Nikola Mrkšić

Semi-supervised Learning Methods for Data Augmentation

Computer Science Tripos

Trinity College

April 23, 2013

Proforma

Name:	Nikola Mrksic
College:	Trinity College
Project Title:	Semi-supervised learning methods for data augmentation
Examination:	Computer Science Tripos, Part II, 2013
Word Count:	12788
Project Originator:	Dr Sean Holden
Supervisor:	Dr Sean Holden

Original Aims of the Project

The original goal of this project was to investigate the extent to which data augmentation schemes based on semi-supervised learning algorithms can improve classification accuracy in supervised learning problems. The objectives included determining the appropriate algorithms, customising them for the purposes of this project and providing their Matlab implementations. These algorithms were to be used to develop a robust system for achieving data augmentation in arbitrary application areas. For evaluation purposes, a general framework for assessing the quality of data augmentation achieved was to be constructed.

Work Completed

The project met and exceeded all of the success criteria. A survey of theoretical results underlying data augmentation has been conducted. Full, general implementations of Bayesian Sets, Spy-EM and Roc-SVM algorithms, as well as their proposed extensions have been implemented. A general scheme for achieving data augmentation in binary and multi-class classification has been developed and successfully applied to the three application areas proposed. An evaluation framework for assessing the quality of data augmentation was implemented and used to give statistical significance to the results obtained.

Special Difficulties

None.

Declaration

I, Nikola Mrksic of Trinity College, being a candidate for Part II of the Computer Science Tripos, hereby declare that this dissertation and the work described in it are my own work, unaided except as may be specified below, and that the dissertation does not contain material that has already been used to any substantial extent for a comparable purpose.

Signed

Date

Contents

Acknowledgements

This project was completed under supervision of Dr Sean Holden, whom I would like to thank for his invaluable assistance, support and guidance throughout my studies. I would also like to thank Dr Arthur Norman, Dr Simone Teufel, Professor Jon Crowcroft and Professor Katherine Heller for all the helpful advice and suggestions they provided.

Chapter 1

Introduction

In this chapter, the task of data augmentation is presented and framed as a semi-supervised machine learning problem. The necessary theoretical assumptions are outlined and a general proof of utility of unlabelled data in improving the classification error in an idealised setting is provided.

1.1 Supervised Learning

Supervised learning algorithms generate a function $f : X \to Y$ that maps potential inputs to desired outputs, also known as labels. The desired function maps any $x_i \in X$ to a specific label $y_i \in Y$. The algorithm is trained using a list of input-output pairs (x_i, y_i). In the case where the set of labels Y is finite, the problem is known as classification; otherwise, the problem is known as regression.

The basic assumption of supervised learning is that the (x_i, y_i) pairs are independent and identically distributed random variables drawn from an underlying probability distribution on $X \times Y$. The function f obtained by learning from the training data tries to capture the probability density function of this distribution. The main condition required for supervised learning to work (that is to be able to generalise from a finite training set to potentially infinitely many "unseen" test cases) is that the *smoothness assumption of supervised learning* holds. Informally, it requires that if the points x_1 and x_2 are *close*, their corresponding outputs (labels) y_1 and y_2 should be *close* as well.

1.2 Semi-supervised Learning

Classifier performance is highly dependent on the nature of the data to be classified. Across different application areas, the prediction quality correlates with the amount of labelled data used for training the classifier. In applications ranging from text classification and speech recognition to different biomedical applications, gathering unlabelled data is usually cheap and straightforward: large amounts of text can be gathered online, speech can be recorded automatically and protein sequences can be acquired at industrial speeds. On the other hand, training data has to be labelled either by a human expert or through a set of physical experiments, making the acquisition of a *sufficiently* large training set expensive, time consuming, and *potentially* infeasible as a result.

Due to the abundance of the unlabelled data available, we are interested in how this data can be used to improve the accuracy of the classifiers produced. This is the task of semi-supervised learning.

Semi-supervised learning algorithms use two different data sets for training: $X_l = ((x_1, y_1), ..., (x_l, y_l))$, the set of inputs for which the corresponding labels are available, and a set of unlabelled data $X_u = (x_{l+1}, ..., x_{l+u})$, for which no labels are available. Given these data sets as input, the algorithm tries to create the same prediction function as in the case of supervised learning. However, in addition to using the labelled data for training, it attempts to use the unlabelled data to increase the quality of the prediction. The unlabelled data can increase the quality of the prediction only if the distribution of $p(x)$ observed from the unlabelled data carries information that is useful in the inference of $p(y|x)$.

To formalize this notion, we generalise the supervised learning assumption to obtain the (informal) *semi-supervised smoothness assumption*:

If x_1 and x_2 are points that are *close* to each other in a *high density region*, then their corresponding outputs y_1 and y_2 should be *close* as well. By transitivity, it follows that all points in the same *cluster* are likely to have their respective outputs clustered as well.

1.3 Data Augmentation

The performance of supervised learning algorithms improves with the size of the data set used for training the classifier. In application areas containing a limited amount of labelled, but a large amount of unlabelled data, *data augmentation* schemes are used to create larger (*augmented*) training data sets by incorporating some of the unlabelled examples into the labelled data set.

For each of the classes (labels) present in the data set, unlabelled examples most likely to belong to that class are identified. These examples, with their anticipated labels, become part of the training data set. Then, this *augmented* data set is used to retrain the classifier (for example, a Support Vector Machine, presented in Chapter 2), in hope that the data introduced may reduce the *classification error* of the classifier built.

In general, constructing data augmentation schemes that result in both simple and fast algorithms is a highly non-trivial task, as successful strategies vary greatly with the nature of data present in different applications.

Under certain assumptions about the nature of the data model, namely that all of the examples were generated using the same *mixture model* and that there exists a one-to-one correspondence between the generative components of this model and the labels present in the data set, it is possible to show that unlabelled data does *carry information* about the parameters of this mixture model. A full discussion and the proof of this claim are given in Appendix A.

However, this result does not yield a mechanism for achieving a reduction in classification error using unlabelled data, which is what the principle goal of data augmentation is. In fact, it is not always the case that this reduction can be achieved: with an infinite amount of labelled data, one can build an optimal classifier without the unlabelled data. Similarly, given an unlimited amount of unlabelled data but no labelled data, one could estimate the parameters exactly but matching them to the actual labels would be impossible.

Fortunately, building upon the result derived in Appendix A, one can show that with a finite amount of labelled and an infinite amount of unlabelled data, definite improvement can be achieved [3]: the classification error approaches the optimal one exponentially fast as the size of the labelled set increases. Unfortunately, little is known about the case when the sets of labelled and unlabelled data are both finite. Further theoretical arguments relevant for understanding the fundamental limits of data augmentation are presented in Chapter 3 and Appendix A.

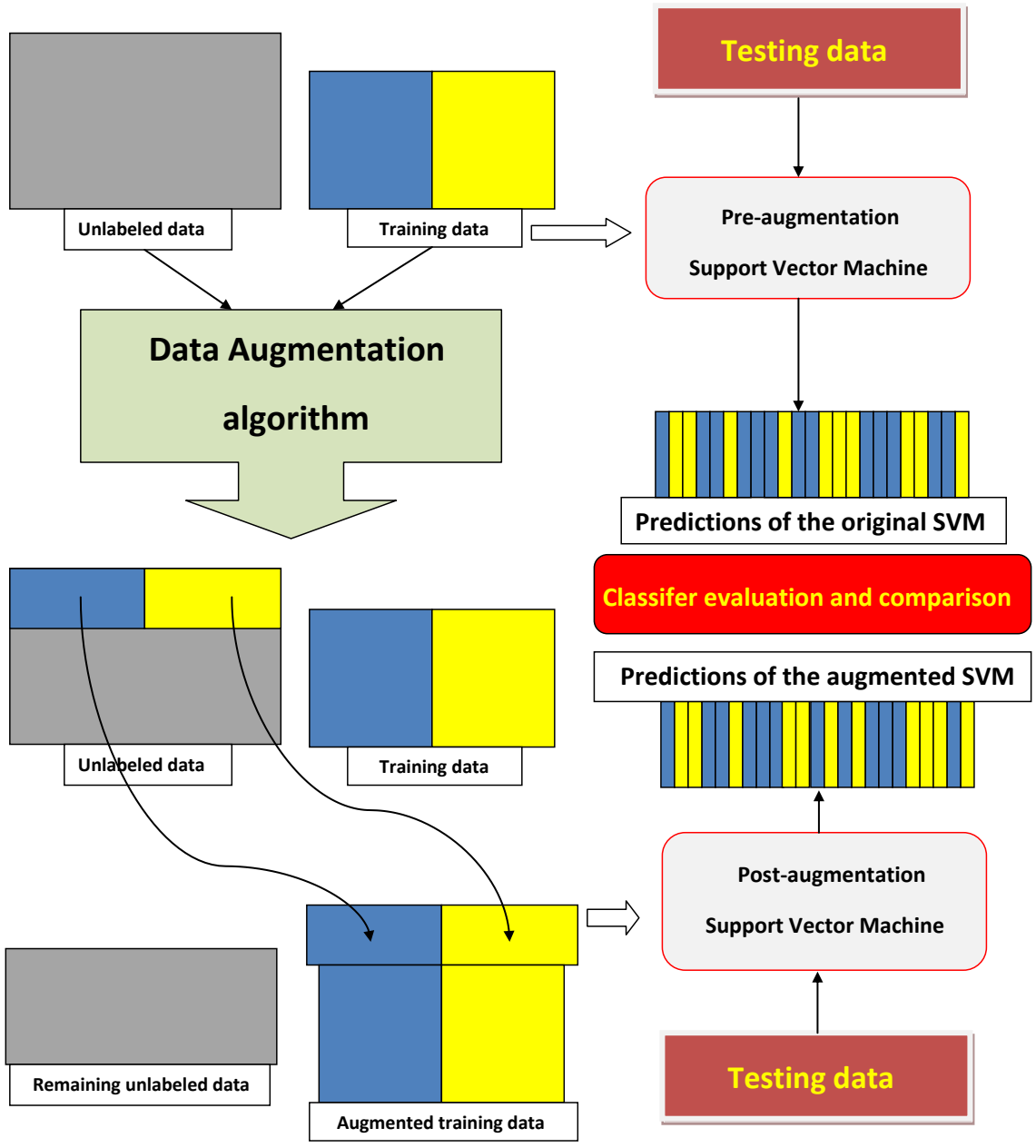


Figure 1.1: Flow diagram of the data augmentation process.

Chapter 2

Preparation

This chapter presents most of the research and planning conducted before the implementation of this project started. It contains my starting point, the rationale behind choices made in the implementation, an outline of the software engineering paradigm used and a description of the algorithms used for classification.

2.1 Starting Point

At the start of the project, I had no knowledge of machine learning whatsoever. Consequently, all the algorithms used and the computational learning theory presented had to be learned and absorbed throughout the course of this project. The original project idea proposed the use of Bayesian Sets algorithm for achieving data augmentation. The theoretical results presented, as well as the use of *Spy-EM* and *Roc-SVM* algorithms are my own refinements to the project proposal, identified through a thorough survey of associated literature.

I had no knowledge of Matlab prior to starting work on this project, and no knowledge of any experimental methods used in the subsequent evaluation.

2.2 Requirements Analysis

The project proposal outlined the idea of using different semi-supervised machine learning algorithms to achieve data augmentation across different application areas. The project consisted of three principle components:

1. Understanding the theoretical boundaries of the reduction in classification error achievable through data augmentation.
2. Identifying and implementing algorithms and statistical techniques applicable to data augmentation.
3. Establishing a uniform criteria to measure the success of different data augmentation algorithms across different application areas. Subsequently, implementing a system which would bring all of these components together to empirically determine the extent to which data augmentation can aid classification.

2.2.1 Theoretical Background

The first step in refining the project proposal was to identify the theoretical results that could allow us to more effectively determine which algorithms are likely to be most effective at boosting classifier accuracy. To this extent, a broad literature survey was conducted [3, 4, 7, 11, 12]. Understanding the material required familiarisation with the relevant aspects of computational learning theory, including the probably approximately correct(PAC) learning framework and the use of Vapnik Chervonenkis (VC) dimensions. Results most relevant to my work are presented in Chapter 3 and Appendix A.

2.2.2 Algorithms for Achieving Entity Set Expansion

Initially, the following algorithms were proposed for the problem of entity set expansion:

- Bayesian Sets algorithm[6] was to be used as the principle data augmentation method and was to act as a representative of the ranking methods.
- Spy Expectation Maximisation algorithm (*Spy-EM*[10, 11]) was proposed as an extension, acting as a representative of the classification methods.

Through further consideration of the related work, another *potential* extension was identified. This was the *RocSVM* algorithm[8], a method based on a paradigm akin to *Spy-EM*, but applicable to continuous input data (unlike *Spy-EM*, which supported only binary data). Therefore, implementing *RocSVM* was incorporated into the project goals, promising the *potentially* most powerful [8] and general approach to achieving data augmentation.

2.2.3 Choosing the Benchmark Classifier

For the sake of meaningful evaluation of the quality of data augmentation achieved, a *uniform measure* of the improvement in classification accuracy achieved through data augmentation had to be established. The simplest, most elegant solution was to use the same classifier across all application areas.

A survey of relevant literature [1] suggested that support vector machines (SVMs) could provide the benchmark classifier. Namely, SVMs are applicable to most classification and regression problems without significant tuning. Using SVMs across all application areas was a rational decision for the sake of this project: we are interested in improving the performance of *arbitrary classifiers* through data augmentation, not in building optimal classifiers through domain specific knowledge.

The alternative approach would have been to use classifiers specifically tailored for each of the application areas considered. As a result, we would obtain insights into using very specific classifiers in very specific applications, thereby restricting our ability to reliably compare the performance of the same data augmentation algorithm across different applications. Moreover, it would be hard to draw any *general* conclusions about the potential of data augmentation.

SVMs are a very powerful tool applicable to a wide range of problems in machine learning. In addition to the practical consideration of allowing consistent evaluation, using *SVMs* was beneficial for the following reasons:

- A technique applicable to improving {SVM performance in any setting would be highly reusable: it would provide a wrapper method for boosting the performance of any (existing and new) supervised learning application which has a body of unlabelled data available to it.
- SVM performance is well understood and reliable library implementations exist(*LIBSVM*, SVM^{light}). Therefore, choosing SVMs as our means of classification minimised the risk of this component becoming a bottleneck in developing the final data augmentation evaluation system.

Therefore, Support Vector Machines were chosen as the benchmark classifier. Hence, the principle measure of data augmentation quality would be the improvement in SVM classification performance caused by training the SVM with the *augmented* data set produced by our semi-supervised algorithms (Figure 1.1).

2.2.4 Application Areas Considered

The extent to which data augmentation can aid classification was investigated in three different application areas. The first two deal with *two-group classification* of instances consisting of *binary features*, whereas the third data set consists of *continuous features* and deals with *multi-class classification*.

1. **Text classification:** *Reuters21578* text categorisation data set. This is a well known data set dealing with a standard problem in machine learning and natural language processing.

2. **Prediction of biomolecular activity**: *KDD Cup 2001*, Task 1 (Binding to Thrombin) data set. Achieving augmentation with this data set was expected to be very hard, as well as computationally difficult.

3. **Supervised learning for theorem proving**: augmentation of the data set used in recent research about using supervised learning to guide automated theorem provers.[2] Its inclusion in the results depended on the successful implementation of *all* the proposed *extensions*, including *RocSVM* and *multi-class classification*.

Details of these experiments and the data sets used are presented in Chapter 3.

2.3 Project Methodology

The target system consisted of four principle components (figure 2.2). As discussed in the previous section, project goals included application of three different data augmentation schemes to three different application areas. Due to the differing nature of these, different classification schemes had to be used for binary and multi-class classification. Hence, the exact work schedule was highly unpredictable as the implementation of the more advanced schemes depended on success in previous stages.

Prior to actual implementation and evaluation, no mechanism was available to assess how successful each of the data augmentation schemes would be in each of the application areas. As outlined in the previous sections, each of them had several potential weaknesses and liabilities, making the list of project requirements very susceptible to change.

