E-mail Classification in the Haystack Framework

by

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Abstract

This thesis describes the design and implementation of a text classification framework for the Haystack project. As part of this framework, we have built a robust Java API that supports a diverse set of classification algorithms. We have used this framework to build two applications: Cesium, an auto-classification agent for Haystack that is Haystack's first real autonomous agent, and PorkChop, a spam-filtering plugin for Microsoft Outlook. In order to achieve suitable training and classification speeds, we have augmented the Lucene search engine's document indexer to compute forward indexes. Finally, unrelated to text classification, we describe the design and implementation of Cholesterol, Haystack's highly optimized RDF store.

Thesis Supervisor: David R. Karger
Title: Associate Professor

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Chapter 1

Introduction

The goal of the Haystack project is to help users visualize and manage large amounts of personal information. This thesis expands Haystack's information management mechanisms to include automatic classification functionality. While Haystack stores a large variety of information, and the algorithms implemented in this thesis can be applied to any type of textual information, the focus of the research is on the classification of e-mail messages.

The average corporate computer user receives over 39 e-mail messages a day [9], with some "knowledge workers" receiving hundreds of e-mail messages a day. The sheer volume of e-mails received by the average user means that even casual users of e-mail have need of effective information management strategies. The nature of typical e-mail communication means that classification is an effective e-mail organization tool. A typical user may receive personal, work, and school e-mails via the same e-mail account; grouping e-mails into these three categories is an effective way to help this user manage their information. The goal of this thesis is to develop an automatic classification system that learns from a user's existing e-mail categorizations and automatically sorts new e-mails into these categories.

To accomplish this goal, I have developed a robust machine learning framework. The framework consists of tools to parse documents and convert them into a format suitable for the machine learning algorithms, pre-processors that clean the document data, machine learning algorithms, and a methodology for evaluating the performance

of classifiers. The machine learning algorithms, however, are the backbone of the learning framework. Broadly speaking, a machine learning algorithm tries to build a generalized model from its training data – such as a set of already categorized e-mail messages – and then applies this model to test data – such as new, incoming e-mail messages.

One of Haystack's primary goals is to help users manage semi-structured information, but machine learning problems are typically very structured; the fact that a specific document is a member of a set of categories implies that it is not a member of all other categories. This strict categorization scheme does not mesh well with Haystack's notion of semi-structured data. Some of the learning algorithms in this thesis have been augmented to handle so-called "fuzzy" categories. Fuzzy categories allow clients of the learning framework to qualify their assertions about documents; not only can classifiers handle typical assertions like, "I am certain that document d is in category c," classifiers can now model uncertainty, such as "document d is probably not in categories a and b."

The learning framework is used to implement two applications: PorkChop, a spam filtering plugin for Microsoft Outlook, and Cesium, a Haystack agent that automatically categorizes arbitrary text data and is Haystack's first real autonomous agent. Cesium makes use of the learning framework's fuzzy categorization capabilities.

1.1 Related Work

The scope of this thesis is fairly broad, ranging from the novel information management techniques in Haystack, to state-of-the-art machine learning techniques, to spam filtering and e-mail autoclassification tools. This related work section discusses the Haystack project, which is the primary end user of of the learning framework developed in this thesis, and talks, in general, about the spam detection problem. Related machine-learning algorithms are discussed in Chapter 4, where they are evaluated in the context of the algorithms implemented in Haystack. This section provides a broad overview of the spam detection problem; specific spam detection programs are

discussed in Chapter 6, where they are compared to PorkChop, a spam filter built using the learning framework.

1.1.1 Haystack

Haystack is a powerful information management tool that facilitates management of a diverse set of information. One of Haystack's key strengths is that it does not tie the user to any specific ontology; Haystack can not only handle a diverse set of data (i.e. e-mail messages, appointments, tasks, etc.), but it can store and display the data in user-defined formats. Haystack provides a uniformly accessible interface for different types of information, regardless of the information's format or original source. For example, it may be useful to incorporate the contents of e-mail attachments (in various forms like PDF or Postscript) into the text classification machinery.

