall or F-Measure, against the cost-insensitive baseline.

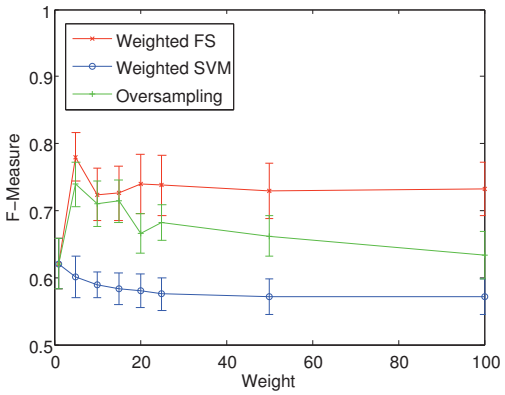
Algorithm	**Δ Pre**	**Δ Rec**	**Δ F-Measure**
wJMI	6.3	5.1	5.7
weighted SVM	-17.0	10.4	-7.0
Oversampling	-8.9	11.5	-0.6

Table 7.3: MNIST results, digit 4. Each value is the difference (x 100) in Precision, Recall or F-Measure, against the cost-insensitive baseline.

Algorithm	**Δ Pre**	**Δ Rec**	**Δ F-Measure**
wJMI	18.5	18.5	18.5
weighted SVM	-22.6	26.7	-6.7
Oversampling	0.1	24.3	10.5



(a) F-Measure on the digit "4" with 95% Confidence, across 10-fold CV.

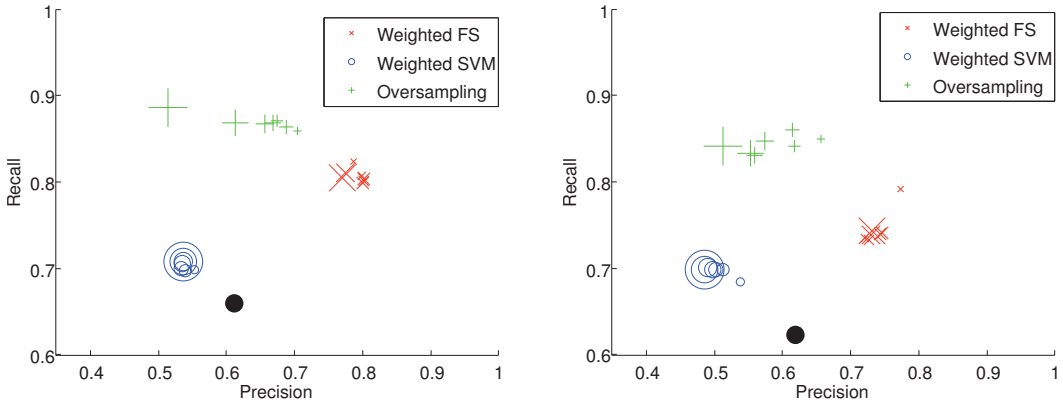


(b) F-Measure on the digit "9" with 95% Confidence, across 10-fold CV.

Figure 7.4: MNIST Results, with both "4" and "9" as the costly digits, using $w(y = (4 \vee 9)) = \{1, 5, 10, 15, 20, 25, 50, 100\}$ and (w)JMI, F-Measure.

We might also wish to understand the performance of our weighted measure when we upweight two classes simultaneously. We investigated this by upweighting both "4" and "9" in the same run, as these digits are often confused by pattern recognition systems. In Figure 7.4 we present the results as we increase the weights on both 4s and 9s, in terms of the F-Measure. In Figure 7.5 we present the same experiments as a scatter plot of precision and recall. We can see that in this case the weighted SVM fails to differentiate between 4s and 9s, and is dominated by both the oversampling and our weighted feature selection. Again the oversampling improves the recall of the upweighted classes, and the weighted feature selection improves both precision and recall, though the improvement in recall is less than the oversampling approach. We note that our technique is successful in improving both precision and recall in both of the upweighted classes, showing it has selected features which can differentiate between 4s and 9s.