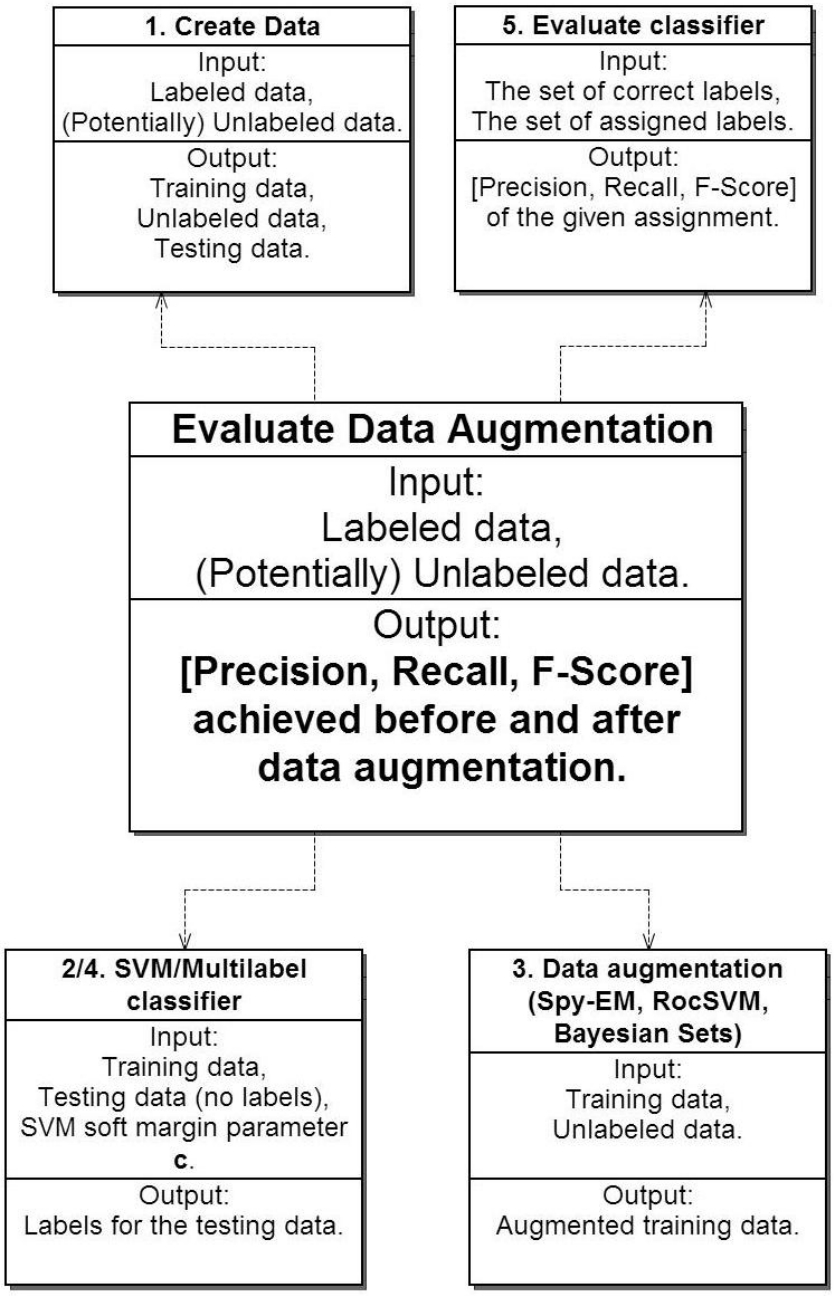


Figure 2.1: Component diagram of the data augmentation evaluation system.

Furthermore, the list of proposed extensions to the project was extensive. The ambitious nature of the goals presented required careful management of expectations to ensure that the primary success criteria were fulfilled notwithstanding potential complications encountered when tackling more advanced goals, such as the *Roc-SVM* algorithm or augmenting the theorem proving data.

A very important consideration in choosing our development model was the fact that results of data augmentation achieved with simpler algorithms on simpler data sets were necessary to determine the direction of subsequent implementation, modify requirements, and *potentially* limit the scope of the project.

Finally, as most of the data augmentation schemes(*Spy-EM, Roc-SVM*) are very computationally demanding, and as processing the biomedical data promised to be borderline intractable, having the entire system able to run at least some of the data augmentation schemes early on was instrumental in being able to obtain all the results required in time.

Taking all of these requirements into account, the development paradigm chosen for this project was ***evolutionary prototyping***[5].

2.3.1 Evolutionary prototyping

Evolutionary prototyping is a form of software prototyping that builds each prototype in a quality manner: the process includes a requirements specification, design documentation and thorough testing. In each development cycle, only the *well understood* requirements are implemented. Subsequently, the prototype is used experimentally to shed more light on the remaining requirements (those less understood), as well as to identify new requirements.

Evolutionary prototyping delivers incremental *functional* systems, with *each iteration* providing a system meeting a set of *well defined* requirements. This paradigm was ideal for the needs of this project, as it catered perfectly to our need to start obtaining results about simpler schemes and simpler application areas while work on the more complicated ones was still under way.

More importantly, the constant requirements feedback warranted by this method proved to be instrumental in providing enough versatility and early warning signals to streamline my efforts towards a smooth and successful completion of all the success criteria and all of the proposed extensions.

2.4 Relevant Algorithms

This section presents two of the algorithms used as building blocks for the data augmentation schemes and the experiment setup presented in Chapter 3. Existing implementations of Support Vector Machines and Naive Bayesian classifiers available from Matlab's Machine Learning toolbox were used in this project.

2.4.1 Naive Bayes Classifier

In statistics and machine learning, classification refers to the problem of identifying to which category (of the given set of categories) a new observation (also known as *instance* in machine learning) belongs to, based on the training data which consists of observations for which the categories (classes) are known. Instances are characterised by a vector of explanatory variables known as *features*.

The probability model for a classifier is represented by the conditional distribution $\Pr(C \mid F_1, ..., F_n)$, where C represents the set of classes and $F_1 \dots F_n$ stand for the *feature vectors* spanning the space of potential observations.

The Naive Bayes classifier makes the assumption of *conditional independence between features* of the observations: for any features F_i and F_j, it must hold that $\Pr(F_i \mid C, F_j) = \Pr(F_i \mid C)$. Even though this is not the case in most data sets, it is a common assumption and it often results in very good performance. This assumption is useful as it can be used to simplify the probability model.

First, the expression for conditional probability can be rewritten using Bayes' theorem:

$$\Pr(C \mid F_1 \dots F_n) = \frac{\Pr(C)\Pr(F_1 \dots F_n \mid C)}{\Pr(F_1 \dots F_n)} \tag{2.1}$$

The denominator represents the normalisation constant, which can be omitted.

Repeatedly unfolding the definition of conditional probability (and omitting all the normalisation factors) yields:

$$\frac{\Pr(C)\Pr(F_1 \dots F_n)}{\Pr(F_1 \dots F_n)} \propto \Pr(C)\Pr(F_1 \mid C)\Pr(F_2 \dots F_n \mid F_1, C)$$

$$\propto \Pr(C)\Pr(F_1 \mid C)\Pr(F_2 \mid C, F_1)\Pr(F_3 \dots F_n \mid F_1, F_2, C)$$

$$\propto \quad \Pr(C)\Pr(F_1 \mid C)\Pr(F_2 \mid C, F_1)\Pr(F_3 \mid C, F_1, F_2)\ldots\Pr(F_n \mid F_1 \ldots F_{n-1}, C)$$

Applying the assumption of conditionally independent features to the final expression yields:

$$\Pr(C \mid F_1 \ldots F_n) = \frac{\Pr(C)\Pr(F_1 \ldots F_n)}{\Pr(F_1 \ldots F_n)} \propto \boxed{\Pr(C)\prod_{i=1}^{n}\Pr(F_i|C)} \tag{2.2}$$

The *prior* for this model, $\Pr(C)$, can be estimated by observing the frequency of each class in the training data available. The conditional probability distributions of each feature, $\Pr(F_i \mid C)$ depend on the joint probability distribution $\Pr(F_i, C)$, as $\Pr(F_i \mid C) = \Pr(F_i, C)/\Pr(C)$. Hence, they can be estimated from the training data by dividing the number of occurrences of each *(feature, class)* pair with the (already estimated) prior of that class (the *bag of words* approach).

Despite the fact that the feature independence assumption is often inaccurate, Naive Bayes classifiers have been successfully used in a wide range of applications. Their popularity stems from their practicality: the decoupling of features allows one to estimate each feature's probability distribution independently and thus avoid the *curse of dimensionality*, which occurs with many data models that scale exponentially with the number of features.

2.4.2 Support Vector Machines

Support vector machines are a very popular supervised learning model used for two-group classification and regression analysis. [15]

Given a set of training instances, the SVM training algorithm builds a model that assigns new examples into one category or the other. The SVM model represents instances as points in a high-dimensional space, mapped in such a way that the points representing instances of the two categories are separated from each other by a gap that is as wide as possible. SVMs construct a hyperplane (or a set of hyperplanes) in that high-dimensional space in order to split the two classes into two distinct subspaces (Figure 2.2). Subsequently, new examples are classified according to the subspace of the model space that they are mapped to.

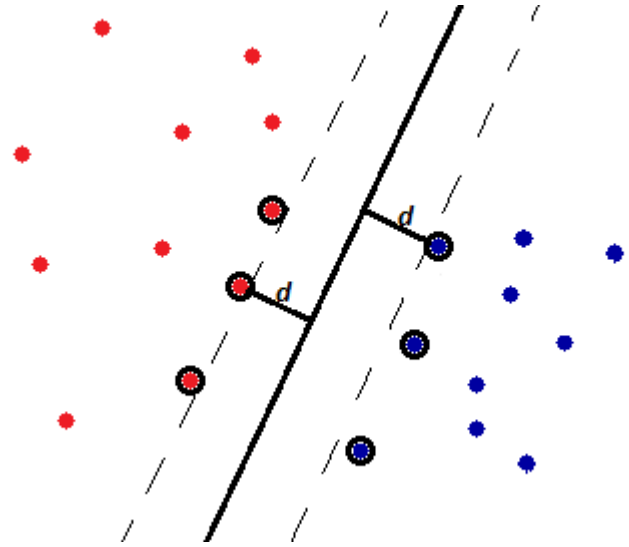


Figure 2.2: The optimal decision line is as far from points of both classes as possible.[1]

Support vector machines are a direct product of work done in *computational learning theory*. If f denotes the target classifier, let $L(f((x)), y)$ be the function that measures its error of prediction (the *loss function*): this can be the square error function, the negative log marginal likelihood function, etc. Then, one can obtain the parameters of the *optimal decision function* by minimising the *expected error of classification* on all data:

$$R(f) = E[L(f(x), y] = \int_y \int_x L(f(x), y) \Pr(\mathbf{x}, y) dx dy \tag{2.3}$$

As $\Pr[\mathbf{x}, y]$ is not available, $R(f)$ can not be computed. Instead, it is replaced with the *sum* of errors across all *training data* (the *empirical risk function*).

Out of all classifiers that *separate* the training data, SVMs choose the *optimal* one by *maximising* the *minimal* distance from the set of all training points (irrespective of class membership) to the separating hyperplane (Figure 2.2). This principle is known as *empirical risk minimisation*. A relatively small number of data points known as *support vectors* are required to determine the exact position of the optimal decision hyperplane.

In real world data sets, it is rarely the case that the separating hyperplane can perform error-free classification of the training data. There are two different approaches to tackling these *non-separable* data sets:

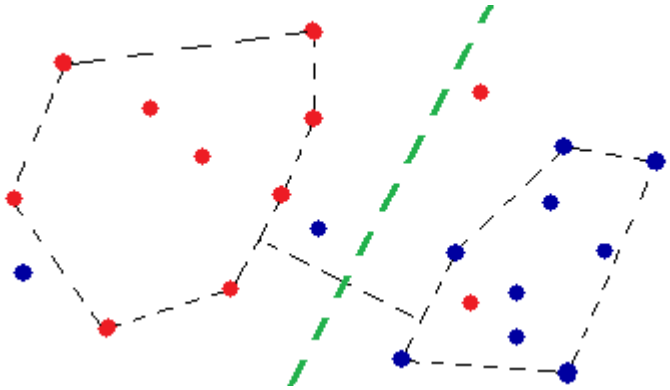


Figure 2.3: Soft margin SVM: here, outlier points are 'ignored'; the decision plane still maximises the distance from the convex hulls of the *reduced* sets of the two classes.[1]

Soft margin classification: if the data is not linearly separable, we might still try to split the majority of the data points *as cleanly* as possible, using the same approach as for the separable data. If no separating hyperplane exists, the *soft margin method* will allow *some of the examples* to be misclassified (Figure 2.3).

Non-linear SVMs are the alternative approach. These use the *kernel trick* to map the initial (non-separable) data points onto a higher-dimensional space where they become separable (Figure 2.4). This mapping is achieved by a non-linear kernel function such as the Gaussian radial basis function or the hyperbolic tangent.

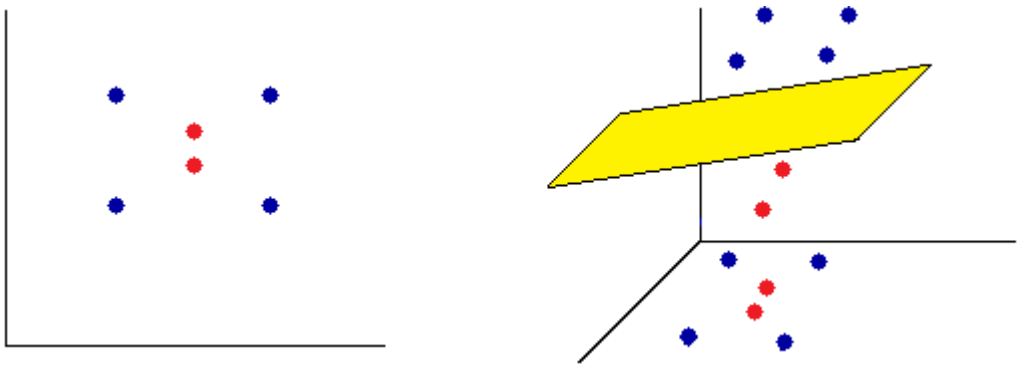


Figure 2.4: Using the *kernel trick* to separate an inseparable 2D training set.[1]

2.5 Languages and Tools

Matlab was deemed to be the most suitable language for implementing the algorithms required for this project. Furthermore, Matlab is omnipresent in machine learning, so this decision facilitated subsequent reuse of these algorithms (of which there are no open-source implementations available) by the research community.

Throughout the course of the project, a number of additional tools were used:

1. C++ was used to pre-process the data sets used.
2. Subversion and Tortoise SVN were used for version control.
3. TeXnicCenter was used to write the dissertation.
4. GeoGebra, MS Word and Paint were used to draw the diagrams for the dissertation.
5. Microsoft Excel was used for some of the evaluation work.

Chapter 3

Implementation

This chapter presents the data augmentation system created, focusing on the partially supervised algorithms developed for the problem of entity set expansion. Theoretical arguments behind the implementation choices made are analysed and the specific requirements of each of the application areas are considered.

3.1 Overview

The implementation work undertaken for this project consisted of solving two separate problems: *entity set expansion* and *data augmentation*.

Entity set expansion: given a set S of seed entities of a particular class S and a set D of candidate entities, determine which of the entities in D belong to S. In other words, *expand* the set S based on the given seeds.

This part of the project consisted of identifying and implementing algorithms for achieving entity set expansion, as well as understanding the theoretical assumptions required in order for these algorithms to work. Three different algorithms were implemented: Bayesian Sets, *a ranking method*, and *Spy-EM* and *Roc-SVM*, which are *classification methods*.

Data augmentation: given a supervised machine learning problem that has unlabelled data available to it, label some of the unlabelled examples and add them to the training set so that the use of this new, augmented data set boosts the accuracy of the classifier produced.

This part of the project consisted of creating a system that first uses the entity set expansion algorithms to achieve data augmentation and subsequently measures how successful the augmentation was. Data augmentation was attempted in three different application areas.

These two problems are interdependent. In a way, entity expansion could be regarded as a stand-alone problem. However, the challenges faced in using these algorithms for data augmentation provided valuable feedback for the subsequent direction of their development, in accordance with the evolutionary prototyping paradigm adopted. For the sake of clarity, the work on the problem of entity set expansion will be covered first. Subsequently, the way in which these algorithms were used to achieve and assess data augmentation will be presented.

3.2 Partially Supervised Learning

Partially supervised learning algorithms are a special class of semi-supervised learning algorithms. They learn from a set of *positive* examples P and a *mixed* set of *unlabelled* examples U (hence termed PU learning). The mixed set is implicitly assumed to contain both positive and negative examples. The key characteristic of PU learning is that *no negative training examples* are available for learning. This contrasts the typical classification context, in which the training data contains instances of *every possible class*.

Partially supervised learning algorithms create binary classifiers that decide whether an instance belongs to the positive set P or not. These classifiers can then be used to extract the hidden positives from the mixed set U. Hence, these algorithms are ideal building blocks for our data augmentation schemes. Given the training set T, consisting of different classes P_i ($T = \bigcup_i P_i$) we aim to expand each of these classes with additional examples drawn from the mixed set. To do this, each of the classes $P_i \subset T$ is treated as the positive set and expanded using examples from the mixed set U.

The only major concern is that the knowledge about the negative sets (which is available for each of these classes: $N_i = T \setminus P_i$) is not used in entity set expansion. However, this knowledge will be utilised during the subsequent data augmentation stages to *purify* the augmented sets, that is to minimise the number of wrongly labelled examples introduced.

In face of imbalance in the distribution of negative data in the training and testing sets (as is the case with our biomolecular data and many real world data sets),

the use of negative data can degrade the quality of classification[9]. When this imbalance (known as the *selection bias*) is encountered, PU learning algorithms offer a superior approach to traditional binary classification [9]. Therefore, in order to provide data augmentation schemes that are as general as possible, entity set expansion was treated as a positive unlabelled learning problem.

3.2.1 Theoretical Foundations

Prior to deciding to base data augmentation on partially supervised learning, a detailed investigation of relevant work was conducted: [3, 4, 7, 11, 12]. The theoretical results used to justify the decision to use PU learning for achieving data augmentation are presented in *Appendix A*. Partially supervised classification is treated using the *probably approximately correct* (*PAC*) framework to show that a classifier with an *arbitrarily low* classification error can be produced given *sufficiently large* sets of positive and unlabelled examples. This result is by no means trivial, as *no labelled negative data* is introduced at any point. Indeed, it comes as a surprise that a classifier deciding membership of P can approach *perfect precision* **and** *perfect recall* **without** using *any negative examples* for training.

Detailed discussion and proofs of these claims are given in Appendix A. The theorem presented there yields sufficient conditions on the sizes of P and U required so that partially supervised learning can (in theory) produce an *arbitrarily good* classifier. This result provides the theoretical foundation to all the approaches to entity set expansion employed in this project. Together with the theoretical grounding of the utility of unlabelled data (also presented in Appendix A), it completes the computational learning theory argument showing that data augmentation, as framed and implemented in this project, promises (at least in theory) to be a well-founded scheme that can aid classification through use of unlabelled data.