Haystack's ability to handle arbitrary ontologies and visualization schemes means that augmenting Haystack's e-mail handling facilities to incorporate an e-mail categorization agent required very few changes to the existing Haystack code. The automatic classification agent simply monitors all incoming e-mail, and annotates each message with one or more predicted categories. The user interface to configure the agent and display its predictions was simple to build with Haystack's robust Slide UI framework.

The paper "Haystack: A Platform for Creating, Organizing, and Visualizing Information using RDF" [8] provides an excellent overview of the motivation, structure, and implementation of the Haystack project; consult that paper for a more thorough overview of precursors to and the history of Haystack.

1.1.2 Spam Detection

Spam detection is a "killer application" for machine learning techniques. Some estimates put the volume of Spam at over 30% of all e-mail messages transmitted daily over the Internet. Not only is spam e-mail an unnecessary burden on e-mail servers, it is a nuisance to users, and is potentially offensive. This section describes common spam filtering techniques, current spam filtering tools, and argues that spam filters

backed by robust machine learning algorithms are vastly more effective than static rules-based spam filters.

Most current spam detection tools work by comparing incoming e-mail messages to a database of manually-compiled rules. Typical filtering methods include:

- Whitelists (approved non-spam e-mail addresses) and blacklists (known spammer e-mail addresses, domains, and ISPs).

- The presence of anomalous e-mail message headers (forged senders, etc.) and e-mail message headers that indicate that a message was generated by a bulk e-mail sending program.

- Searching the message for certain pre-defined words, phrases, or types of text (such as sentences in ALL CAPS).

The advantage of these types of e-mail filters is that they don't require any training – they can immediately start filtering spam e-mail, even if there is very little initial data (i.e. the user has only received a few e-mail messages). However, rules based filters have no ability to adapt to a specific user's e-mail. For example, a sex education worker might receive a high number of important work-related e-mails that have common spam keywords in them. The adaptive nature of machine learning algorithms makes them more powerful than rules based filtering for a number of reasons:

- *Machine-learning algorithms can adapt to an individual's e-mail.* People who maintain rules-based filters for spam detection often include personal information – such as their home telephone number or zip code – in their personal set of spam rules [7]; personal information (other than your e-mail address and perhaps your first name) is highly unlikely to be present in spam e-mail, and is thus an excellent discriminator. While rules-based filters must be manually programmed with personal information, machine learning algorithms will automatically learn good discriminants.

- *The "spam score" of a message computed by a rules-based filter is somewhat arbitrary.* Most rules-based filters work by assigning each characteristic of an

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e-mail a spam score; if the score for a specific e-mail message exceeds a set limit, then the message is classified as spam. How many points should an e-mail get for having the word "sex" in it? A machine learning algorithm's logic is based on empirical observation of its training corpus, not a human's guess.

- *Static rules-based spam filters cannot adapt to changing patterns in e-mails.* Spam detection tools reduce the profitability of spam to its senders; spammers will obviously try to look for ways around them. As rules-based filters have become more widely deployed, some spammers have tried to evade simple word-blocking spam filters by, for example, writing the word "porn" as "p0rn". Rules-based filters must be updated to reflect changing trends in spam content, but machine-learning algorithms can automatically adapt to changes in spam; they might misclassify the first few messages, but as long as the user is diligent about correcting the learner's mistakes, the new type of spam will quickly be caught. In fact, a machine learning algorithm is likely to learn that the word "p0rn" is an excellent discriminator between spam and legitimate e-mail – an ever better discriminator than the word "porn".