Finally we compare our weighted method against the SpreadFX algorithm by Forman [43]. In Forman's paper he suggests the extension of the SpreadFX algorithm to use a random sampler on a non-uniform distribution. We create such a distribution by normalising our weight vector so that it sums to one, and then use it in the Rand-Robin scheduler. This leads to a cost-sensitive feature selection algorithm, though it is quite different from our approach. SpreadFX converts any given multi-class problem into a series of $|Y|$ one-versus-all binary problems, then performs feature selection on each sub-problem. The scheduler is then used to select features from each of the rankings constructed on the sub-problem. This



(a) Precision/Recall plot for the digit "4", the marker size indicates the weight w.

(b) Precision/Recall plot for the digit "9", the marker size indicates the weight w.

Figure 7.5: MNIST Results, with both "4" and "9" as the costly digits, using $w(y = (4 \vee 9)) = \{1, 5, 10, 15, 20, 25, 50, 100\}$ and (w)JMI, Precision/Recall plot.

has two important drawbacks in terms of the information theoretic measures we have used: first the runtime complexity scales with the number of classes, and second it is harder to use a multivariate ranking technique such as JMI, as it is unclear what the set of selected features should be. One further issue is that the feature selection process becomes stochastic, unlike the rest of the algorithms we consider throughout this thesis. As it is difficult to construct multivariate ranking techniques using Spread-FX we compare SpreadFX against wMIM rather than the wJMI used throughout the rest of the cost-sensitivity experiments. In Table 7.4 we present the average improvement in precision, recall and F-measure compared against the cost-insensitive method. This table is identical to Table 7.2 in terms of experimental methodology except that it uses MIM instead of JMI. We also present a bar chart comparing the different methods with "4" as the costly digit (this figure uses an identical setup to Figure 7.2a, except using MIM instead of JMI). We can see that SpreadFX performs equivalently or better than our proposed weighted feature selection criteria, though it is not statistically significantly better. The SpreadFX approach is reminiscent of multi-label approaches as it assumes independence between the feature sets for each label. In contrast weighted feature selection criteria such as wMIM and wJMI score highly features which are useful for predicting multiple classes, especially if multiple classes have been upweighted.

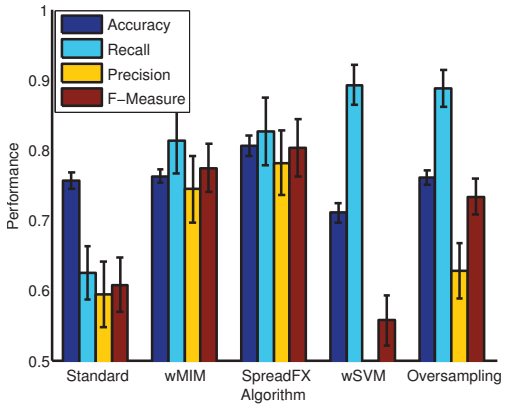


Figure 7.6: MNIST Results, using wMIM comparing against SpreadFX, with "4" as the costly digit.

Table 7.4: MNIST results, averaged across all digits. Each value is the difference (x 100) in Precision, Recall or F-Measure, against the cost-insensitive baseline.

Algorithm	δ **Precision (%)**	δ **Recall (%)**	δ **F-Measure (%)**
wMIM	3.9	4.4	4.2
Weighted Classifier	-13.5	10.3	-4.1
SpreadFX	6.0	6.6	6.4
Oversampling	-6.7	11.3	1.0

7.4.2 Document Classification

We chose 5 document classification datasets from Han and Karypis [52] (the datasets are listed in Table 7.5). We tested these datasets using the same procedure as the MNIST datasets, selecting 50 features with either our wJMI criterion, or the standard JMI criterion and classifying using either a normal or weighted SVM. We ran each experiment using 10-fold cross validation where each class was upweighted in turn with $w(y) = 10$, and present the Wins/Draws/Losses at the 95% confidence interval in Table 7.6. The first three columns are comparing against the cost-insensitive method, and we see that the weighted feature selection improves the F-measure in some cases, but the weighted SVM and oversampling approaches degrade performance in many cases. When comparing the weighted feature selection against the weighted classifier or oversampling (the last two columns) we see that the weighted feature selection improves upon weighted classification in many cases, particularly with the ohscal dataset, which was the largest dataset we tested, with 11162 examples and 11465 features.