These proofs rely on many assumptions. Indeed, it is unclear whether (or if at all) these assumptions hold in any of the application areas proposed. Moreover, the theory presented yields no constructive (or efficient) method for implementing PU classification or using the constructed classifiers to achieve data augmentation.

Henceforth, the discussion moves away from the theoretical aspects and focuses on the algorithms used, the data augmentation scheme developed and the results obtained in the suggested application areas. As will be shown in the experiments, schemes powered by PU learning can be successful at data augmentation, thus providing empirical support for the theoretical arguments presented.

3.3 Spy Expectation Maximisation Algorithm

Spy-EM algorithm was first proposed for the task of partially supervised classification in [11]. It is a heuristic technique based on Naive Bayes classifiers and the *expectation-maximisation* (*EM*) algorithm.

Expectation-maximisation is an iterative method for finding *maximum likelihood parameters* for statistical models based on incomplete data. The *expectation step* fills in the missing values using estimates of their expected values based on existing data and the *current estimates* of the parameters. The *maximisation step* calculates the parameters most likely to have generated the values obtained in the *expectation step*. The two steps are repeated until the parameters converge.

In partially supervised classification, available data corresponds to the positive set P and the missing data corresponds to U. Let c_1 and c_2 denote the positive and the negative *class*.[1] Obviously, $\Pr[c_1 \mid x_i] = 1$ for all $x_i \in P$, but no information is available about $\Pr[c_1 \mid x_i]$ if $x_i \in U$. Therefore, the expectation step will have to estimate $\Pr[c_1 \mid x_i]$ for each $x_i \in U$ (line 5). Then, the maximisation step will compute the parameters $\Pr[f_j \mid c_1]$ and $\Pr[c_1]$ that are most likely to have produced the values assigned to $\Pr[c_1 \mid x_i]$ in the expectation step (line 7).

Algorithm 1.1 *Spy-EM* Step 1: Initialisation via expectation-maximisation

Input: P and U, the sets of positive and unlabelled examples

1: **function** INITIAL-EM(P, U)

2: $C \leftarrow \text{TrainNB}(P, U)$ ▷ Train the initial Naive Bayes classifier

3: **while** parameters of C change **do**

4: **for each** unlabelled example $x_i \in U$ **do**

5: $\boxed{\Pr[c_1 \mid x_i]} \leftarrow \text{posterior}(C, x_i)$ ▷ new probability that $x_i \in P$

6: **for each** feature f_j of x_i **do**

7: ***Recalculate*** $\Pr[f_j \mid c_1]$ and $\Pr[c_1]$ for the updated $\boxed{\Pr[c_1 \mid x_i]}$

8: **end for**

9: **end for**

10: ***Retrain*** C using new values of $\Pr[f_j \mid c_1]$ and $\Pr[c_1]$

11: **end while**

Output: C, the classifier obtained via expectation maximisation

[1] Focus on the positive class c_1. All results for c_2 follow directly, as $\Pr[c1 \mid x_i] = 1 - \Pr[c2 \mid x_i]$.

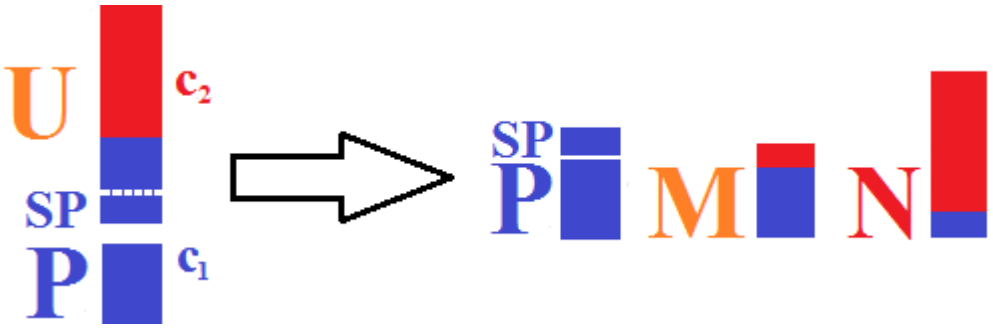


Figure 3.1: Extracting the set of *reliable negatives* N from the unlabelled set U.

Naive Bayes classifiers can be used as the basis of the *EM* algorithm, as shown above. The initial values for the prior $\Pr[c_1]$ and the conditional probabilities $\Pr[f_j \mid c_1]$ are estimated from the training data, as explained in Chapter 2.

Initially, all the unlabelled data is treated as negative, and *EM* iterates until the assignment of labels to U converges. The original paper ([11]) claims that the algorithm converges quickly; indeed, in the experiments, *Initial-EM* usually took no more than 4-5 iterations to converge.

Initial-EM can be used as a stand-alone classifier. Given *easily separable* data sets, it exhibits good performance. However, the method is highly biased towards positive samples. Given harder data sets, it tends to classify all of the examples as positives. To achieve better performance, the method should balance the influence that the positive and the (unknown) negative set have on classification. For this purpose, a set of *reliable negatives* N has to be extracted from U. *Initial-EM* provides information about which $x \in U$ are likely to belong to c_1, and which ones are not. However, making confident assertions about the class membership of any $x \in U$ is difficult: none of their labels are available to begin with or to provide a subsequent basis for comparison.

The *key trick* employed by *Spy-EM* is to move a *randomly sampled subset* of P, the *spy set* SP, into the mixed set U. If we apply *EM* to $P \setminus SP$ and $U \cup SP$, the behaviour of *the spy elements* from SP will be identical to the behaviour of the *hidden positives* in U. Therefore, those elements that *do not* behave in that same way are *more likely* to be the actual negatives and should be put into the reliable negatives set N. Consequently, the remaining set of unlabelled examples $M = U \setminus N$ contains a higher proportion of positives than U did. Therefore, the *ExtractRN* algorithm decomposes U into sets M and N, both of higher *purity* (the proportion of positives/negatives) than U (Figure 3.1).

Algorithm 1.2 *Spy-EM* Step 2: Extracting reliable negatives

Input: positive set P, unlabelled set U, sampling rate s

1: **function** ExtractRN(P, U)
2: $SP \leftarrow \text{sample}(P, s)$
3: $U' \leftarrow U \cup SP$
4: $P' \leftarrow P \setminus SP$
5: $C \leftarrow$ Initial-EM(P', U') ▷ Use *EM* to build the classifier
6: **for each** $x_i \in U'$ **do**
7: $\boxed{\Pr[c_1 \mid x_i]} \leftarrow \text{posterior}(C, x_i)$ ▷ *EM* posterior probabilities
8: **end for**
9: *Choose threshold* **t** *using posteriors assigned to spy positives in EM*
10: $N \leftarrow \emptyset$, $M \leftarrow \emptyset$
11: **for each** $x_i \in U$ **do**
12: **if** $\Pr[c_1 \mid x_i] \leq t$ **then** $N \leftarrow N \cup x_i$
13: **else** $M \leftarrow M \cup x_i$
14: **end for**

Output: the set of reliable negatives N and the remaining mixed set M

Choosing the threshold t (line 9) used for decomposing U is non-trivial. To extract all spy positives from U' into M, we should set t to $\min\{\Pr[c_1 \mid s] \mid s \in SP\}$. In a noiseless setting, this is a reasonable approach. However, most data sets include some outliers which cause the value of t to be lower than *most of the negatives*, making this bound inapplicable. In practice, choosing t so that l% of the examples have $\Pr[c_1 \mid x] \leq t$ proved to work well for any l between 5 and 20 per cent. In the experiments, varying l changed the number of iterations required for convergence, but had no effect on the final classifier produced.

Finally, given the positive set P, the reliable negatives set N and the remaining mixed set M, the *EM* algorithm is employed once again. It estimates the parameters most likely to have generated the labels for the sets of P and N, with the remaining mixed set M representing the missing data. Using the obtained parameters, the final (Naive Bayes) classifier is produced. Posteriors assigned by this classifier are used to determine which of the $x \in M \cup N$ actually belong to c_1. These are the *hidden positives* that will be used to achieve *data augmentation*.

As shown in the pseudo code below, the posterior probabilities of examples in both M and N are allowed to change between subsequent *EM* iterations (whereas the posteriors of P remain fixed). This is the reason why the *noise level* l can be set to any value between 5 and 20 per cent. If there are too many hidden positives in the set of reliable negatives N, the *EM* algorithm will correct their posteriors after a sufficient number of iterations, pulling them closer to c_1.

Algorithm 1.3 *Spy-EM* Step 3: Building the final classifier

Input: positive set P, reliable negatives set N, mixed set M

1: **function** FINAL-EM(P, N, M)

2: **for all** $x_i \in P$ **let** $\Pr[c_1 \mid x_i] := 1$ ▷ posteriors of P **remain fixed** in *EM*
3: **for all** $x_i \in N$ **let** $\Pr[c_1 \mid x_i] = 0$ ▷ **not fixed** in *EM*

4: $C \leftarrow$Initial-EM(P, N) ▷ Build the first classifier without considering M

5: **for each** example $x_i \in M$ **do**
6: $\Pr[c_1 \mid x_i] =$posterior(C, x_i) ▷ estimate posteriors for M using C
7: **end for**

8: $C_f \leftarrow$ EM($\mathbf{Pr}[c_1 \mid \mathbf{x}]$) ▷ Run *EM* with the new posteriors for M and N

Output: C_f, the final classifier for extracting *hidden positives* from $N \cup M = U$

The final run of *EM* produces a sequence of classifiers, the last of which is *not necessarily the optimal one*. Further discussion of the stopping criteria used can be found in [11].

Most of the work in *Spy-EM* consists of training Naive Bayes classifiers required for expectation maximisation. The complexity of training an NB classifier is $O(n')$, where n' represents the number of non-zero elements in the *feature matrix* of the training data. Assuming that the number of iterations required for *EM* to converge is bounded, as was the case in our experiments, it follows that the complexity of *Spy-EM* is at most $O(n \cdot f)$, n being the number of examples, f the number of features. In two of our application areas, the data sets are sparse, with each feature vector containing a limited number of non-zero attributes. Consequently, the complexity of *Spy-EM* comes closer to $O(n)$.

3.4 Rocchio-SVM Algorithm

Spy-EM is based on the *expectation-maximisation* algorithm implemented using Naive Bayes classifiers. The algorithm was originally designed for text classification, where feature vectors consist of binary indicators stating whether certain words appear in the document or not. In this setting, the priors required for Naive Bayes classification can be estimated from the training data. By design, *Spy-EM* is unable to perform classification if feature vectors consist of continuous attributes, as is the case with the theorem prover data set. An alternative scheme applicable to such data sets can be implemented using the *Roc-SVM* algorithm.

Roc-SVM is a partially supervised learning algorithm first proposed by Li and Liu in [8]. As in *Spy-EM*, a set of *reliable negatives* N is extracted from U and subsequently used to build the final classifier. However, instead of expectation-maximisation, *Roc-SVM* uses *support vector machines* to build that classifier.

To extract the set of reliable negatives N, *Roc-SVM* employs the *Rocchio classifier*. The method first computes the *centroids* (also known as the *prototype vectors*) of P and U. Then, for all the unlabelled examples $x \in U$, it computes the *cosine similarity* between their feature vectors $\vec{d_x}$ and the two centroid vectors. All instances closer (more similar) to the negative centroid become members of the set of reliable negatives N.

Algorithm 2.1 *Roc-SVM* Step 1: Rocchio classification

Input: P and U, the sets of positive and unlabelled examples

1: **function** ROCCHIO(P, U)

2: $\vec{c^+} := \alpha \frac{1}{|P|} \sum_{\vec{d} \in P} \frac{\vec{d}}{||\vec{d}||} - \beta \frac{1}{|U|} \sum_{\vec{d} \in U} \frac{\vec{d}}{||\vec{d}||}$

3: $\vec{c^-} := \alpha \frac{1}{|U|} \sum_{\vec{d} \in U} \frac{\vec{d}}{||\vec{d}||} - \beta \frac{1}{|P|} \sum_{\vec{d} \in P} \frac{\vec{d}}{||\vec{d}||}$

4: $N \leftarrow \emptyset$

5: **for** the feature vector $\vec{d_x}$ of every unlabelled example $x \in U$ **do**

6: **if** $\text{sim}(\vec{c^+}, \vec{d_x}) \leq \text{sim}(\vec{c^+}, \vec{d_x})$ **then** ▷ $\text{sim}(\vec{c}, \vec{d}) = \frac{\vec{c} \cdot \vec{d}}{||\vec{c}|| ||\vec{d}||}$

7: $N \leftarrow N \cup \{x\}$

8: **end for**

Output: the set of reliable negatives N

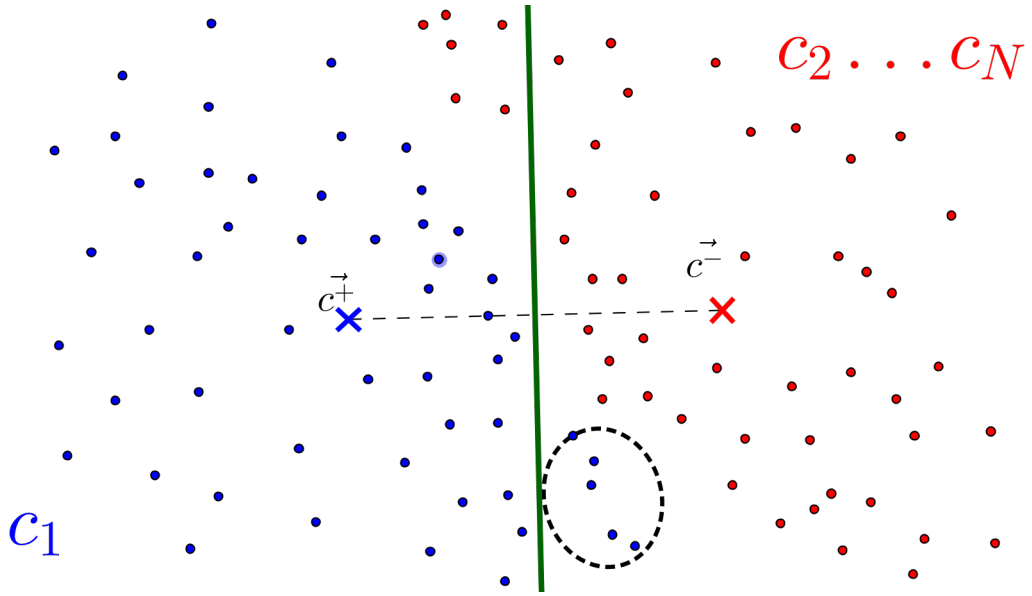


Figure 3.2: Rocchio classifiers are not able to remove all positives from N. [8]

Rocchio classification could be used as a stand-alone method for extracting N. This method performs classification using a separating hyperplane equidistant from the two centroids. If the actual decision boundary is not represented by (that) linear hyperplane, Rocchio tends to misclassify many examples close to the boundary chosen (Figure 3.2).

Lower purity of N does not degrade *Spy-EM* performance because additional iterations of *EM* relabel the positives in N. However, *Roc-SVM* builds the final classifier using support vector machines, which are much more susceptible to noise than *EM* is. Therefore, purging as many positives from N as possible is of paramount importance for subsequent *SVM* performance.

P consists of examples from a single (positive) class c_1. Conversely, the mixed set U may include negative examples of many different classes $c_2 \ldots c_N$. If this is the case, the centroid vectors used in Rocchio are not representative of any of the negative classes. These inadequate centroids tend to pull some of the hidden positives into N, causing its purity to deteriorate (Figure 3.2).

To account for different negative classes, *K-means clustering* can be used to separate the obtained negative set RN into K clusters, $N_1 \ldots N_K$, each (hopefully) representing *distinct* negative classes. Rocchio classification is then employed (again) to identify members of RN closer to at least one of the *new negative clusters* than to the positive set P. These examples become members of the final negative set N. This method outperforms the stand-alone Rocchio classifier [8].

Algorithm 2.2 *Roc-SVM* Step 2: K-means clustering for negatives extraction
Input: P and U, the sets of positive and unlabelled examples

function ROCCHIO WITH K-MEANS(P, U)
  $RN \leftarrow$ Rocchio(P, U)
  Randomly choose k initial cluster centres from RN ▷ K = 10 was used in the experiments
  Perform *K-means clustering* to separate RN into $N_1 \dots N_k$
  for $i = 1$ to k **do**
    $\vec{p_i} := \alpha \frac{1}{|P|} \sum_{\vec{d} \in P} \frac{\vec{d}}{||\vec{d}||} - \beta \frac{1}{|N_i|} \sum_{\vec{d} \in N_i} \frac{\vec{d}}{||\vec{d}||}$
    $\vec{n_i} := \alpha \frac{1}{|N_i|} \sum_{\vec{d} \in N_i} \frac{\vec{d}}{||\vec{d}||} - \beta \frac{1}{|P|} \sum_{\vec{d} \in P} \frac{\vec{d}}{||\vec{d}||}$
  end for

  $N \leftarrow \emptyset$
  for the feature vector $\vec{d_x}$ of every example $x \in RN$ **do**
    if $\exists \vec{n_i} \forall \vec{p_j} [\text{sim}(\vec{d_x}, \vec{n_i}) \geq \text{sim}(\vec{d_x}, \vec{p_j})]$ **then**
    $N \leftarrow N \cup \{x\}$ ▷ x is closer to *some* negative than to *all* positives
  end for

Output: the set of reliable negatives N

K-means Rocchio extracts a negative set of high purity by enforcing *very rigid criteria* for including examples into N. This strictness can cause the resulting set to become too small to warrant a good classifier [8]. Fortunately, a method similar to expectation-maximisation can be employed to *iteratively* grow the negative set.