Some spam researchers [6] predict that adaptive spam detection algorithms will mean the death of spam. The only way spammers will be able to craft messages that escape an adaptive spam filter is to make their messages indistinguishable from your ordinary e-mail. Spam messages are mostly sales pitches, so unless your regular e-mail is mostly sales pitches, it's unlikely that a majority of spam would get through an adaptive spam filter. As text learning algorithms become better and better at distinguishing spam sales pitches from the normal flow of e-mail, they predict that the torrent of spam will slow to a trickle.

Static rules-based spam detection algorithms do have their place in a robust spam solution; it's hard, for example, to get a machine learning algorithm to learn whether an e-mail has a malformed header or not, but it's easy to write a rule to detect this. Adaptive machine learning algorithms are powerful, but they aren't a panacea; the best spam detection systems will most likely use static rules alongside state of the

art machine learning algorithms. The combination of the expressive power of static rules and the adaptiveness of machine learning algorithms is sure to form the basis of a very formidable spam detection solution.

1.2 Overview

This thesis is divided into six sections.

Chapter 2 discusses the design considerations involved in building a text classification system. One important aspect of any text classification system is its document representation scheme; most machine learning algorithms cannot process raw text documents, and a document representation scheme defines how a text document is presented to the machine learning algorithms. The most common document representation is a "bag-of-words" or "word frequency vector," which is simply a histogram of the words in a given document. These word frequency vectors are computed by Lucene, which was customized to efficiently store this data and is described in Chapter 3. Once all documents have been translated into word frequency vectors, a number of pre-processing algorithms may be run. These pre-processing algorithms help remove noise and clean the word frequency vectors before they are input into the machine learning algorithms.

The machine learning algorithms are the backbone of the learning framework, and are described in Chapter 4. Broadly, each algorithm takes as input a set of word frequency vectors already labeled with categories, builds a model from this training data, and then applies that model to the test data. If a classifier's input data is semi-structured, then the boundaries between categories are much less distinct; portions of the learning framework support "fuzzy" category membership. The learning framework supports three different types of classifiers: *binary classifiers*, which determine if a document is in a class, *multi-class classifiers*, which label a test document with exactly one class out of a possible field of many classes, and *multi-label classifiers*, which label a test document with any number of labels. All types of classifiers can process structured training information, and the framework provides binary classifiers

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and multi-label classifiers that can handle semi-structured data. Java interfaces are used extensively, and similar classifiers can be swapped in and out with no significant code modifications. The various classifiers implemented in this thesis have been benchmarked using standard test corpora, and the algorithms perform on par with published implementations.

The learning framework was used to build two applications: Cesium, an auto-classification agent for Haystack, and PorkChop, a spam-filtering plugin for Microsoft Outlook. Cesium is discussed in Chapter 5, and PorkChop is discussed in 6.

Finally, the Cholesterol database is the backend RDF store for the Haystack project and is an integral part of Haystack. It is not directly related to the learning framework, but I performed a significant amount of development work on Cholesterol. Cholesterol is described in Chapter 7.

Chapter 2

How to Build a Text Classification System

This section describes how to build a text classification system. As the name implies, the goal of a text classification system is to process a document and label that document as a member of one or more groups. A text classifier takes as input a set of training documents, each labeled as a member of one or more groups, and tries to learn a model from this training data. The specifics vary by algorithm, but classification models, in general, try to identify which features of the training documents can be used to separate the training documents among their assigned classes. Some learning algorithms can also handle semi-structured data, where documents can be labeled as "probably" a member of a category, or "definitely" not a member of a category, and this uncertainty about training labels influences the classification model. Once a model has been built from the training data, the classifier analyzes test documents and uses the model to assign these documents labels.