Table 7.5: Summary of text classification datasets.

Dataset	Features	Examples	Classes
fbis	2000	2463	17
la12	31472	6279	6
ohscal	11465	11162	10
re0	2886	1504	13
re1	3758	1657	25

Table 7.6: Document classification results: F-Measure W/D/L across all labels, with the costly label given $w(y) = 10$.

Data	wJMI	wSVM	Oversample	wJMI v wSVM	wJMI v Oversample
fbis	4/13/0	1/13/3	5/11/1	7/10/0	2/15/0
la12	1/5/0	0/3/3	0/5/1	4/2/0	2/4/0
ohscal	2/8/0	0/0/10	0/1/9	10/0/0	10/0/0
re0	0/13/0	0/13/0	0/13/0	0/13/0	0/13/0
re1	1/24/0	0/25/0	0/25/0	2/23/0	0/25/0

7.5 Chapter Summary

In this chapter we looked at the effects of choosing a different loss function than the joint likelihood we considered in the previous three chapters. We saw that choosing a cost-sensitive conditional likelihood allowed the derivation of cost-sensitive feature selection criteria, based upon Guiaşu's weighted information theory. We proved several essential properties of the weighted mutual information measure to ensure it's suitability as a selection criterion.

As with the criterion derived in Chapter 4, some assumptions are necessary to produce a feature selection criterion which is estimable across many datasets. We thus investigate a weighted variant of JMI as it was found to perform the best in our empirical study from Chapter 5, and a weighted variant of MIM as a baseline.

We show how the cost-sensitive nature of our new criteria allows the construction of a cost-sensitive system from a *cost-insensitive* classifier coupled with the *cost-sensitive* feature selection. This compares favourably with other cost-sensitive techniques based around altering either the classifier or the training data.

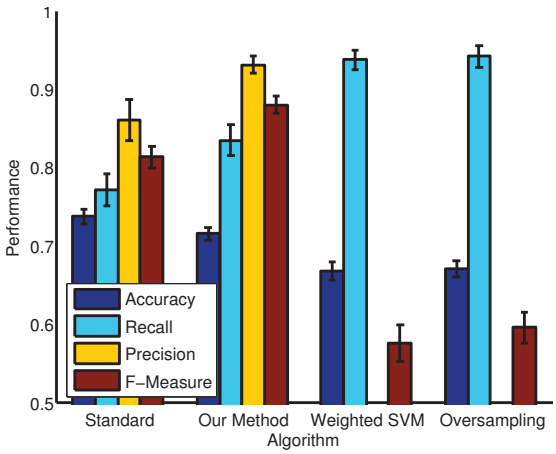


Figure 7.7: Ohscal results. Cost of mis-predicting class 9 is set to ten times more than other classes. The weighted SVM and oversampling approaches clearly focus on producing high recall, far higher than our method, however, this is only achievable by sacrificing precision. Our approach improves precision *and* recall, giving higher F-measure overall.

Chapter 8

Conclusions and future directions

We began this thesis by reviewing the literature on information theoretic feature selection. This literature contained a forest of different selection criteria based upon different permutations of information theoretic functions, with little understanding of the objective functions such criteria optimise. Our first result showed that using an information theoretic criterion implies the objective function is the log-likelihood of a particular model. We then proceeded to explore the literature relating the different criteria to the one derived from the likelihood. Once we had explained the literature we investigated the specific benefits of our framework, looking at extensions which incorporate prior knowledge or cost-sensitivity. We now provide a detailed summary of the contributions of this thesis, providing answers to the questions posed in the first chapter.

8.1 What did we learn in this thesis?

The contributions of this thesis arose by considering the questions stated in Chapter 1. We now review those questions, summarising the answers provided by this thesis.