The first SVM is trained using only P and N and used to extract $W_1 \subseteq M$, the set of examples in M likely to be negative. The next SVM is trained using P and the *new negative set* $N \cup W_1$. This step is repeated until the (final) SVM built can extract no new negatives from the remaining mixed set M_i. Thus, $M_i \subseteq M$ represents the set of hidden positives identified by *Roc-SVM*.

This iterative method has its drawbacks. As SVMs are very sensitive to noise, inclusion of a small number of positives from M into N in any iteration can cause an avalanche effect: the algorithm may pull many similar positives into the negative set by the time it terminates. Consequently, the performance of the classifiers produced falls into a downward spiral.

We can determine whether this method went awry by observing how the final SVM performs on the positive set. If it classifies more than 5% of examples in P as negatives, that means that too many positives were pulled into the negative set. If so, we revert to the first SVM, trained using only P and N (lines 12-14).

Algorithm 2.3 *Roc-SVM* Step 3: Building the final classifier

Input: positive set P, mixed set M, reliable negatives set N

1: **function** ROC-SVM(P, M, N)

2: $i := 1$, $N_i \leftarrow N$, $M_i \leftarrow M$

3: $C_i \leftarrow$ TrainSVM(P, N_i) ▷ use only P and N to build the first SVM

4: $W_i \leftarrow \{x \in M_i \mid \text{SVMClassify}(C_i, x) = -1\}$ ▷ *negatives* C_1 identifies in M

5: **while** $W_i \neq \emptyset$ **do** ▷ until no more negatives can be extracted from M

6: $N_{i+1} \leftarrow N_i \cup W_i$ ▷ move new negatives to the negative set

7: $M_{i+1} \leftarrow M_i \setminus W_i$ ▷ ...and remove them from the mixed set

8: $i \leftarrow i + 1$

9: $C_i \leftarrow$ TrainSVM(P, N_i) ▷ build the next SVM using the expanded N

10: $W_i \leftarrow \{x \in M_i \mid \text{SVMClassify}(C_i, x) = -1\}$ ▷ generate $W_i \subseteq M_i$ using C_i

11: **end while**

12: $p \leftarrow \dfrac{|\{x \in P \mid \texttt{SVMClassify}(C_i, x) = 1\}|}{|P|}$ ▷ Final SVM's *recall* on set P

13: **if** $p \geq 0.95$ $C_\texttt{f} := C_i$ ▷ if recall is high, use the final SVM

14: **else** $C_\texttt{f} := C_1$ ▷ otherwise, revert to the first SVM

Output: the final classifier $C_\texttt{f}$

In addition to providing a partially supervised algorithm for data sets with real valued attributes, *Roc-SVM* tends to outperform *Spy-EM* [8]. These improvements come at the expense of efficiency. *Roc-SVM* trains a sequence of SVMs in order to build the final classifier. SVM training has a quadratic and a cubic component. Estimating the exact complexity is hard, but we can expect training times of the order of (at least) $O(n^2)$, n being the number of training examples. Assuming a *constant* number of iterations in Step 3, *Roc-SVM's* best-case complexity is $O(n^2)$, still vastly inferior to *Spy-EM's* $O(n)$.

3.5 Bayesian Sets

Bayesian sets [6] are an information retrieval inspired algorithm for entity set expansion. Contrary to *Spy-EM* and *Roc-SVM*, which build classifiers to decide membership of the positive set P, Bayesian sets *rank* all examples of the data set D by their *likelihood* of belonging to P. Formally, given the *query set* $Q \subset D$, the goal of the algorithm is to order all items in D by their *similarity* with elements of Q, so that the elements of Q hidden in D feature highly in the ranking produced.

Bayesian Sets take a probabilistic model approach, assuming all examples are independently and identically distributed from some parametrised statistical model $P(\mathbf{x} \mid \theta)$, where θ represents the model parameters. In this setting, examples belonging to the same concept class (in this case Q) must have been generated using the same set of parameters θ_Q.

Therefore, the marginal probability $P(\mathbf{x} \mid Q, \theta_Q)$ can be used to estimate $\Pr[\mathbf{x} \in Q]$. θ_Q is unknown, so we average across the possible values of θ according to $P(\theta)$, the *prior* density on θ, to obtain $P(\mathbf{x} \mid Q)$. Furthermore, to account for the biasing effect of longer examples (longer documents, proteins) being less frequent and thus having a lower marginal probability, we *normalise* the scoring metric to obtain:

$$score(\mathbf{x}) = \frac{P\left(\mathbf{x} \mid Q\right)}{P(\mathbf{x})} = \frac{P(\mathbf{x}, Q)}{P(\mathbf{x})P(Q)} \approx \frac{Pr[\mathbf{x} \in Q]}{\Pr[\mathbf{x} \notin Q]} \tag{3.1}$$

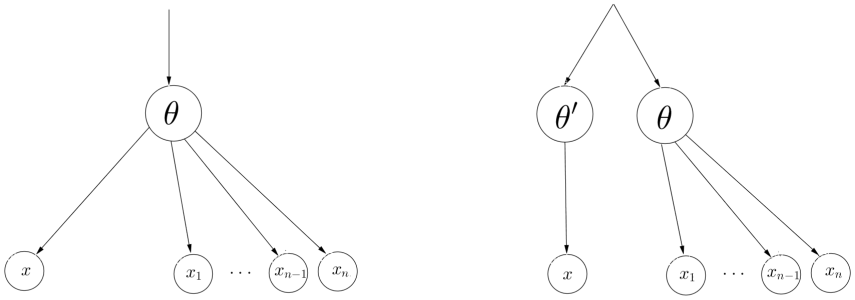
Using basic rules of probability, $P(\mathbf{x})$ and $P(\mathbf{x} \mid Q)$ can be expressed as:

$$P(\mathbf{x}) = \int P(\mathbf{x} \mid \theta) P(\theta) d\theta \tag{3.2}$$

$$P(Q) = \int \prod_{\mathbf{x_i} \in Q} P(\mathbf{x_i} \mid \theta) P(\theta) d\theta$$

$$P(\theta \mid Q) = \frac{P(Q \mid \theta) P(\theta)}{P(Q)}$$

$$P(\mathbf{x} \mid Q) = \int P(\mathbf{x} \mid \theta) P(\theta \mid Q) d\theta \tag{3.3}$$



$P(x, Q)$ $P(x)P(Q)$

Figure 3.3: the *score* function compares the probabilities of the data being generated by the two graphical models given above.[6]

The scoring metric reflects the ratio between $\Pr[\mathbf{x} \in Q]$ and $\Pr[\mathbf{x} \notin Q]$ (Equations 3.2-3.3, Figure 3.3). As such, this score can not be normalised to obtain $\Pr[\mathbf{x} \in Q]$, as this would require integration over all θ, which would be intractable.

However, *score* does provide an adequate measure of likelihood, since $\forall \mathbf{x_1}, \mathbf{x_2} \in D$. $\Pr[\mathbf{x_1} \in Q] \leq Pr[\mathbf{x_2} \in Q] \Rightarrow score(\mathbf{x_1}) \leq score(\mathbf{x_2})$. Therefore, it can be used to impose the desired ordering between the elements of D. Once the scoring function has been implemented, the Bayesian Sets algorithm is trivial:

Algorithm 3.1 *Bayesian Sets algorithm*

Input: set of items D, query set $Q = \{\mathbf{x_i}\} \subset D$

1: **function** BAYESIAN SETS(Q, D)

2: **for each** $\mathbf{x} \in D$ **do**

3: ***compute*** $score(\mathbf{x}) = \dfrac{P(\mathbf{x} \mid Q)}{P(\mathbf{x})}$

4: **end for**

Output: the list of all elements in D, sorted by decreasing scores

Intractability and difficulties in choosing the probability models and priors are recurring themes in most approaches based on Bayesian inference, including this one. If we limit our discussion to data sets featuring binary attributes, that is if for all $x_i \in D$ it holds that $x_{i,1} \ldots x_{i,n} \in \{0, 1\}$, then we can choose the probability models and their priors in a way that will make the integrals in equations 3.2 and 3.3 analytical.

Model the marginal probability $P(\mathbf{x} \mid \theta)$ using the *Bernoulli distribution*:

$$P(\mathbf{x_i} \mid \theta) = \prod_{j=1}^{n} \theta_j^{x_{i,j}} (1 - \theta_j)^{1 - x_{i,j}} \tag{3.4}$$

The distribution $P(\theta)$ is said to be a *conjugate prior* for the likelihood $P(\mathbf{x} \mid \theta)$ if the posterior probability $P(\theta \mid \mathbf{x})$ belongs to the *same family* of probability distributions as the prior. The use of conjugate priors can vastly simplify the task of inference. Therefore, model the prior $P(\theta)$ using the conjugate prior of the Bernoulli distribution, given by the *Beta distribution*:

$$P(\theta \mid \alpha, \beta) = \prod_{j=1}^{n} \frac{\Gamma(\alpha_j + \beta_j)}{\Gamma(\alpha_j)\Gamma(\beta_j)} \theta_j^{\alpha_j - 1} (1 - \theta_j)^{\beta_j - 1} \tag{3.5}$$

α and β represent *hyperparameters* of this distribution. In the experiments, these were set to $\alpha = c \cdot \mathbf{m}$, $\beta = c \cdot (1 - \mathbf{m})$, where $c = 2$ represents the *Dirichlet coefficient* and $\mathbf{m}$ represents the *mean vector* of all $\mathbf{x} \in D$.

From these assumptions, it follows that $P(\theta \mid \mathbf{x})$ is a Beta distribution as well. Its hyperparameters, α' and β', can be expressed as closed-form expressions of α, β and $\{x_{i,j}\}$. As a result, the integrals in equations 3.2 and 3.3 become analytical, making *exact inference* possible. Furthermore, as shown in [6], the use of Bernoulli and Beta distributions for $P(\mathbf{x} \mid \theta)$ and $P(\theta)$ reduces the computation of the list of *log scores* $s_1 \ldots s_N$ to a single (sparse) matrix multiplication:

$$\mathbf{s} = c + \mathbf{X}\mathbf{q} \qquad s_i = \log(score(\mathbf{x_i})) \tag{3.6}$$

$\mathbf{X}$ is the N by n *feature matrix* of D, and c and $\mathbf{q}$ are auxiliary values computed in linear time using the hyperparameters and the feature matrix $\mathbf{X}$:

$$c = \sum_{i=1}^{n} \log(\frac{\alpha_i + \beta_i}{\alpha_i + \beta_i + N} \frac{\beta_i'}{\beta_i}) \qquad q_i = \log(\frac{\alpha_i' \beta_i}{\alpha_i \beta_i'}) \tag{3.7}$$

For sparse feature matrices $\mathbf{X}$, the multiplication in Equation 3.6 can be implemented *very efficiently*, lowering the computational complexity of the algorithm to the order of *O(N)*, where $N = |D|$. Even though Bayesian Sets have the same asymptotic complexity as *Spy-EM*, there is practically *no overhead* associated with their execution, making them (by far) the fastest entity expansion algorithm implemented in this project.

The following table provides the top twenty results obtained by applying Bayesian Sets to the MovieLens data set (1643 films described by binary attributes). The query set $Q = \{172, 181, 210\}$ consists of two Star Wars films and an Indiana Jones film (all directed by George Lucas). Bayesian Sets return a range of sci-fi films akin to Star Wars, but the Indiana Jones film is not even in the top twenty results, although its influence (presumably) manifests itself through the presence of films such as the African Queen and Operation Dumbo Drop, which have little to do with the two Star Wars films present in the query.

Film ID	Score	Film Name
181	**9.58508**	**Return of the Jedi (1983)**
50	9.58508	Star Wars (1977)
172	**9.34084**	**Empire Strikes Back, The (1980)**
271	7.99097	Starship Troopers (1997)
498	7.14069	*African Queen, The (1951)*
897	5.20461	Time Tracers (1995)
450	5.20461	Star Trek V: The Final Frontier (1989)
449	5.20461	Star Trek: The Motion Picture (1979)
380	5.20461	Star Trek: Generations (1994)
373	5.20461	Judge Dredd (1995)
230	5.20461	Star Trek IV: The Voyage Home (1986)
229	5.20461	Star Trek III: The Search for Spock (1984)
228	5.20461	Star Trek: The Wrath of Khan (1982)
227	5.20461	Star Trek VI: The Undiscovered Country (1991)
222	5.20461	Star Trek: First Contact (1996)
82	5.20461	Jurassic Park (1993)
62	5.20461	Stargate (1994)
121	5.01092	Independence Day (ID4)
110	4.40121	*Operation Dumbo Drop (1995)*
1239	4.35433	Cutthroat Island (1995)

Users searching for films akin to Star Wars will be satisfied with these results. However, the perceived quality of the ranking produced is highly dependant on the user, as there is no *correct answer* to a query. Indeed, different users might prefer different rankings, given the potential ambiguity of the query sets or the specific user's perception of similarity. Therefore, measuring the quality of the ranking produced is a highly non trivial task, as discussed in subsequent sections.

3.5.1 Iterative Bayesian Sets

As presented in the Evaluation, data augmentation via Bayesian Sets proved to be inferior to *Spy-EM* and *Roc-SVM* in most application areas. In accordance with the evolutionary prototyping paradigm, a final extension to Bayesian Sets was formulated in the last stages of the project.

Blind (pseudo) relevance feedback is a technique for achieving automatic query expansion in information retrieval systems. As used in this problem, the technique applies Bayesian Sets to obtain the ranking of D for the given query set. Then, the top K results in the ranking are added to the query set Q. This process is repeated until a new iteration identifies no new elements to be added to the query set. In the experiments, $K = 30$ and $K \in (0.05N, 0.2N)$ were attempted.

Algorithm 3.2 *Iterative Bayesian Sets*

Input: set of items D, query set $Q = \{\mathbf{x_i}\} \subset D$

1: **function** ITERATIVE BAYESIAN SETS(Q, D)

2: $i \leftarrow 1,\ Q^0 \leftarrow \emptyset,\ Q^1 \leftarrow Q$ ▷ auxiliary variables, the initial query

3: **while** $Q^i \neq Q^{i-1}$ **do** ▷ until the query converges

4: $R_i[1 \dots N] \leftarrow$ Bayesian Sets(Q^i, D) ▷ ranking of D using the i-th query

5: $Q^{i+1} \leftarrow Q^i \cup \{R[1], R[2] \dots R[K]\}$ ▷ add the top K elements to the query

6: $i \leftarrow i + 1$

7: **end while**

Output: $R_f[1 \dots N]$, the ranking of D produced using the final query

In some application areas, as shown in the Evaluation, pseudo relevance feedback managed to improve data augmentation achieved using Bayesian Sets by a substantial margin.

3.6 Application Areas Considered

The extent to which the proposed algorithms can be used to achieve data augmentation was investigated in three different application areas.

3.6.1 Text Classification

Reuters21578 text categorisation collection contains Reuters news documents from 1987, labelled manually by Reuters personnel. The total number of categories is 672, but many of them occur very rarely. Some documents belong to many different categories, others to only one and some have no category at all.

For the purpose of the experiment, a subset of this data set representing feature vectors of the two most frequent labels was used. Hence, we are dealing with binary classification where feature vectors (input) used for classification consist of discrete binary data: each feature vector is represented by 18933 binary features, each indicating the presence of some word in the given article.

Of the three data sets used, this is the '*simplest*' one, in that both categories are abundant in the training data (approximate $3:2$ ratio of the two classes). The training set T_r consists of 4108 articles, whereas the testing set T_s consists of 1660 articles. The distributions of the two classes in the training and testing data sets are the same, and the unlabelled data set U is drawn from the training data set. Consequently, T_r, T_s and U all have the same class distribution.

3.6.2 Prediction of Biomolecular Activity for Drug Design

KDD Cup 2001, Task 1: 'Binding to Thrombin' data set, produced by DuPont Pharmaceuticals Research Laboratories, is related to drug design.

Drugs are usually small organic molecules. The first step in designing a new drug is to identify and isolate the receptor to which the drug should bind. In this case, this is the Thrombin site. The next step in drug design is to test many small molecules to determine which of them are able to bind to that site. These molecules are known as the *active* compounds.

The data set contains examples of both active and inactive compounds. For each compound, a list of binary attributes is provided, each of them describing whether the structure of that molecule possesses a certain three-dimensional property

or not. The goal is to create a classifier able to precisely recognise an active compound given the list of properties that its 3D structure satisfies.

Fundamentally, this task is no different from the text classification one: it deals with binary classification of data consisting of binary attributes and the unlabelled set U is drawn from T_r. However, it is much more challenging for the following reasons:

1. There is a great imbalance between the number of active and inactive compounds in the training data set: only 42 of the 1909 examples represent the active compounds.

2. Even more problematic (at least from a practical perspective) is that the number of binary attributes is *very large*: $139,351$ binary features are used to represent each compound.

3. Finally, the problem exhibits *selection bias*: the distribution of active and inactive compounds in T_r and U differs from the distribution encountered in the testing data set T_s.

3.6.3 Supervised Learning for Theorem Proving

In this problem, related to automated theorem proving, the goal is to use supervised learning to guide an automated theorem prover. The theorem prover available can use five different heuristics to try to prove a first order logic statement. Given attributes for these statements such as the number of variables per logical connective or the average number of times that variables are repeated in the statement, we want to help the prover decide which of the five heuristics would be best for tackling that given statement. [2]

The training data contains attributes for a collection of statements, labelled with information about which of the five heuristics was fastest at proving them. The unlabelled data is the set of problems that *no heuristic* could solve within a certain time limit. An important distinction from the first two application areas is that the attributes describing the examples to be classified are no longer binary, or even discrete: they are now represented by *continuous data*.