However, a fully functional text classification system requires much more than machine learning algorithms. This chapter provides an overview of all of the constituent parts of an text classification system, with the exception of the specifics of the machine learning algorithms, which are discussed in Chapter 4. Machine learning algorithms can't process raw text; text documents must first be converted into a computer-friendly document representation. Section 2.1 discusses common document

5	standard
1	management
4	oil
.	
.	
1	under
3	of
1	venture

STANDARD OIL SRD TO FORM FINANCIAL UNIT

Standard Oil Co and BP North America plan to form a venture to manage the money market activities of both companies. BP North America is a subsidiary of British Petroleum Co Plc BP, which also owns a 55 pct interest in Standard Oil.

The venture will be called BP/Standard Financial Trading and will be operated by Standard Oil under the oversight of a joint management committee.

Figure 2-1: A word frequency vector

representations and how they shape the nature of the classification problem. Once a text document has been converted into a computer-friendly representation, a number of pre-processing algorithms can be run on the data. These pre-processing algorithms, which are discussed in Section 2.2 "clean" the document representation by exploiting properties of the English language to remove extraneous features, reduce noise, and improve the ability of the classifier to generalize. Section 2.3 provides an overview of the Java APIs provided by the Haystack Learning Framework to generate a computer-friendly document representation from a text document and to pre-process a corpus of documents.

Once the computer-friendly document representation has been cleaned via the pre-processing algorithms, it is ready to be fed into the classifier. Chapter 4 provides an in-depth discussion of the machine-learning algorithms implemented in this thesis; Section 2.4 discusses various high-level aspects of machine learning. Specifically, Section 2.4 motivates the structured and semi-structured classification frameworks and addresses a number of practical issues one must take into consideration when designing a real-world classifier.

Finally, Section 2.5 discusses various methodologies for evaluating the performance of a classifier.

2.1   Document Representation

The simplest way to represent a text document is the "bag-of-words" or "word frequency vector" representation. A word frequency vector is produced by tokenizing a document using a tool like Lucene (Chapter 3), and building a histogram of the
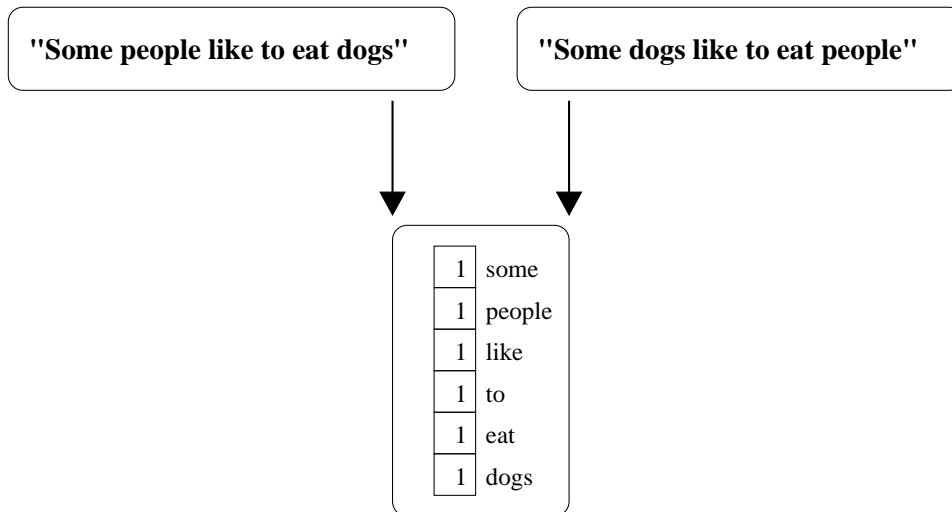
Figure 2-2: Two semantically different sentences generate the same word vector
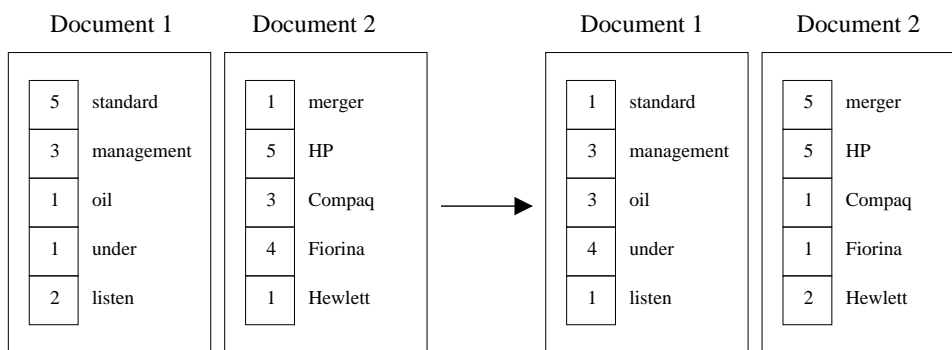
Figure 2-3: An illustration of Rennie and Rifkin's experiment [17]