8.1.1 Can we derive a feature selection criterion which minimises the error rate?

We answered this question in Chapter 4 by considering the joint likelihood of a discriminative model as our objective function. This likelihood is maximised by having a high predictive probability for all the true labels of a training dataset,

when using parameters which have a high probability *a priori*. It is a proxy for the error rate as high likelihood is a sufficient condition for a low error rate, though it is not a necessary one. We saw that this likelihood could be expanded into a series of terms with each term relevant for a particular component of the error. We repeat Equation 4.10 for clarity below,

$$-\ell \approx \mathbb{E}_{\mathbf{x},y}\left\{ \log \frac{p(y^i|\mathbf{x}^i,\boldsymbol{\theta})}{q(y^i|\mathbf{x}^i,\boldsymbol{\theta},\tau)} \right\} + I(X_{\neg\boldsymbol{\theta}};Y|X_{\boldsymbol{\theta}}) + H(Y|X) - \frac{1}{N}\log p(\boldsymbol{\theta},\tau).$$

The first term denotes the quality of our predictor compared to the optimal predictions for the selected feature set, this takes the form of a KL-Divergence, and is zero when our predictor makes the optimal predictions. The second term denotes the quality of our selected feature set compared to the full feature set, this takes the form of a conditional mutual information and is zero when our selected feature set contains all the relevant information. The third term denotes the quality of the data itself, and the final term is the prior probability of the model parameters. We can therefore think of Equation 4.10 as expanding the likelihood thus,

$$-\ell \approx \text{predictor} + \text{feature set} + \text{data} + \text{prior}, \tag{8.1}$$

where we wish to minimise the first three terms, and maximise the fourth. In general we can do little to adjust the quality of our training data, and we should not adjust our priors based upon the data, therefore the first two terms are the quantities we can minimise. Making the filter assumption from Definition 8 allows us to first select a feature set which maximises the likelihood, and then to build a classifier which maximises the likelihood based on that feature set.

One further insight based upon this expansion is that filter methods which choose to maximise this likelihood are in effect wrapper methods using a perfect classification model. Even the filters themselves appear to be simple classifiers, as they construct a probability distribution and measure its predictive performance with a KL-Divergence. This perspective shows that when choosing to maximise the joint likelihood filters and wrappers differ only in the method by which they search the feature space, and the assumptions made by the classification model. Using a classification model with few assumptions and maximising the model likelihood can be seen as a filter maximising the mutual information of the feature set.

Returning to the specific problem of filter feature selection we can derive the optimal selection criterion. If we choose to iteratively maximise the likelihood by selecting (or removing) features greedily then we should select the feature which maximises (minimises) the conditional mutual information between that feature and the class label, conditioned upon the selected feature set plus the prior term for the current feature set. We note that in the iterative updates the prior term is a ratio therefore if we use a flat uninformative prior, the prior term cancels. This leads to a maximum likelihood update rule based solely upon the conditional mutual information. With this derivation and the iterative update rules we are ready to answer the next question, by linking our derived updates to the selection criteria from the literature.

8.1.2 What implicit assumptions are made by the information theoretic criteria in the literature?

We looked at this question in Chapter 5, considering the criteria from the literature as approximations to our optimal criterion derived in Chapter 4. We considered the link to our optimal criterion assuming there was a flat prior over the possible feature sets, as the criteria we investigated did not include prior knowledge. This link makes explicit the objective function underlying each of the published criteria, namely the joint likelihood of a discriminative model.

As the optimal criterion is intractable to estimate, each of the published criteria make *implicit* assumptions which reduce the complexity of the estimation problem. These assumptions make the criteria *approximate iterative maximisers of the joint likelihood*. The main theoretical difference between the criteria is whether they assume the features are class-conditionally independent. Without this assumption there is an additional class-conditional term in the criteria. One other important theoretical point is whether they provide a mechanism to *balance* the relative magnitude of the redundancy terms against the relevancy term. To ascertain how these differences impact the criteria in practice, we conducted an empirical study of 9 different heuristic mutual information criteria across 22 datasets. We analysed how the criteria behave in large/small sample situations, how the stability of returned feature sets varies between criteria, and how similar criteria are in the feature sets they return. In particular, we looked at the following empirical questions:

How do the theoretical properties translate to classifier accuracy?