In the original work, the problem was treated as five separate supervised learning problems. Our task is to decide which heuristic should be used to attempt to prove a new statement, that is to *classify* new examples into one of these five categories. We are interested in whether a reduction in the classification error

can be achieved using the unlabelled set of statements U to *augment* the (five) labelled sets used for training the classifiers, $T_{r_1} \dots T_{r_5}$.

There were three (new) major challenges associated with this task:

1. The input data is *continuous*, making the use of data augmentation algorithms such as *Spy-EM* impossible, as they require binary attributes as input. Bayesian Sets require stronger assumptions about the model generating the data and still have no *efficient* implementation for continuous data [6]. Therefore, tackling this task was conditional on successful incorporation of the final project extension, the *Roc-SVM* algorithm.

2. The statements provided as input to the classifier are to be labelled with one of the *five* heuristics offered: the one most likely to prove them. Hence, this task deals with *multi-class* classification. As a result, the development of a multi-class classification scheme was another prerequisite for considering this application area.

3. Unlabelled data U does *not* have the same distribution as the training data $T_{r_1} \dots T_{r_5}$. On the contrary, it is the set of statements *not* proved using these heuristics. Therefore, it is questionable whether *this* unlabelled set contains any information applicable to making informed decisions about these heuristics.

3.7 Data Augmentation

Support vector machines were used as the *benchmark classifier* for all three tasks. The SVM is first trained using T_r, the original training data. Then, the algorithm creates the augmented training set T_r^+ by labelling examples from U, the unlabelled set. The new data set is then used to train another SVM. The success of data augmentation is reflected through the *difference in the classification error* between these two classifiers.

As discussed in the Preparation, SVMs support two-group classification of examples with both discrete and continuous features. As such, they can be applied to the first two tasks directly. Task III boasts five different classes, but SVMs can be used to build a multi-class classification scheme as well.

The operation of the data augmentation scheme is the same across all three tasks (Algorithm 4.1, Figure 3.4). For each of the K classes in the training set, the algorithm identifies which examples in U are likely to belong to that class.

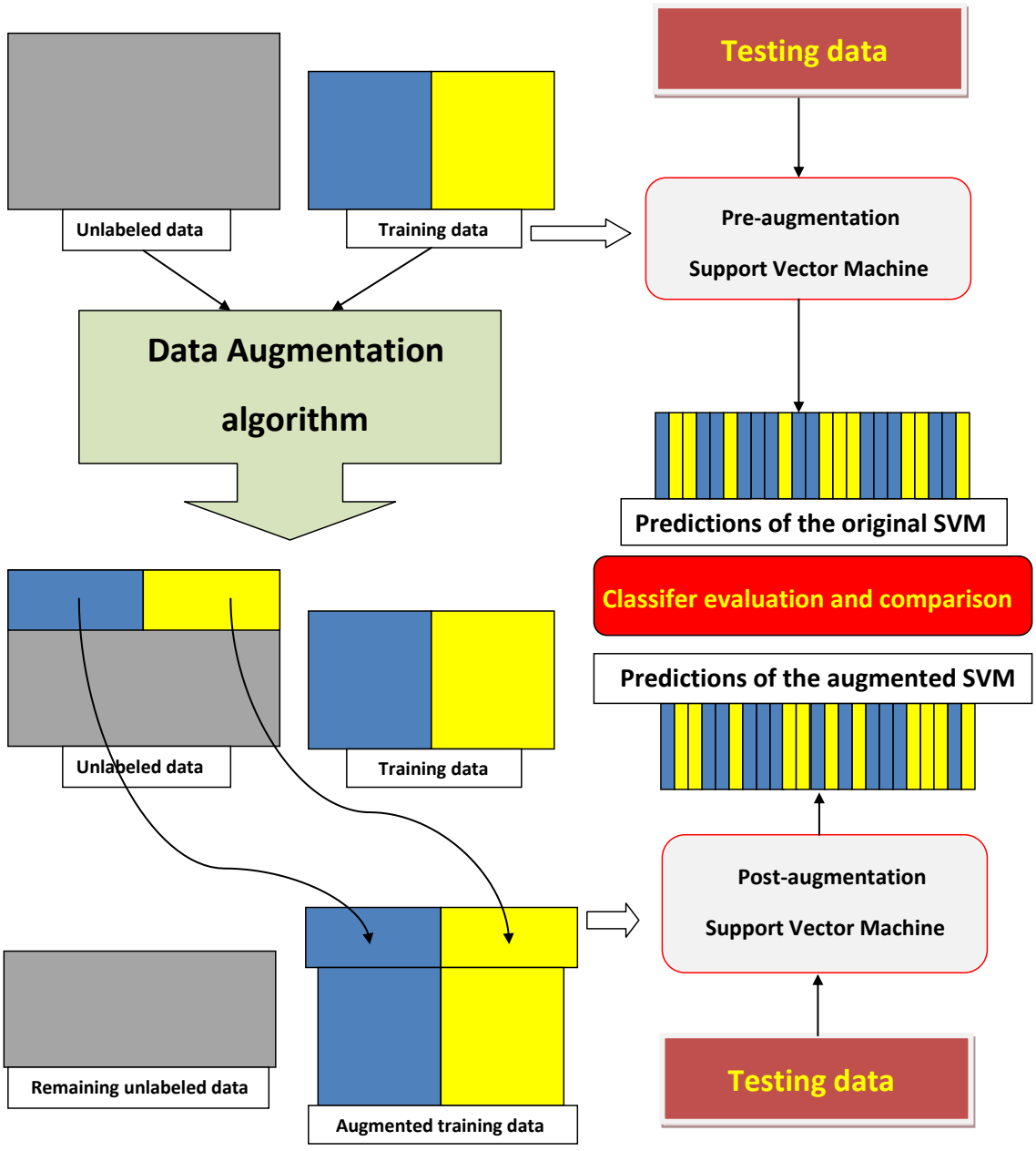


Figure 3.4: Flow diagram of the data augmentation process.

The *hidden members* of each of the K classes are identified using the three entity set expansion algorithms implemented. The set of training examples that belong to the i-th class, T_{r_i}, acts as the positive set to be expanded using the unlabelled set U. The newly identified members of the i-th class are then added to T_{r_i} in order to obtain the augmented set $T^+_{r_i}$.

Support vector machines are very sensitive to noise. Therefore, the success of data augmentation depends on achieving a good trade-off between *creating a (substantially) larger training data set* and *introducing too much noise* (wrongly labelled examples) into the training set. In the experiments, erring on the conservative side (adding *fewer elements* in order to achieve *higher purity* of the augmented data set) proved to be the superior approach.

By definition, PU learning makes no use of the negative classes. However, once the augmented data set T^+_r has been created, our data augmentation scheme tries to extract some marginal utility from the fact that instances of all classes are available. In order to maximise the purity of the augmented set, the algorithm eliminates all examples identified as members of multiple classes from T^+_r (lines 5-11). As shown in the Evaluation, removing these *unreliable examples* from the augmented data set immensely improved the subsequent classification error.

Algorithm 3.2 *Data augmentation*

Input: Training set $T_r = T_{r_1} \cup \ldots \cup T_{r_K}$, unlabelled set U

1: **function** AUGMENTDATA($T_{r_1} \ldots T_{r_K}, U$)

2: **for each** class $i \in (1, K)$ **do** ▷ K = 2 for Tasks I, II; K = 5 for Task III
3: $T^+_{r_i} \leftarrow$ Entity Set Expansion (T_{r_i}, U) ▷ T_{r_i} is used as the positive set
4: **end for**

5: $S \leftarrow \emptyset$
6: **for each** class $i \in (1, K)$ **do** ▷ find all duplicates
7: **for all** $j \in [1, K]$ **do**
8: **if** $i \neq j$ **then** $S \leftarrow S \cup \{T_{r_i} \cap T_{r_j}\}$
9: **end for**
10: $T^+_{r_i} \leftarrow T^+_{r_i} \setminus S$ ▷ remove duplicates
11: **end for**

Output: $T^+_{r_1} \ldots T^+_{r_K}$, the augmented training sets for each class

Of the three methods used to achieve entity set expansion (line 3), there is not much to say about *Spy-EM* and *Roc-SVM* algorithms. As explained in their respective sections, they produce classifiers that decide membership of each of the K classes present in the training set T_r. As such, they yield a subset of U for each class, $T_{r_i}^+$, to be used for augmenting that class in the training set T_{r_i}. After these augmented sets are obtained, all that is left is to make sure that no example from U is introduced into more than one training class. As the K classifiers created provide no information about the preference for membership between classes, the safest approach is to not use these unreliable examples at all (lines 5-11).

Unlike *Spy-EM* and *Roc-SVM*, Bayesian Sets do not provide binary decisions about class membership. Instead, for each of the K classes, they provide a ranking of all elements in U by their likelihood of belonging to that class. As these likelihoods do not represent the actual probabilities, they can not be used to determine a clear cut-off criteria for the number of the top d_i elements in the i-th ranking to be included into each $T_{r_i}^+$. As making an informed decision proved to be very hard, two simple methods for setting the value of d_i were adopted:

1. If the class distributions in T_r and U are the same, the number of elements of each class in U can be reliably estimated from the class distribution observed in T_r.

2. Set each d_i to the number of elements of that class included into the augmented data set $T_{r_i}^+$ by *Spy-EM*. Although this is quite an ad-hoc approach, it has proven useful for the sake of comparing Bayesian Sets to *Spy-EM*, as will be shown in the Evaluation.

Hence, armed with these methods for extracting the hidden members of each class from U, we are almost in a position to start the evaluation of the extent to which data augmentation is possible in each of the suggested application areas.

3.7.1 Multi-class Classification

In Task III, each example $\mathbf{x}$ is represented by a set of (real-valued) metrics of a first order logic statement and belongs to one of the K (five) classes. To achieve data augmentation, we first need to construct f, the classifier deciding which heuristic should be used to attempt to prove an unseen statement $\mathbf{x}'$. Having built that function, *Roc-SVM* can be used for attempting data augmentation, that is reducing the classification error of f.

Two different methods that use SVMs to create multi-class classification schemes have been implemented: *one-vs-all* and *all-vs-all*.

In *one-vs-all classification*, K different classifiers (SVMs) are built. Given a new example $\mathbf{x}$, $f_i(\mathbf{x})$ decides membership of class i (whether $\mathbf{x}$ belongs to class i or not). f_i is trained using T_{r_i} (training examples of class i) as the positive set and $T_r \setminus T_{r_i}$ (the remaining examples) as the negative set. Subsequently, classification is performed using:

$$f(\mathbf{x}) = \underset{i \in 1...K}{\operatorname{argmax}} f_i(\mathbf{x}) \tag{3.8}$$

All-vs-all classification schemes build $\frac{K(K-1)}{2}$ different classifiers to decide preference between all pairs of classes. Let $f_{i,j}$ denote the SVM used to determine preference between classes i and j, trained using T_{r_i} as the positive set and T_{r_j} as the negative set. $f_{i,j}(\mathbf{x}) = 1$ if $\mathbf{x}$ is more likely to belong to class i; otherwise, $f_{i,j}(\mathbf{x}) = -1$. As the final class of an example $\mathbf{x}$, choose:

$$f(\mathbf{x}) = \underset{i}{\operatorname{argmax}} \left(\sum_{j \neq i} f_{i,j}(\mathbf{x}) \right) \tag{3.9}$$

In our experiments, all-vs-all classification managed to outperform the baseline algorithm (always choosing the most frequent class from T_r), whereas one-vs-all *did not*. As a result, the all-vs-all classification scheme based on support vector machines was used as *the benchmark classifier* for Task III.

Chapter 4

Evaluation

This chapter evaluates the performance of the PU algorithms and the data augmentation scheme implemented. The system designed to provide statistically significant insights into the extent to which data augmentation improves classification is presented and used to analyse the three application areas suggested.

The data augmentation scheme presented is based on three different algorithms for achieving entity set expansion. Therefore, the first step in evaluating the performance of this scheme is to determine how well these methods perform entity set expansion in the application areas suggested. Subsequently, an experiment for measuring the extent to which data augmentation can reduce the classification error is presented. The experiment was designed to facilitate direct statistically significant comparison between the three methods. Finally, the specific problem of using each method for data augmentation in each data set is addressed.

In order to reason about the quality of the classifiers produced, both for entity set expansion and in Tasks I - III (application areas), five standard measures were employed. The classifier produced is used to classify all examples in the test set: let TP denote the number of true positives (positives examples classified as such), TN the number of true negatives, FP of false positives (positives classified as negatives) and FN of false negatives. Then, define:

1. *Accuracy*: the proportion of examples (both positives and negatives) classified correctly:

$$ACC = \frac{TP + TN}{TP + TN + FP + FN} \tag{4.1}$$

2. *Classification error*: the proportion of examples classified incorrectly:

$$ERR = \frac{FP + FN}{TP + TN + FP + FN} = 1 - ACC \tag{4.2}$$

3. *Precision* (also known as positive predictive accuracy): the proportion of positives among all elements classified as positive:

$$PR = \frac{TP}{TP + FP} \tag{4.3}$$

4. *Recall* (also known as sensitivity): the proportion of positive examples correctly identified as such:

$$RC = \frac{TP}{TP + FN} \tag{4.4}$$

5. *F-score*: harmonic mean of precision and recall. This measure will be used as a holistic measure of the quality of the classifier:

$$F = \frac{2\ PR\ RC}{PR + RC} = \frac{2\ TP}{2\ TP + FP + FN} \tag{4.5}$$

All of these measures range between 0 and 1, with higher values representing the better ones. *Precision* and *F-Score* are the principle measures we will use to compare the quality of the classifiers produced.

4.1 Entity Set Expansion

The differences in entity set expansion quality between *Spy-EM* and *Roc-SVM* are relatively minor [8]. Therefore, consideration of *Roc-SVM* will be delayed until the next section. The performance of *Spy-EM* and Bayesian Sets will be compared in three different data sets:

1. *20Newsgroups* text categorisation collection. This data set was used for testing and verifying that the implementation of *Spy-EM* produced results comparable to those presented in [11].

2. *Reuters21578* text categorisation collection, used in Task I.

3. *KDD Cup 2001*, Task 1 (Binding to Thrombin) data set, used in Task II.

Table 4.1: Entity Set Expansion in 20Newsgroups data set

Positives in U	**Bayesian Sets**			**Spy-EM**		
	Precision	Recall	F-Score	Precision	Recall	F-Score
90%	0.759	0.846	0.800	0.778	0.866	0.820
67%	0.678	0.893	0.771	0.676	0.891	0.769
20%	0.326	0.946	0.485	0.325	0.942	0.483

Table 4.2: Entity Set Expansion in Reuters21578 data set

Positives in U	**Bayesian Sets**			**Spy-EM**		
	Precision	Recall	F-Score	Precision	Recall	F-Score
90%	0.664	1.000	0.798	0.663	0.999	0.797
67%	0.587	1.000	0.739	0.586	0.998	0.738
20%	0.282	1.000	0.440	0.282	1.000	0.440

As discussed in the Implementation, finding a cut-off criteria for Bayesian Sets is non-trivial. In this section, the second approach is taken: the element count set by *Spy-EM* is reused. Clearly, this boundary does not represent the ideal cut-off for Bayesian Sets. However, it provides a good setting for comparing the purity of the expanded entity sets produced by these two algorithms.

Precision and recall are measures best suited to assess the quality of entity set expansion; accuracy and classification error will be used to assess the subsequent classifiers produced. All three data sets were attempted with several different proportions of positives left in the unlabelled set U, as shown in the tables. The fewer positives are left in U, the worse the subsequent performance is, as clearly shown by the results obtained.

The results obtained in 20Newsgroups and Reuters21578 experiments reveal stark similarities between the performance of these algorithms. With fewer positives left in U and a greater proportion of them in P, the performance of the two algorithms converges, showing that Bayesian Sets can match and even improve on *Spy-EM's* performance. Indeed, given a cut-off criteria tailored for Bayesian Sets, it is not unreasonable to believe that they could be capable of outperforming *Spy-EM*.

Table 4.3: Entity Set Expansion in KDDCup2001 data set

Positives in U	**Bayesian Sets**			**Spy-EM**		
	Precision	Recall	F-Score	Precision	Recall	F-Score
90%	0.264	0.632	0.372	0.286	0.684	0.403
67%	0.194	0.655	0.299	0.225	0.759	0.347
20%	0.060	0.556	0.109	0.072	0.667	0.130

The biomolecular data set is by far the most difficult one used in this project. Unlike the first two data sets, there is a very small number of positive examples in the whole data set. In the three experiments presented, Bayesian Sets exhibit performance inferior to that achieved by *Spy-EM*. The performance of both classifiers is somewhat anomalous: both precision and recall *decrease* with the number of positives revealed to the algorithm. However, the difficulty of this data set must be taken into account when evaluating these results: when only 10% of the positives (4 of them) are revealed, more than half of the positives in U (24 of them) are extracted. As shown later, SVMs do not come close to replicating this performance despite taking *much longer* to train.

4.2 Setting up the Experiment

In order to assess the quality of data augmentation and make statistically significant comparisons between different methods, the experiment setup must ensure that data augmentation via different methods is attempted using the same data sets. Figure 4.1 shows a scheme of the system implemented to evaluate data augmentation in Tasks I, II and III. The body of examples is first split into the training set T and the testing set T_s. The training set is decomposed into the *reduced training set* T_r and the unlabelled set U, with sampling rates of $s = 10\%$, $s = 33\%$ and $s = 80\%$ used to extract T_r in the experiments (Figure 4.1).

The *pre-augmentation* SVM is trained using the reduced training set T_r. The accuracy and F-Score achieved by this classifier on the testing set T_s act as the **baseline** for classifier performance in the experiments: if the data augmentation schemes aid classification, the performance of the classifiers produced must improve on the baseline classifier.