number of occurrences of each word in the document. It is relatively easy to compute a word frequency vector from a text document, and these word vectors are convenient to work with. However, any information about phrases within the document is lost.

At first approximation, it seems obvious that grouping relevant word pairs in the vector representation will be useful to the classifier – "machine learning" is more useful than "machine" and "learning." However, it's important to group the right word pairs; grouping the phrases "the dog" and "a dog" may actually decrease the accuracy of the classifier (both phrases refer to the same concept – a "dog"). It is computationally infeasible to generically determine which word pairs it would be advantageous to group without any higher order, domain specific information.

The Independence Assumption

Due to the intractability of determining which word pairs are relevant and which word pairs are not relevant, most text classification systems impose a simplifying "independence assumption", which states that each word in a document is independent of all other words in the document. While it does seem logical that grouping word pairs would be helpful to a classifier, a number of studies have borne out the independence assumption. Rennie and Rifkin [18] found no improvement classifying two different datasets with non-linear SVM kernels over linear SVM kernels, and Yang and Liu [28] duplicated this result on the Reuters-21578 dataset. Furthermore, Rennie and Rifkin have run experiments that show that randomly scrambling word frequencies between documents yields a classifier with the same accuracy for a linear SVM (see Figure 2-3) [17]. The independence assumption dramatically shapes the nature of text classification algorithms.

2.1.1   CRM114 Phrase Expansion Algorithm

The CRM114 spam filter (discussed in Section 6) is a spam filtering tool with a novel approach to feature generation. While the general logic when designing machine learning systems is to use as few features as possible (to reduce computation time and to prevent overtraining), the CRM114 spam filter generates as many features as possible from the document text.

CRM114 moves a 5-word sliding window over the document, and generates every possible combination of subphrases for that 5-word window (see Figure 2-4). The author has no solid theoretical background for reversing common practice, but CRM114's impressive accuracy using a Naive Bayes classifier lends some credence to his design decisions. While his work is preliminary, unverified, and not solidly theoretically founded, it's worth examining; a tokenizer that implements CRM114-style phrase expansion algorithm is discussed in Section 2.3.1.

The Standard | Oil Corporation announced | that, effective today, it would...

oil   oil corporation   oil corporation announced
corporation   oil announced
announced   corporation announced
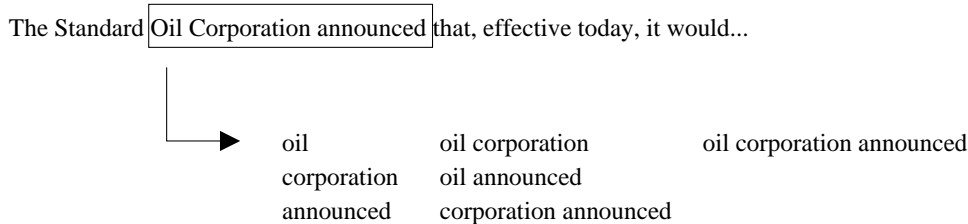
Figure 2-4: The CRM114 phrase expansion algorithm with a chunk size of 3 words

2.2 Feature Selection and Other Pre-Processing

Pre-processing algorithms use properties of English to clean a corpus before it is presented to the machine learning algorithms. Four document cleaning techniques are described in this section: stemming, stop word removal, Zipf's law, and IDF. Zipf's law, stop word removal, and IDF are typically used in machine learning systems, and usually improve classification accuracy by reducing noise and removing extraneous data. There is a much less clear-cut case for stemming words.