Summarising the performance of the criteria under the above conditions, including the class-conditional term is *not* always necessary. Various criteria, for example mRMR, are successful without this term. However, without this term criteria are blind to certain classes of problems, *e.g.* the MADELON dataset (see Section 5.3), and will perform poorly in these cases. Balancing the relevancy and redundancy terms is however *extremely* important — criteria like MIFS, or CIFE, that allow redundancy to swamp relevancy, are ranked lowest for accuracy in almost all experiments. In addition, this imbalance makes the criteria unstable, causing them to become sensitive to small changes in the supplied data.

How stable are the criteria to small changes in the data?

Several criteria return wildly different feature sets with just small changes in the data, while others return similar sets each time, hence are 'stable' procedures. As we might expect the most stable was the univariate mutual information as it has the simplest distributions to estimate, followed closely by JMI [110, 80]; while among the least stable are MIFS [6] and ICAP [58].

How do criteria behave in limited and extreme small-sample situations?

In extreme small-sample situations, it appears the above rules (regarding the conditional term and the balancing of relevancy-redundancy) can be broken — the poor estimation of distributions means the theoretical properties do not translate immediately to performance.

Do the different criteria return different feature sets?

We might ask how the theoretical differences between the criteria impact the selected feature sets, and so using the stability measures we compared the feature sets returned by each of the criteria with each other criterion. If we visualise the differences using multi-dimensional scaling (see Figure 5.5) we can see a cluster of criteria which "balance" the relevancy and redundancy terms (or ignore redundancy completely in the case of MIM), and each criterion which does not balance the terms is very different from all other criteria. This explains why the empirical performance of many of the criteria is so similar.

Having explained the behaviour and performance of the criteria in the literature we looked at the other benefits provided by our probabilistic framework for feature selection.

8.1.3 Developing informative priors for feature selection

One major benefit of our joint likelihood approach to feature selection is the natural incorporation of domain knowledge in the form of priors over the selected feature set $\boldsymbol{\theta}$. In Chapter 6 we looked at simple forms for these priors, and showed how to combine them with selection criteria from the literature. During this process we saw how the IAMB algorithm for Markov Blanket discovery can be seen as another special case of our joint likelihood framework, operating under a specific sparsity prior. We used this insight to extend IAMB to include other information in the prior, specifically to include domain knowledge over the presence or absence of nodes in the Markov Blanket. This result shows local structure learning algorithms using conditional independence testing as instantiations of a likelihood-based score and search technique, similar to the result by Cowell [25] for global structure learning algorithms. As we might expect the inclusion of correct knowledge improved the recovery of the Markov Blanket in several artificial datasets. However the performance still improved even when half the supplied "knowledge" was incorrect. This improvement was greatest when using complex datasets and small amounts of data.

8.1.4 How should we construct a cost-sensitive feature selection algorithm?

In Chapter 7 we answer this question by *deriving* a cost-sensitive feature selection criterion directly from a cost-weighted likelihood. This weighted likelihood minimises an upper bound on the empirical risk. The derived criterion is based upon a *weighted* mutual information, which generalises Shannon's mutual information to incorporate the importance (or cost) of certain states. To allow the use of such a function we proved two novel properties of this weighted measure, namely the chain rule, and the non-negativity of information. Our derived criterion works with costs which depend solely upon the label, as otherwise the non-negativity property will not necessarily hold.

We then empirically tested this cost-sensitive criterion against several other

methods for creating cost-sensitive classification systems. We showed that using *cost-sensitive* information theoretic feature selection effectively converts a *cost-insensitive* classifier into a cost-sensitive one, by adjusting the features the classifier sees. We see this as an analogous process to that of adjusting the data via over or undersampling to create a cost-sensitive classifier, but with the critical difference that we do not artificially alter the data distribution. We found that while classical cost-sensitive classifiers traded off precision to improve recall, our new cost-sensitive feature selection methodology improved both precision and recall in the upweighted class(es).

As this thesis is of finite size there are obviously many interesting areas which remain for future study in the field of information theoretic feature selection, and we review some of them in the next section.

8.2 Future Work

While this thesis has consolidated much work in information theoretic feature selection, allowing many techniques to be described as instantiations of a likelihood-based framework, it has also revealed several interesting areas for future work.