All three schemes attempt to augment T_r using examples from U, each of them producing a separate augmented data set T_r^+. These data sets are used to train

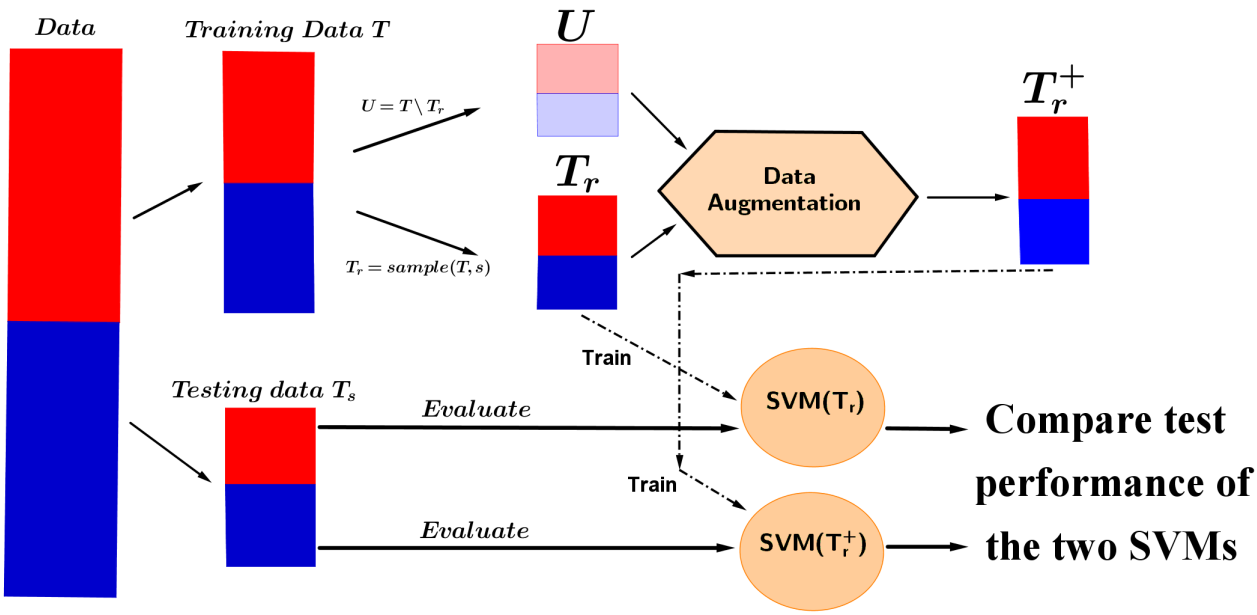


Figure 4.1: The experiment used to evaluate the quality of data augmentation.

their respective *post-augmentation* SVMs. The differences in performance between the *post-augmentation* SVMs and the baseline (*pre-augmentation*) SVM represent the success of the data augmentation achieved in the given experiment.

The **ceiling** for the classifier performance *in all experiments* (for *any sampling rate* s) is determined by training an SVM using the whole training set ($s = 100\%$, $T_r = T$, $U = \emptyset$) and evaluating it using T_s. The post-augmentation SVMs can not outperform this one, as it is trained using the best training set that can be obtained from T_r and U.

If applicable to the specific data set, each of the data augmentation schemes (Bayesian Sets, *Spy-EM*, *Roc-SVM*) is applied to the *same instances (samples)* of T_r and U. Furthermore, the accuracy of the classifiers produced is evaluated against the *same testing set* T_s. As a result, confident assertions about the differences in performance between these three methods can be made:

As long as the testing set T_s is sufficiently large ($|T_s| > 30$), the *Central Limit Theorem* warrants that the distribution of the errors in that sample can be approximated by a Gaussian distribution. If so, the *Z-Score test for comparing learned hypotheses* can be used to establish statistical significance of the differences between classifiers. Let $err_{T_s}(C)$ denote the testing error of classifier C evaluated on T_s. Then, the difference in classification performance between two classifiers C_1 and C_2 is reflected by their *z-score*:

$$\boxed{z = \frac{d}{\sigma_d}} \qquad where \qquad d = |err_{T_s}(C_1) - err_{T_s}(C_2)|$$

$$\sigma_d = \sqrt{\frac{err_{T_s}(C_1)(1 - err_{T_s}(C_1)) + err_{T_s}(C_2)(1 - err_{T_s}(C_2))}{|T_s|}} \tag{4.6}$$

The *z-score* itself represents the distance from the sample mean to the population mean in units of the standard error: each value of z corresponds to some p such that $P[Z > z] = p$, where $Z \sim N(0, 1)$. For any z, the value of the corresponding p can be computed using a standard table of the cumulative distribution of $N(0, 1)$.

This *p-value* represents the probability (significance level) of the *null hypothesis* which assumes that the two samples (classifications of C_1 and C_2) are drawn from the same underlying distribution. When the *p-value* is less than 0.01, the null hypothesis is rejected. If so, the differences between classification accuracies of C_1 and C_2 are due to an underlying cause with a certainty of $100(1-p)\%$. Thus, if $p < 0.01$, these differences have *statistical significance*.

Having implemented this evaluation system, we are finally in a position to make statistically relevant claims about the extent to which this data augmentation scheme reduces classification error in the three application areas suggested.

4.3 Text Classification

The results of data augmentation with the Reuters21578 data set are shown in Table 4.4. *Spy-EM* and *Roc-SVM* achieve *formidable performance*: both improve on the *baseline* in *all* experiments, usually by a substantial margin. The worse the pre-augmentation SVM performance is and the more unlabelled data is available, the greater the *relative improvement* in classification accuracy by *Spy-EM* and *Roc-SVM* is.

The *Z-score test* reveals that the differences between the classifiers produced by *Spy-EM* and *Roc-SVM* are *not statistically significant* ($p > 0.01$ in all of the experiments). On the other hand, the differences between baseline SVMs and the ones produced by these two schemes are statistically relevant in the first two

Table 4.5: Reuters21578 data augmentation without the *purification step*.

$\|\mathbf{T_r}\| : \|\mathbf{T}\|$	**Baseline SVM**		**Bayesian Sets SVM**		***Spy-EM* SVM**		***Roc-SVM* SVM**	
	Accuracy	F-Score	Accuracy	F-Score	Accuracy	F-Score	Accuracy	F-Score
10%	0.855	0.774	0.624	0.642	**0.916**	**0.898**	**0.879**	**0.819**
33%	0.907	0.868	0.783	0.747	**0.934**	**0.916**	**0.929**	**0.899**
80%	0.933	0.906	0.869	0.830	0.922	0.894	**0.942**	**0.921**
Ceiling (100%):	Accuracy: **0.946**				F-Score: **0.926**			

experiments ($p < 0.01$). Thus, these two schemes achieve statistically significant improvements in classification accuracy, with neither of them being the clear favourite.

In cases when only a small amount of unlabelled data is available and the extent to which performance can be improved is negligible (as in the third experiment), these two schemes still manage to improve performance. This *non performance decreasing property* is highly elusive: in such settings, data augmentation schemes usually construct SVMs inferior to the pre-augmentation ones. The reason why these two schemes consistently improve accuracy in this task is that, as explained in Chapter 3, the algorithm *purifies* the augmented set T_r^+ by removing those elements that appear in augmented sets of both classes: $T_r^+ = T_r^+ \setminus \{T_{r_1}^+ \cap T_{r_2}^+\}$.

The performance of the *Spy-EM* scheme deteriorates without the *purification step*: unlike before, *Spy-EM* actually degrades the SVM accuracy in the third experiment (Table 4.5). The *Roc-SVM* scheme was originally designed to perform much more conservative set expansion than *Spy-EM*. As such, it exhibits avid performance even without purification, managing to boost SVM accuracy in all experiments (Table 4.5). According to the *Z-score* test, the differences between these versions of *Spy-EM* and *Roc-SVM* become statistically significant ($p > 0.01$ in 2/3 experiments). Without purification, Spy-EM exhibits more variability in performance: it outperforms *Roc-SVM* in the first experiment but pushes the accuracy below the baseline in the third experiment (Table 4.5).

Bayesian Sets using the number of elements included by *Spy-EM* as the cut-off criteria clearly exhibit vastly inferior performance to *Spy-EM* and *Roc-SVM*. Data

augmentation via Bayesian Sets consistently degrades classification performance. SVMs constructed using the Bayesian Sets' augmented data sets perform below the baseline in all three experiments. Thus, in accordance with the evolutionary prototyping paradigm, the Iterative Bayesian Sets algorithm was designed in an attempt to improve on the original scheme. As can be seen in Table 4.6, the scheme substantially outperforms the original Bayesian Sets one. While being the only data augmentation scheme to actually construct an SVM which *reaches the ceiling performance*, Iterative Bayesian Sets still fall short of matching the *consistent quality* or the *extent* of data augmentation achieved by *Spy-EM* and *Roc-SVM*. In fact, the *Z-Score test* reveals that the differences in performance between pre-augmentation SVMs and the ones produced by this scheme are *not statistically significant*.

Table 4.6: Reuters21578 data augmentation, regular versus Iterative Bayesian Sets.

$\lvert\mathbf{T_r}\rvert : \lvert\mathbf{T}\rvert$	**Baseline SVM**		**Bayesian Sets SVM**		**Iterative BS SVM**	
	Accuracy	F-score	Accuracy	F-Score	Accuracy	F-Score
10%	0.853	0.766	0.722	0.562	**0.856**	**0.772**
33%	0.915	0.877	0.705	0.621	0.910	0.870
80%	0.932	0.905	0.823	0.758	**0.946**	**0.926**
Ceiling (100%):	Accuracy: **0.946**			F-Score: **0.926**		

4.4 Biomolecular Activity Prediction

The goal of this task is to build a classifier identifying active (positive) compounds given information about the 3D structure of their molecules. As the number of negatives vastly exceeds the number of positives in the data set, a high accuracy no longer warrants that the classifier performs the given task well. Indeed, a function classifying all examples as negatives has a high accuracy while being of no use for this task. Instead, the precision and recall of the classifier have to be optimised. Therefore, *F-Scores* were used for comparison of the different classifiers produced.

Table 4.7: Data augmentation in the biomolecular activity prediction data set.

$\lvert\mathbf{T_r}\rvert : \lvert\mathbf{T}\rvert$	**Baseline SVM**			**Bayesian Sets SVM**			***Spy-EM* SVM**		
	Precision	Recall	F-Score	Precision	Recall	F-Score	Precision	Recall	F-Score
10%	0.143	0.007	0.013	0.182	0.120	**0.145**	0	0	0
33%	0.158	0.020	0.036	0.167	0.113	**0.135**	0.118	0.073	**0.091**
80%	0.191	0.027	0.047	0.165	0.107	**0.130**	0.135	0.080	**0.100**
Ceiling (100%):	Precision: **0.294**			Recall: **0.033**			F-Score: **0.060**		

Table 4.7 shows the results achieved using the augmentation schemes based on Bayesian sets and *Spy-EM*. Data augmentation via *Roc-SVM* proved to be intractable for this data set given the computational resources available.

Given the complexity of this data set (139,351 binary features), the amount of data available (1909 examples) did not suffice for the SVM to learn enough about this problem. Therefore, it does not come as a surprise that all baselines, as well as the ceiling of the SVM performance are *incredibly poor*. The underlying cause for this, more than the huge number of features, is that the problem exhibits *selection bias*: T_r contains 2.2% whereas T_s contains 23.6% of positive examples. Consequently, the SVMs trained are very '*reluctant*' to assign positive labels.

Clearly, SVM performance can benefit immensely from the addition of extra positives into T_r. Indeed, in all experiments, both Bayesian Sets and *Spy-EM* raise SVM performance far *above* the ceiling value: Bayesian sets induce at least a *three-fold* increase of the SVM's *F-Score*. The main reason for the enormous scale of this improvement is that adding more positives into T_r mitigates the disastrous effects that *selection bias* has on the subsequent testing error.

SVMs are very susceptible to noise: wrongly labelled examples introduced into an already small training set can completely ruin subsequent SVM performance. This is the case with *Spy-EM* in the first experiment: the post-augmentation SVM reverts to labelling all examples as negatives.

The *Z-Score test* confirms that both schemes improve on the baseline SVMs, as well as on the ceiling SVM. In all three experiments, the differences in the classifiers produced by the two schemes are statistically significant, with Bayesian Sets being the clear favourite.

The performance of the augmented SVMs is still far from impressive. Nonetheless, the *magnitude* of the *relative improvement* in performance achieved by these data augmentation schemes attests to their ability to reduce classification errors in difficult problems without utilising any domain-specific knowledge.

4.5 Supervised Theorem Proving

As explained in the previous sections, data augmentation in this problem could only be attempted using the *Roc-SVM* algorithm. Table 4.8 summarizes the results achieved. As there are five different classes, accuracy is the only metric appropriately reflecting the differences in quality between the classifiers produced.

The results achieved by the baseline and ceiling SVMs are still far from impressive, barely improving on the accuracy of 0.298 achieved by the classifier which always picks the most frequent class. Unlike in the two previous tasks, the SVM performance does not monotonously grow with the size of the training set T_r. In fact, different $T_r = sample(T, s)$ seem to produce classifiers with accuracies randomly scattered around 0.320, obtained using $T_r = T$ for training the SVM.

The insufficient amount of training data is the primary cause for this variability in results. Another reason for the meagre performance exhibited by this classifier is that the voting scheme implemented uses no meaningful mechanism for resolving ties, which occur frequently with only five different classes available.

Table 4.8: Data augmentation in the supervised theorem proving data set.

$\lvert\mathbf{T_r}\rvert : \lvert\mathbf{T}\rvert$	**Baseline SVM**	***Roc-SVM* SVM**
	Accuracy	Accuracy
5%	**0.335**	**0.346**
10%	0.316	**0.369**
20%	0.313	**0.361**
33%	**0.345**	*0.313*
50%	0.259	**0.333**
80%	0.326	*0.201*
Ceiling (100%):	0.320	

Table 4.9: Data augmentation using statements not proven by any of the five heuristics.

$\|\mathbf{T_r}\| : \|\mathbf{U}\|$	**Baseline SVM**	***Roc-SVM* SVM**
	Accuracy	Accuracy (average)
1 : 10	**0.3601**	0.321
1 : 2		0.334
1 : 1		0.337
4 : 1		0.340

The *Roc-SVM* scheme achieves *substantial improvements* in SVM performance when U is significantly larger than T_r (experiments 1, 2, 3). When U is not large enough, the impact *Roc-SVM* has is somewhat arbitrary: it may either degrade (experiments 4,6) or boost SVM performance (experiment 5).

The *Z-Score test* reveals that the differences in performance between baseline SVMs and the ones produced using the *Roc-SVM* scheme are *statistically significant*. However, as the underlying multi-class classifier (based on SVMs) is very susceptible to noise introduced through data augmentation, the post-augmentation SVMs *do not always improve* on the performance achieved by the pre-augmentation ones.

Therefore, applying the *Roc-SVM* augmentation scheme makes sense only when the amount of unlabelled data *greatly exceeds* the amount of labelled data available. Indeed, only when U was much larger than T_r (experiments 1,2,3) did the *Roc-SVM* scheme consistently *improve* SVM performance over many repetitions of these experiments.

An additional data set from the original work [2] was available for the purposes of evaluation. Examples in U' consist of features of FOL statements that none of the heuristics could prove within a specified time limit. As these statements do not belong to any of the five classes, data augmentation using subsets of U' only degraded the accuracy of the SVM produced (Table 4.9). The more of the examples from U' were introduced, the more the classification accuracy suffered.

Chapter 5

Conclusion

The principle goal of this project was to investigate the extent to which *data augmentation* using semi-supervised learning algorithms can improve classification performance. The final data augmentation scheme substantially improves classification accuracy in all of the application areas considered.

The initial success criteria consisted of implementing Bayesian Sets and *Spy-EM* and using them for data augmentation in different application areas. The project itself was highly underspecified since two of the data sets were not available until the later stages of the project. Hence, in accordance with the evolutionary prototyping paradigm adopted, the data augmentation system was built incrementally, developing progressively harder augmentation schemes and evaluating them using progressively harder data sets until all the success criteria were satisfied.

During the early stages of the project, Bayesian Sets were envisioned as the chief instrument for achieving entity set expansion. Further research indicated that partially supervised learning algorithms such as *Spy-EM* could be used to build data augmentation schemes with formal grounding in computational learning theory (Appendix A).

The *RocSVM* algorithm was identified as the only method capable of operating on data sets with real-valued attributes. As a result, it was incorporated into the project goals. The implementations of these entity expansion algorithms produced results comparable to those obtained in [6, 8, 10].

The subsequent data augmentation scheme utilises these algorithms to *augment* the *training data* of support vector machines used to perform the classification itself. A substantial amount of effort was put into further refining Bayesian Sets and establishing an appropriate *cut-off criterion* for their ranking.

The final system built to evaluate these schemes was designed to provide *statistically significant* results about the extent to which data augmentation affected classifier performance. It was successfully implemented and applied to the three application areas proposed:

1. **Text classification:** the schemes based on *Spy-EM* and *Roc-SVM* achieved substantial improvements in classification: both of them produced SVMs with performance levels comparable to the ceiling performance. Bayesian Sets proved to be inadequate for this data set, not managing to improve accuracy even after pseudo relevance feedback was used to improve the original augmentation scheme.

2. **Biomolecular activity prediction:** Bayesian Sets and *Spy-EM* achieved *formidable results*, improving classification accuracy by *an order of magnitude*. Not only did this scheme effectively utilise the unlabelled data to expand the training set, but it managed to mitigate the negative effects that the *selection bias* had on classification, thus confirming the claims given in [9]. Furthermore, Bayesian Sets revealed their underlying potential by outperforming *Spy-EM* using a very ad-hoc cut-off criterion.