A side benefit of most pre-processing techniques is that they reduce the computational complexity of the classification problem by removing words from the data set. In other learning problems, it may be paramount to dramatically reduce the number of words – features – in the corpus, generally because 1) the learning algorithms cannot scale to large numbers of features, and 2) the majority of the features have absolutely no predictive value. However, there is no pressing need to perform feature selection in text classification systems because:

- *The learning algorithms are generally designed to scale to large numbers of features.* The machine learning algorithms discussed in Chapter 4 are well-suited for text classification problems, where there may be tens-of-thousands of features.

- *There are no completely irrelevant features.* Joachims [12] ranked the features in the "acq" category of the Reuters dataset by their information gain – a common metric for determining the value of a specific feature – divided the words into six sections, and then trained six classifiers on the data. A classifier that is trained on only the worst data (i.e. the words judged least relevant by the

information gain metric) still performs significantly better than average. This implies that it's good to have all of the features in the document; a good text classifier should learn many features, and there are few completely irrelevant features.

Most text classification systems still perform some form of pre-processing, but the goal of the pre-processing is not to make the problem computationally tractable or to eliminate irrelevant features; the pre-processing algorithms used in text classification systems typically clean the data, reduce noise, and try to increase the ability of a classifier to generalize.

The Haystack Learning Framework provides four different pre-processing methods.

2.2.1 Stop Word Removal

Stop word removal is an easy-to-implement pre-processing step that removes common words that are known to contribute little to the semantic meaning of an English document. Typical stop words include "the," "of," "is," etc. Lucene provides a mechanism to remove stop words when tokenizing a document.

2.2.2 Zipf's law

Zipf's law says that the r-th most frequent word will occur, on average, $\frac{1}{r}$ times the frequency of the most frequent word in a corpus. This implies that most of the words in the English language occur infrequently. Removing extremely rare words not only reduces dimensionality, it also improves classifier accuracy; the logic is that rare words might have excessive discriminatory value.

The default pre-processor in the Haystack Learning Framework removes any words that occur only once or twice in the entire corpus.

2.2.3 Inverse Document Frequency

The inverse document frequency (IDF) algorithm is used to reduce the effect of common words on a classifier and increase the effect of uncommon words on the classifier.

The rationale is that common words have little discriminatory value, while relatively uncommon words are more effective in separating document classes. Once a word frequency vector has been computed for every document in the corpus, the IDF algorithm can be applied to each document. The IDF formula is as follows:

$$IDF(W_i) = log\left(\frac{|D|}{DF(W_i)}\right) \tag{2.1}$$

$|D|$ represents the total number of documents in the corpus, and $DF(W_i)$ represents the number of documents word W_i is present in. It is intuitive from Equation 2.1 that the inverse document frequency of a word is low if it appears in many documents. The logic is that words that appear in a large percentage of documents are of little value in discriminating between documents. While words that appear only once or twice in the entire corpus are removed (in accordance with Zipf's law), the inverse document frequency is highest when a word appears in fewer documents.

The IDF formula is applied to each document as follows:

$$d_{IDF} = [Frequency(W_1) * IDF(W_1), ..., Frequency(W_n) * IDF(W_n)] \tag{2.2}$$

The weight of each word in a document (the number of times that word appears in the document) is scaled by the IDF of that word in the entire corpus. Common words like "is" and "the" may appear frequently in each document (i.e. their $Frequency(W_i)$ is large), but because they appear in many documents in the corpus, their IDF will be low.