The first area arises from the derivation in Chapter 4. In that chapter we constructed a probabilistic framework to find the Maximum a Posteriori solution to the feature selection problem. A natural extension of this work would be to investigate a fully Bayesian solution to the feature selection problem. Our work finds the modal value of the posterior distribution over $\boldsymbol{\theta}$, but it is well known that the MAP solution may not be close to the center of mass of the full posterior [10], and thus it may not accurately represent the posterior distribution. A Bayesian solution to the feature selection problem would allow detailed investigations of the posterior for $\boldsymbol{\theta}$, possibly highlighting feature sets which more accurately represent the posterior distribution. We expect that such a solution would take the form of a Dirichlet process across the space of possible $\boldsymbol{\theta}$ values, though we have invested little time in deriving such a solution.

The second area is based upon the insights gained into filter feature selection from Chapters 4 & 7. In those chapters we began by choosing a particular objective function to maximise, respectively the joint likelihood and weighted conditional likelihood. In each case we derived different selection criteria, though both were based upon information theory. There exist many other filter criteria,

many of which do not have links to precise objective functions. It may be interesting to investigate the links between a criterion such as the Gini Index [34], and derive the objective function implied by the choice of such a criterion. It is interesting to note that the log-likelihood is an instance of a *proper scoring function* [44], and other such scoring functions may also have links to feature selection criteria. One obvious extension would be to develop feature selection from a likelihood which combines both priors over $\boldsymbol{\theta}$, and differing misclassification costs, to unify the methods proposed in Chapters 6 and 7.

The third area is based upon the literature in information theoretic feature selection which we examined in Chapter 5. There we saw how the majority of published criteria make specific assumptions about the underlying distributions, and how all the criteria made the assumption that there are only pairwise interactions between features. Relaxing this assumption leads to more complex information theoretic terms, which consequently have higher data requirements to ensure they accurately estimate the mutual information. An interesting topic of study would be to combine this insight with work on entropy estimation [83] or analysis of the variance of the mutual information [56], to determine for any given dataset how many of these complex terms it is possible to estimate accurately, then adjusting the feature selection criterion accordingly. This would allow an adaptive feature selection criterion which adjusts to the amount of available data, behaving like J_{cmi} when there are many thousands or millions of datapoints, and scaling back through JMI towards MIM as the number of datapoints shrinks.

The fourth area is more theoretical in nature, and relates to the weighted mutual information used in Chapter 7. In that chapter we defined the weighted mutual information so that the weights are a function of a single variable, rather than both variables in the mutual information. We proved how this ensures the non-negativity of the measure, which is important for feature selection to ensure we are maximising the likelihood. However the original weighted conditional likelihood of Dmochowski *et al.* [31] does not include this constraint, and the weights are allowed to depend upon both $\mathbf{x}$ and y. In this case it is possible for the weighted mutual information to take negative values, and a very interesting subject is the nature of such negative values. This gives rise to some interesting questions: "What does a negative I_w imply about the nature of the relationship between X and Y?", and "What does it imply about the cost-sensitive problem that we wish to optimise?".

The final area involves extending the techniques presented in this thesis to new problems. The material on priors in Chapter 6 considered very simple priors, and more performance may be available by utilising more complex and informative priors. The material on cost-sensitivity is framed in the context of multi-class problems as those are more likely to exhibit the property where each label has a different group of predictive features. Exploring two class problems where this is the case, and extending the framework to cope with multi-label datasets would provide interesting applications of the weighted feature selection approach.

One topic which we chose not to consider in this thesis is the interaction between the search method and the feature selection criterion. Preliminary work suggests that for some of the criteria examined in Chapter 5 the choice of search method is irrelevant to the feature set returned. Forward searches, backwards searches and floating searches all returned the same (or very similar) feature sets, across a number of datasets. Also using the sum of $J(X_j)$ over the whole selected feature set as the objective function returned the same feature sets as the more greedy search methods mentioned earlier. It would be interesting to do a more extensive empirical study to see if this strange effect is borne out across many datasets as it implies the choice of search method has little relevance compared to the choice of selection criterion. This is a rather counter-intuitive result given the performance gains made with other feature selection criteria when changing the search method (*e.g.* Pudil *et al.* [91]), and suggests there may be a deeper insight into why information theory does not need complex search techniques.

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