3. **Supervised theorem proving:** this part of the project dealt with a *continuous* data set consisting of five different classes. A multi-class classification scheme based on SVMs was implemented and the *Roc-SVM* augmentation scheme successfully improved its classification accuracy using unlabelled data drawn from a separate subset of training data. Subsequently, the system built revealed that the body of unlabelled examples available from the original research project could not be utilised to achieve data augmentation in the original work.

In addition to providing an open-source library for achieving entity set expansion and data augmentation in arbitrary data sets, work on this project generated some interesting ideas for further research:

- **Spy Bayesian Sets**: Bayesian Sets provide the most efficient scheme out of the ones implemented. However, their performance is inhibited by the absence of a clear criterion for establishing the cut-off point in the rankings produced. The use of *spy positives* for extracting *reliable negatives* proved to be instrumental for the success of *Spy-EM* and *Roc-SVM*. Hence, incorporating this idea into (Iterative) Bayesian Sets may yield an entity set expansion algorithm superior to all algorithms considered in this project.

- **Further evaluation:** the results obtained in this project clearly show that the augmentation schemes developed reduce the classification error when support vector machines are used as the underlying classifiers. However, to establish the applicability of this scheme to real world supervised learning problems, a thorough investigation of its impact on application-specific classifiers tailored to each of the application areas should be conducted.

Bibliography

[1] Christopher M. Bishop. *Pattern Recognition and Machine Learning*. Springer-Verlag, New York, NY, USA, 2006.

[2] James P. Bridge, Sean B. Holden, and Lawrence C. Paulson. Machine learning for first-order theorem proving: learning to select a good heuristic. *Submitted to Journal of Automated Reasoning*, 2013.

[3] V. Castelli and T. Cover. On the exponential value of labeled samples. *Pattern Recognition Letters 16:105-111*, 1995.

[4] Olivier Chapelle, Bernhard Schlkopf, and Alexander Zien. *Semi-Supervised Learning*. MIT Press, Cambridge, MA, USA, 2006.

[5] Alan M. Davis. Operational prototyping: A new development approach. *IEEE Software, Volume 9 Issue 5, September 1992*, 1992.

[6] Zoubin Ghahramani and Katherine A. Heller. Bayesian sets. *Advances in Neural Information Processing Systems 18*, 2006.

[7] Benjamin Letham, Katherine Heller, and Cynthia Rudin. Growing a list. *Submitted to ICML*, 2013.

[8] Xiao-Li Li and Bing Liu. Learning to classify text using positive and unlabeled data. *Proceedings of Eighteenth International Joint Conference on Artificial Intelligence*, 2003.

[9] Xiao-Li Li, Bing Liu, and See-Kiong Ng. Negative training data can be harmful to text classification. *Proceedings of the 2010 Conference on Empirical Methods in Natural Language Processing*, 2010.

[10] Xiao-Li Li, Bing Liu, Lei Zhang, and See-Kiong Ng. Distributional similarity vs. pu learning for entity set expansion. *Proceedings of the ACL 2010 Conference Short Papers*, 2010.

[11] Bing Liu, Wee Sun Lee, Philip S Yu, and Xiao-Li Li. Partially supervised classification of text documents. *Proceedings of the Nineteenth International Conference on Machine Learning*, 2002.

[12] Kamal Nigam, Andrew McCallum, Sebastian Thrun, and Tom Mitchell. Learning to classify text from labeled and unlabeled documents. *Proceedings of the Fifteenth National Conference on Artificial Intelligence*, 1998.

[13] Leslie Valiant. A theory of the learnable. *Machine Learning, 20*, 1984.

[14] V. Vapnik and A. Chervonenkis. On the uniform convergence of relative frequencies of events to their probabilities. *Theory of Probability and its Applications, 16*, 1971.

[15] Vladimir Vapnik and Corinna Cortes. Support-vector networks. *Machine Learning, 20*, 1995.

Appendix A

Computational learning theory

This appendix contains the theoretical arguments used to justify the use of partially supervised learning to achieve data augmentation, as attempted in this project. It contains proofs of two major arguments. Informally:

1. Partially supervised learning can yield *arbitrarily* good classifiers.
2. Unlabelled data carries information relevant to the task of classification.

Furthermore, this appendix introduces the relevant concepts in computational learning theory, such as the PAC learning framework and the VC dimension.

A.1 Theoretical Foundation of Partially Supervised Learning

This section provides a theoretical foundation of partially supervised learning, as framed in Chapter 3.2.

Let X denote the space of feature vectors of possible instances and let $Y = \{0, 1\}$ denote the set of possible outcomes: 1 for positives, 0 otherwise. Assume that all of the examples $(x, y) \in X \times Y$ are independently and identically distributed random variables drawn from some fixed probability distribution over $X \times Y$.

Let $\Pr_D[A]$ denote the probability of event A if the examples are drawn from some probability distribution D. For a finite set of examples L, let $\Pr_L[A]$ denote the probability of event A if the examples are uniformly drawn from L.

The input of the algorithm consists of the positive set P with n_1 elements drawn from $D_{X|Y=1}$, the conditional distribution of all positives, and the unlabelled set U with n_2 elements drawn from D_X, the marginal distribution on X.

The learning algorithm produces the classifier by choosing a function f from the class of functions $F : X \to \{0, 1\}$. The task of learning is equivalent to the task of minimising the expected error of f, that is the probability that the chosen classifier f makes a wrong prediction.

The best possible classifier of all $f \in F$ is the one that minimises the expected error, that is the probability of making wrong predictions:

$$
\begin{aligned}
\Pr[f(X) \neq Y] &= \Pr[f(X) = 1 \wedge Y = 0] + \Pr[f(X) = 0 \wedge Y = 1] \\
&= \Pr[f(X) = 1] - \Pr[f(X) = 1 \wedge Y = 1] + \Pr[f(X) = 0 \wedge Y = 1] \\
&= \Pr[f(X) = 1] - \Pr[Y = 1] + \Pr[f(x) = 0 \wedge Y = 1] + \Pr[f(X) = 0 \wedge Y = 1] \\
&= \Pr[f(X) = 1] - \Pr[Y = 1] + 2\Pr[f(x) = 0 \wedge Y = 1] \\
&= \Pr[f(X) = 1] - \Pr[Y = 1] + 2\Pr[f(x) = 0 \mid Y = 1]\Pr[Y = 1]
\end{aligned}
$$

The first thing to note is that $\Pr[Y = 1]$ is constant. Therefore, minimising the expression given above involves simultaneously minimising $\Pr[f(X) = 0 \mid Y = 1]$ and $\Pr[f(X) = 1]$. However, (X, Y) is drawn from D, which we know nothing

about. Hence, to obtain a method of choosing the best classifier, we need to transform the task of minimising the error across D to one that deals only with the sets P and U. Intuitively, we can only hope to find a *good* approximation to the best classifier given limited knowledge of D (obtained through P and U).

We shall focus on the *noiseless case*: classification settings such that there exists $f_t \in F$ such that $Y = f_t(X)$ for every example (X, Y) drawn from D. The noisy case, where all labels Y are flipped with some probability and the target classification function $f_t \notin F$ is presented in [11].

We want to relate the task of finding a *good* classifier $f \in F$ to the task of minimising $\sum_{i=1}^{n_2} f(X_i)$ (where $X_i \in U$) while maximising $\Pr_P[f(X) = 1]$ at the same time. Therefore, we need to find conditions on the sizes of P and U, n_1 and n_2, under which the function that chooses f by minimising $\sum_{i=1}^{n_2} f(X_i)$ generalises well, that is achieves *good* expected precision and recall across all examples drawn from D.

Formally, we can set this problem in the *probably approximately correct* (PAC) framework [13]: if the target function is any $f_t \in F$, the learning algorithm A needs to produce a function $f \in F$ such that, given enough training data, $\forall \epsilon > 0, \delta > 0. \Pr[E[f(X) \neq f_t(X)] > \epsilon] \leq \delta$. If A can do this for any $f_t \in F$, then A represents a *PAC learning algorithm* for F. However, before we can formally reason about the class of functions F, we need to provide a formal measure of how complicated these classes can be.

Vapnik Chervonenkis (VC) dimension is a measure of the capacity of the probability model used for classification. It is defined as the cardinality of the largest set of examples that the algorithm can *shatter*. An algorithm can *shatter* a set of training examples $T = \{(x_1, y_1) \ldots (x_n, y_n)\}$ if for all potential label assignments to $y_1 \ldots y_n$ there exists some $f \in F$ which makes no classification errors when evaluating T. If T is the greatest set that can be shattered using elements of F, then n represents the VC dimension of F.

The VC dimension reflects the power of the classifier used. A high VC dimension means that a classifier can model complex classifiers but might overfit, whereas a low VC dimension reduces the risk of overfitting but also restricts what the classifier can model. The VC dimension does not depend on the training set used, but solely on the maximum *number* of data points that the model can classify without making an error. Hence, it is an *inherent property* of the function class used to represent the classifiers produced by the learning algorithm. The utility

of VC dimensions stems from the fact that they can be used in conjunction with the training error to obtain a *probabilistic upper bound* on the subsequent testing error for the classifier, that is the classification error on new, unseen data. [14]

For the function class of our classifier $F : X \to \{0, 1\}$ it must hold that $VC(F) \leq \log_2(F)$, as there are two possible label assignments to each $x_i \in X$. Similarly, the Naive Bayes classifier has a VC dimension of no more than $2m+1$, where m represents the number of words used in the classifier [11]. The VC bounds presented henceforth are *not exact*; they are used as an illustration of the rate at which sample sizes have to grow so that the chosen classifier f becomes arbitrarily close to the ideal one, f_t.

Finally, let A' be the algorithm that chooses f by minimising $\sum_{i=1}^{n_2} f(X_i)$. The conditions for A' to be a *PAC learning algorithm* for the *concept class* represented by $F : X \to \{0, 1\}$ are given by the following theorem [11]:

Theorem 1 *Let F be a permissible[1] class of functions of VC dimension d. Let $f_t \in F$ be the target function and let $\nu = E[f_t(X)]$. Let the sets P and U consist of n_1 and n_2 random variables drawn from $D_{X|Y=1}$ and D_X, respectively. Take any $\epsilon > 0$, $\delta > 0$ and assume that $n_1, n_2 > \frac{16}{\epsilon} d \ln(\frac{16e}{\epsilon} \ln \frac{16e}{\epsilon}) + \ln(\frac{24}{\delta})$. Let F' be the subset of F such that all members of F' achieve perfect recall on P. If $f' = \operatorname{argmin}_{f \in F'} \sum_{i=1}^{n2} f(Z_i)$ then with probability of at least $1 - \delta$, it holds that:*
$ER(f') > 1 - \epsilon$ *and* $EP(f') > \frac{(1-\epsilon)\nu}{(1+9\epsilon)\nu+4\epsilon}$ *and* $\mathrm{E[f'(X)} \neq f_t(X)] < (10\nu + 4)\epsilon$.

Proof. To prove this theorem, start from the following one:

Theorem 1.1(Haussler, 1992) *Let $F : Z \to \{0, 1\}$ be a permissible[1] class of functions with VC dimension d. Let $(X_1, Y_1) \ldots (X_n, Y_n)$ be independent identically distributed random variables. For any $\epsilon > 0$, if Φ denotes*

$$\Pr\left[\exists f \in F : \left|\frac{1}{n}\sum_{i=1}^{n} f(X_i, Y_i) - E[f(X, Y)]\right| > \alpha\left(\frac{1}{n}\sum_{i=1}^{n} f(X_i, Y_i) + E[f(X, Y)] + \nu\right)\right]$$

$$\text{then } \Phi \leq 8\left(\frac{16e}{\alpha\nu}\ln\frac{16e}{\alpha\nu}\right)^{d} e^{-\alpha^2\nu n/8}.$$

Therefore, the probabilistic upper bound on the error decreases with the size of the training set n. Thus, if we set the parameters $\alpha = \frac{1}{2}$ and $\nu = 2\epsilon$, and try to substitute the upper bound on the error with any $\delta > 0$, Haussler's theorem specialises to the following claim:

[1] A function class measurability condition not relevant in practice [11].

Corollary 1 *Let F be a permissible class of functions of VC dimension d and let $T = X_1 \ldots X_n$ be a set of independently and identically distributed random variables. By Haussler's theorem, if $n > \frac{16}{\epsilon}\left(d\ln(\frac{16e}{\epsilon}\ln\frac{16e}{\epsilon}) + \ln\frac{8}{\delta}\right)$, then:*

$$\Pr\Big[\ \exists f \in F : (E[f(X) \neq f_t(X)] > 3\Pr_T[f(X) \neq f_t(X)] + \epsilon) \vee \\ (\Pr_T[f(X) \neq f_t(X)] > 3E[f(X) \neq f_t(X)] + \epsilon) \quad \Big] \ \leq\ \delta.$$

The *two separate events in this expression* distinguish between large training errors and overfitting, thus providing a unifying expression for achieving *Structural Risk Minimisation*. Algebraically, the two events result from removing the absolute values present in Haussler's theorem.

Finally, we are in a position to prove Theorem 1:

From Corollary 1, we know that if $n_1 > \frac{16}{\epsilon}\left(d\ln(\frac{16e}{\epsilon}\ln\frac{16e}{\epsilon}) + \ln\frac{24}{\delta}\right)$, then $\boxed{ER(f') \geq 1-\epsilon}$ with probability of at least $1-\delta/3$, as required in the theorem statement. Consequently, $\Pr[f'(X) = 0 \wedge Y = 1] \leq \epsilon\nu$.

From $f' = \text{argmin}_{f\in F'}\sum_{i=1}^{n2} f(Z_i)$ it follows that $\Pr_U[f'(X) = 1] \leq \Pr_U[Y = 1]$:

$$\begin{aligned}
&\Leftrightarrow\ \Pr_U[f'(X) = 1 \wedge Y = 0] + \Pr_U[f'(X) = 1 \wedge Y = 1] \leq \Pr_U[Y = 1] \\
&\Leftrightarrow\ \Pr_U[f'(X) = 1 \wedge Y = 0] \leq \Pr_U[Y = 1] - \Pr_U[f'(X) = 1 \wedge Y = 1] \\
&\Leftrightarrow\ \Pr_U[f'(X) = 1 \wedge Y = 0] \leq \Pr_U[f'(X) = 0 \wedge Y = 1].
\end{aligned}$$

Similarly (again via Corollary 1), if $n_2 > \frac{16}{\epsilon}\left(d\ln(\frac{16e}{\epsilon}\ln\frac{16e}{\epsilon}) + \ln\frac{24}{\delta}\right)$ then with probability of at least $1-\delta/3$, it holds that:

$$\Pr_U[f'(X) = 0 \cap Y = 1] \leq 3\Pr[f'(X) = 0 \cap Y = 1] + \epsilon \ \textit{and}$$
$$\Pr[f'(X) = 1 \cap Y = 0] \leq 3\Pr_U[f'(X) = 1 \cap Y = 0] + \epsilon.$$

Combining the expressions obtained thus far:

$$\Pr[f'(X) = 1 \wedge Y = 0] \leq 3(\ 3\Pr[f'(X) = 0 \wedge Y = 1] + \epsilon\ ) + \epsilon \leq 9\epsilon\nu + 4\epsilon$$

Hence, with probability of at least $1-\delta$, ($1-\delta/3$, even) the *probability of error* can be bounded by:

$$\Pr[f'(X) \neq Y] = \Pr[f'(X) = 0 \wedge Y = 1] + \Pr[f'(X) = 1 \wedge Y = 0] < \\ < \nu\epsilon + 9\epsilon\nu + 4\epsilon = \boxed{10\epsilon\nu + 4\epsilon}, \text{ as required.}$$

Finally, using these results, one can show that the *expected precision* converges to the optimal one at the rate suggested by Theorem 1:

$$
\begin{aligned}
EP(f') &= \Pr[Y = 1 \mid f'(X) = 1] = \frac{\Pr[Y = 1 \wedge f'(X) = 1]}{\Pr[f'(X) = 1]} \\
&= \frac{\Pr[Y = 1 \wedge f'(X) = 1]}{\Pr[f'(X) = 1 \wedge Y = 0] + \Pr[f'(X) = 1 \wedge Y = 1]} \\
&= \frac{\Pr[Y = 1 \wedge f'(X) = 1]}{\Pr[f'(X) = 1 \wedge Y = 0] + \Pr[Y = 1] - \Pr[f'(X) = 0 \wedge Y = 1]} \\
&\geq \frac{ER(f') \Pr[Y = 1]}{\Pr[f'(X) = 1 \wedge Y = 0] + \Pr[Y = 1]} > \boxed{\frac{\nu - \nu\epsilon}{(1 + 9\epsilon)\nu + 4\epsilon}}
\end{aligned}
$$

□

A.2 Theoretical Foundation of Data Augmentation

In this section, a probabilistic framework for describing the classifiers and observations (training/testing data) [12] will be used to give a theoretical grounding for data augmentation:

A *mixture distribution* is the probability distribution of a random variable whose probability density function is a linear combination of density functions of other random variables. Given a finite set of probability density functions $p_1(x)...p_n(x)$ and weights $w_1...w_n$ such that $w_i \geq 0$ and $\sum_{i=1}^{n} w_i = 1$, the probability density function of the mixture distribution is given by: $f(x) = \sum_{i=1}^{n} w_i p_i(x)$. The cumulative distribution function of the mixture distribution is defined analogously.

A *mixture model* is a mixture distribution that represents the probability distributions of observations in the overall population, without requiring that the set of observations identifies the sub-population that an observation belongs to. Unlike mixture distributions, which are used to derive properties of the overall population from the properties of sub-populations, mixture models are used to perform statistical inference about properties of specific sub-populations given only observations on the entire population, without the sub-population membership information revealed.

We shall assume that all of our data was produced by a mixture model, and that there exists a one to one correspondence between its generative components (underlying random variables) and the classes (corresponding to labels).

Under these assumptions, every observation d_i is generated according to a probability distribution given by a mixture model parametrised by θ. The mixture model consists of generative components $c_j \in C$, where $C = \left\{c_1, ..., c_{|C|}\right\}$, and each of these components is parametrised by a disjoint subset of θ. Therefore, an observation is obtained by first selecting a component according to the prior probabilities $P(c_j|\theta)$ and then having that component generate an observation according to its conditional distribution $P(d_i|c_j;\theta)$. Therefore, the probability of any observation d_i can be expressed as a weighted sum over all generative

components:

$$P(d_i|\theta) = \sum_{j=1}^{|C|} P(c_j|\theta)P(d_i|c_j;\theta) \tag{A.1}$$

By our assumption of one to one correspondence between classes and generative components, c_j denotes both the j-th generative component and the j-th class. Let y_i denote the class label for the i-th observation. If observation d_i was generated by component c_j, we enforce the correspondence: $c_j = c_{y_i}$. These class labels are known only for labelled data.

In this environment, the problem of learning concept classes is equivalent to estimating the parameters of the mixture model which produced the given set of observations. Therefore, to prove that unlabelled data is useful for learning concept classes, it suffices to show that it carries information about the parameters θ. This will hold if and only if the learning task is not *degenerate*:

$$\exists d_i, c_j, \theta', \theta''.P(d_i|c_j;\theta') \neq P(d_i|c_j;\theta'') \wedge P(c_j|\theta') \neq P(c_j|\theta'') \tag{A.2}$$

The set of tasks which fail this condition (those tasks for which any parametrisation yields the same outcomes) corresponds to the set of tasks for which learning is impossible. High-dimensional mixture models (such as Gaussian mixture models) always satisfy this condition.

To show that the unlabelled data carries information about the parameters θ, we need to show that θ and D are conditionally dependent, D being the random variable representing the probability distribution of the unlabelled observations:

We need to show $P(\theta|D) \neq P(\theta)$. Assume the opposite, that $P(\theta|D) = P(\theta)$. Hence, $\forall\theta'.P(\theta'|D) = P(\theta')$. Therefore, any two parametrisations θ' and θ'' provide the same *class probabilities* for any observation.

Applying Bayes' rule to our assumption, we find that $\forall\theta', \theta'', P(D|\theta') = P(D|\theta'')$. Substituting this into equation 1.1, we obtain:

$$\forall\theta', \theta''. \sum_{j=1}^{|C|} P(c_j|\theta')P(d_i|c_j;\theta') = \sum_{j=1}^{|C|} P(c_j|\theta'')P(d_i|c_j;\theta'') \tag{A.3}$$

Our non-degeneracy condition(1.2) requires that there must exist an observation d_i such that some of its individual terms in equation 1.3 differ for some parametrisations θ' and θ''. If this is the case, the total probability of the observation must be different with these different parametrisations as well.

This contradicts our conditional independence assumption. Therefore, it follows that $P(\theta|D) \neq P(\theta)$. The parametrisations are conditionally dependent on the observations. This means that unlabelled data *does* carry information about the parameters of the generative model.

Appendix B

Project Proposal

Introduction and Description of the Work

Fundamentally, there exist two different types of tasks in machine learning, based on the desired outcome of the machine learning algorithm: *unsupervised* and *supervised* learning.

Unsupervised learning algorithms are presented with the list of inputs to the function, $x_i \in X$, and the goal of the algorithm is to infer interesting structure from this data. It is typically assumed that the points are drawn i.i.d.(independently and identically distributed) from a common distribution on X. Essentially, the task of unsupervised learning is to estimate the probability density function of that distribution (assuming one exists).

Supervised learning algorithms generate a function $f : X \to Y$ that maps potential inputs to desired outputs, also known as labels. The desired function maps any $x_i \in X$ to a specific label $y_i \in Y$. The algorithm is trained using a list of input-output pairs (x_i, y_i). In the case where the set of labels Y is finite, the problem is known as classification; otherwise, the problem is known as regression.

The basic assumption of supervised learning is that the (x_i, y_i) pairs are independent and identically distributed random variables drawn from an underlying probability distribution on $X \times Y$. The function f obtained by learning from the training data tries to capture the probability density function of this distribution. The main condition required for supervised learning to work (i.e. to be able to generalise from a finite training set to potentially infinitely many "unseen" test

cases) is that the *smoothness assumption of supervised learning* holds. Informally, the condition is that if the points x_1 and x_2 are *close*, their corresponding outputs y_1 and y_2 should be *close* as well.

After estimating $p(x|y)$ using an unsupervised learning procedure, the predictive density can then be inferred using *Bayes theorem*:

$$p(y|x) = p(y)\frac{p(x|y)}{\int_y p(x|y)p(y)\mathrm{d}y} \tag{B.1}$$

This equations forms the basis of *Bayesian inference*, a method in which Bayes' rule is repeatedly used to update the probability estimate for a hypothesis as additional evidence is obtained. It rests on the *Bayesian interpretation* of the concept of probability, which regards it as an abstract quantity either theoretically assigned for representing a certain state of knowledge, or calculated from previously assigned probabilities. This contrasts the traditional *frequentist* view which defines the probability of an event as the limit of its relative frequency in a large number of trials.

Semi-supervised learning algorithms combine these two approaches. The data set X consists of $X_l = (x_1, ..., x_l)$, the set for which the set of labels $Y_l = (y_1, ..., y_l)$ is known, and the set of unlabeled data $X_u = (x_{l+1}, ..., x_{l+u})$. Given this data sets as input, the algorithm tries to create the same prediction function as in the case of supervised learning. However, in addition to using the labeled data for training, it attempts to use the unlabeled data to increase the quality of the prediction. The unlabeled data can increase the quality of the prediction only if the distribution of $p(x)$ observed from the unlabeled data carries information that is useful in the inference of $p(y|x)$.

To formalize this notion, we generalise the supervised learning case to obtain the *semi-supervised smoothness assumption*: If x_1 and x_2 are points that are *close* to each other in a *high density region*, then their corresponding outputs y_1 and y_2 should be *close* as well. By transitivity, it follows that all points in the same *cluster* are likely to have their respective outputs clustered as well.

Data augmentation refers to a family of methods that construct iterative algorithms by introducing unobserved training data. In general, constructing data augmentation schemes that result in both simple and fast algorithms is a highly non-trivial task, as successful strategies vary greatly with the type of data models used in the specific application. It is a common problem in semi-

supervised learning, and the following problem is one of its best known instances, often encountered in problems such as classification of text documents:

Entity set expansion problem: Given a set S of seed entities of a particular class S and a set D of candidate entities, we wish to determine which of the entities in D belong to S. In other words, we expand the set S based on the given seeds.

There is a class of semisupervised learning algorithms that learns from a set of *positive* examples P and a set of *unlabeled* examples U(*PU learning*). The key characteristic of PU learning is that there is *no negative training example* available for learning. This is contrary to the typical classification context, in which the training data consists of a series of examples of *every possible class*.

The problem of *entity set expansion* maps directly to PU learning: the set of seed entities S is the set of positive examples P, whereas the set of candidate entities D maps directly to the set of unlabeled examples U. This means that the existing body of algorithms developed for *PU learning* is directly applicable to entity set expansion, providing a good way to assess the performance of novel approaches to this problem by comparing their performance to the already established ones.

Bayesian sets(Ghahramani et al, 2005) take an information retrieval inspired approach to the problem of entity set expansion. A *relevance criterion* for each $d \in D$ is defined, calculated, and used to sort all the unlabeled data in D in order of the likelihood that they are of the same class as the elements of the candidate set S. This relevance criterion is based on the current understanding of patterns of generalisation in human cognition:

$$score(\mathbf{x}) = \frac{p(\mathbf{x}|D_s)}{p(\mathbf{x})} \tag{B.2}$$

where $D_s \subset D$ represents the concept class of entities of class S. D represents the universe of all entities in this data model.

The input of the Bayesian sets algorithm consists of the set of items D, a probabilistic model $p(\mathbf{x}|\theta)$, $x \in D$, and a prior on the model parameters $p(\theta)$. The query given to the algorithm is the set $D_s = \{x_i\} \subset D$.

The algorithm calculates the $score(x)$ for all $x \in D$. Subsequently, it returns this list of elements as output, sorted by decreasing scores. Each of these scores represents the probability that the specific element belongs to the concept class D_s.

Clearly, the core complexity of this algorithm lies in computing the *score* function. For simple models in which $p(\mathbf{x}|\theta)$ has an independent Bernoulli distribution for all of the candidate's features ($x_i \in \mathbf{x}$) the computation of all the scores can be reduced to a single sparse matrix multiplication. Even using this simple model Bayesian sets exibit avid performance.

The mathematics involved in the computation of the scores is quite involved and will not be further examined here. However, it is important to note that the computational complexity of Bayesian sets is linear with respect to the size of D, even when $p(\mathbf{x}|\theta)$ uses a distribution from the exponential family. The Bayesian sets algorithm is very flexible; it can be used for a wide variety of data (discrete, continuous, text) and with different probabilistic models.

S-EM algorithm: An interesting classifier alternative to Bayesian sets (which are a *ranking algorithm*), is presented in (Partially Supervised Classification of Text Documents, Liu et al., 2002). The algorithm proposed is called the *S-EM algorithm*. It is based on repeated applications of the *Naive Bayesian* classifier and the *Expectation-Maximisation* algorithm, details of which will be omitted here. The algorithm first runs a reinitialisation phase which "grows" the positive set P using an NB classifier trained with the current perception of P to find other likely members of the positive set. It repeats this step until the algorithm converges, i.e. the naive classifier can't find any new members of the positive set.

Subsequently, the algorithm proceeds by using a "spy" technique to identify *reliable negatives(RN)* in the unlabeled set U. This is achieved by training another NB classifier with only a portion of the positive set $P_1 \subset P$. Then, we can track the behaviour, i.e. the subsequent classification of the members of $P \setminus P1$ by the Naive Bayesian classifier. If we assume that the hidden positives in U that we're trying to identify behave similarly to elements of $P \setminus P1$, we can identify some *reliable negatives* from the set U, which are then used to re-train the classifier until it converges to produce the final entity set. The paper contains a theoretical foundation for partially supervised classification, as well as an experimental evaluation of S-EM algortihm's F-Score $F = \frac{pr}{p+r}$, where p is the precision, and r is the recall achieved. This gives us ample justification to use this algorithm as a frame of reference for assessing the performance of Bayesian sets.

(Distributional Similarity vs. PU Learning for Entity Set Expansion, Li et al., 2010) claims that the bidirectional pull of the constructed classifier makes it

superior to ranking methods such as Bayesian sets. Furthermore, they propose an interesting, non-trivial assertion that classification methods produce superior results to ranking methods in general. Even though the S-EM algorithm is at the moment applicable only to text classification, it would be interesting to try to extend it to other data sets supported by Bayesian sets and compare their performance on those data models in an attempt to gain further insight into this proposition.

Resources Required

The most suitable language for implementing these algorithms is *Matlab*. *R* is a viable alternative. We shall aim to implement the whole project in Matlab, potentially adding R interoperability for certain aspects of the projects.

The project will be completed in cooperation with Dr Holden's collaborator, Dr Matthew Trotter of the Celgene Institute for Translational Research Europe (CITRE), Sevilla, Spain. The data set required to examine protein localization and interactions will be provided by Dr Holden's current collaborators at the Anne McLaren Laboratory for Regenerative Medicine. The data set for examining statements used with the theorem prover will be provided by Dr Holden.

Starting Point

Artificial Intelligence I taken in Part 1B.

I will have to familiarise myself with most of Part II Artificial Intelligence II course, as well as do further reading into the field of machine learning, especially the area of semi-supervised learning.

Furthermore, there is a body of approximately five to ten research papers that contain work relevant to this project that I will have to familiarise myself with.

Substance and Structure of the Project

The project involves performing an initial study of the extent to which the Bayesian Sets algorithm of Ghahramani and Heller might be extended and applied within the area of drug design, the identification of protein localization and

interactions, as well as classifying statements used in automated theorem proving. More specifically, we aim to address the problem of *data augmentation* (*entity set expansion*), as defined in the introduction.

As an *optional* part of the project, we will try to create a variation of the S-EM algorithm that would be applicable to problems other than text classification.

The principal goal of the project is to implement a properly tested, documented and optimized open source software library allowing the Bayesian Sets algorithm and extensions to be applied easily to new data sets.

As for the optional part of the project, in case we are successful in deriving a variation of the S-EM algorithm required for application to data models other than text classification, we shall aim to integrate it in the library as well.

The data sets provided will allow us to address problems in:

1. Drug design: Achieving data augmentation for the supervised algorithms applied in this area. The dataset will be provided by Dr Matthew Trotter of the Celgene Institute for Translational Research Europe (CITRE), Sevilla, Spain.

2. Regenerative medicine: Identifying protein localisation and interactions in the context of regenerative medicine. The dataset will be provided by Dr Holden's collaborators at the Anne McLaren Laboratory for Regenerative Medicine.

3. Classification of statements used for a supervised theorem prover: Recent work by Dr Holden applied machine learning techniques to first order theorem proving. We will try to achieve data augmentation on the set of statements attempted by the theorem prover.

Subsequently, the aim of the project is to investigate the performance of the Bayesian set algorithm (and *potentially* our variation of S-EM), producing quantitative comparisons of their performance using the three different data sets available to us.

To quantify how much our data augmentation affected the performance, we will first compute the *F-Score*, *prediction@N* and other metrics to assess the performance of the algorithms implemented. Subsequently, the original algorithms used in these different applications will be applied to our augmented data set to measure the change in their performance.

If our attempt at the extension of S-EM to tasks other than text classification is successful, an examination similar to the one taken in (Li et al., 2010) will be taken to further examine their claim that classification methods are superior to ranking ones.

The project has the following main sections:

1. Familiarisation with the programming language to be used (*Matlab*) and the surrounding software tools. Detailed examination of the Bayesian sets and the S-EM algorithm. An attempt to derive further variations of Bayesian sets, as well as an attempt to extend the S-EM algorithm to problems other than text classification.

2. Development and implementation of the Bayesian sets algorithm and its extensions derived in the first phase. Potentially, development and implementation of the modified S-EM algoritm as well. Creating, optimising, and testing an open source library which will allow direct application of these methods to new, general data sets.

3. Application of the developed software to the data sets available. Thorough examination and quantification of their performance.

4. Experimental evaluation of the performance changes in the three algorithms used with the original data sets after data augmentation.

5. Writing the Dissertation.

Success Criteria

The following should be achieved:

- Development and implementation of the original Bayesian sets algorithm, as well as its further derivations required for application to the three data sets available.

- Implementing, testing, optimising and documenting an open source library to allow application of Bayesian sets to new data sets in order to achieve data augmentation.

- Application of our implementation of Bayesian sets to the three data sets available; measuring how well data augmentation is achieved.

- Experimental investigation of the extent to which data augmentation achieved leads to an improvement in performance in the original application areas.

Extensions

- Derivation and implementation of an extension to the S-EM algorithm that will allow application to problems other than text classification.
- Inclusion of this algorithm as part of the open source library created.
- Application of this algorithm to the data sets available. Measuring the quality of data augmentation achieved.
- Comparison of S-EM algorithm's performance with the performance of Bayesian sets.

Evaluation

The success of data augmentation achieved can be measured using standard metrics such as the *F-score*(prediction, recall), *Prediction@N* and others.

The change in the *subsequent performance* of the classifiers used is harder to measure, due to the different nature of algorithms used in the three application areas considered.

We would like to obtain a *uniform* measure of success of data augmentation across these different data sets. To achieve that, we will first apply a *standard classifier implementation* such as SVM^{light} to all three data sets. Subsequently, we will measure (the change in) its performance after our attempt at data augmentation.

This should yield a result that will be representative of the impact data augmentation can have in these application areas.

Timetable and Milestones

19.10.2012 - 18.11.2012

Background reading in machine learning and semi-supervised learning. Thorough examination of the Bayesian sets algorithm, S-EM algorithm, as well as any other relevant scientific literature. Attempt at deriving further variations of Bayesian sets, and an attempt at generalising the S-EM algorithm.

Milestones: Pseudocode and theoretical background required to start implementation.

19.11.2012 - 16.12.2012

Familiarisation with Matlab and the relevant libraries. Implementation of Bayesian sets and the original S-EM algorithm.

Milestones: A first prototype of the Bayesian sets algorithm.

17.12.2012 - 31.12.2012

Further work on implementing the Bayesian sets and (*potentially*) the modified S-EM algorithm. Testing on the text classification problems available in the literature.

Milestones: A tested version of Bayesian sets. A prototype of the modified S-EM algorithm.

1.1.2013 - 31.1.2013

Final work on the S-EM algorithm. Optimising, testing and documenting the library so that it allows application of these two algorithms to text classification.

1.2.2013 - 15.2.2013

Adapting the library to allow application to the three data sets available.

Milestones: The library can now be easily applied to general data sets.

16.2.2013 - 28.2.2013

Applying the algorithm to the available data sets and measuring the success of data augmentation achieved.

Milestones: Results of evaluation now available.

1.3.2013 - 31.3.2013

Examination into how the use of the newly obtained (augmented) data sets improves the performance of the algorithms used in the three application areas.

1.4.2013 - 15.4.2013

Writing the dissertation.

Milestone: Draft of the Dissertation.

16.4.2013-1.5.2013

Final work on the Dissertation.

Milestone: Final version of the Dissertation. Final version of the library implemented submitted.