2.2.4   Stemming

Stemming normalizes semantically similar words by removing the suffixes of words – i.e. "learning" becomes "learn" and "dogs" becomes "dog." Not only does stemming reduce the dimensionality of the word vector, it increases the ability of the classifier to generalize to different word forms. Lucene (Chapter 3) provides a Porter Word

Stemmer [15], which can optionally be used by clients of the Haystack Learning Framework to normalize word forms.

Stemming isn't a panacea – even the best stemming algorithms will make mistakes. For example, "number" will be translated by a Porter Stemmer to "numb." The decision to use a stemming algorithm to pre-process document data is a trade-off between generalizeability and specificity. If you use a stemmer, then most word forms will be correctly normalized and your classifier will theoretically generalize better when faced with new documents. However, one can argue that by not stemming words, one allows the classifier to capture more detail; for example, "played" implies past-tense, and is distinct from "play," which could be used to represent either present or future tense.

Most text classification systems use IDF, stop words, and Zipf's law to pre-process corpus data; stemming is not nearly as universally applied as the other pre-processing algorithms, as there is evidence that using a stemming algorithm can reduce classification accuracy [20].

2.3 Tokenization and Pre-Processing API

Machine learning algorithms generally expect their input to come in the form of a word frequency vector – a histogram of word frequencies in a document. However, training and test documents are generally provided as flat text; they must be tokenized and assembled into word frequency vectors before they can be fed into the machine learning algorithms. Lucene provides robust tokenization tools, which are wrapped by the learning framework's ITokenizer interface.

Pre-processing and tokenization are discussed together because two useful pre-processing tools – stemming and stop word removal – are most easily done during document tokenization. Section 2.3.1 discusses the Tokenization API, and Section 2.3.2 discusses the document pre-processing API.

2.3.1 Tokenization API

The ITokenizer interface presents a generic interface to tokenization.

```
interface ITokenizer
{
    String next();
    void close();
}
```

Three different tokenizers are provided:

SimpleTokenizer

```
class SimpleTokenizer implements ITokenizer
{
    SimpleTokenizer(Reader r);
    ...
}
```

The SimpleTokenizer performs only rudimentary lexical analysis – it converts all words to lowercase.

AdvancedTokenizer

The AdvancedTokenizer tokenizer provides facilities for stop word removal and stemming. The list of stop words to remove is supplied by Lucene, as is the Porter Stemmer algorithm.

```
class AdvancedTokenizer implements ITokenizer
{
    AdvancedTokenizer(Reader r /* bStopWords = true, bPorterStemmer = true */ );
    AdvancedTokenizer(Reader r, boolean bStopWords, boolean bPorterStemmer);
    ...
}
```

PhraseExpandingTokenizer

The PhraseExpandingTokenizer implements the CRM114 phrase expansion algorithm described in Section 2.1.1.

The PhraseExpandingTokenizer uses another tokenizer (such as a SimpleTokenizer or an AdvancedTokenizer) to parse the incoming document. The *chunk* parameter

```
class PhraseExpandingTokenizer implements ITokenizer
{
    PhraseExpandingTokenizer(int chunk, ITokenizer it);
    ...
}
```

represents the size of the tokenizer's sliding window across the document text. For each $chunk$-sized word group the sliding window is placed over, $2^{chunk} - 1$ phrases are generated. The CRM114 phrase expansion algorithm is explained in Figure 2-4.

2.3.2 Document Cleaning API

Support for document cleaning, which consists of inverse document frequency (IDF) and Zipf's law, is provided by the DocumentCleaner class.

```
class DocumentCleaner
{
    DocumentCleaner(List listDocuments, WordToNumber wtn);
    void cleanDocuments(/* bIDF = true, bZipfs = true */);
    void cleanDocuments(bool bIDF, bool bZipfs);
}
```

2.4   Learning Algorithms

Machine learning algorithms are the centerpiece of any text classification system. The specific machine learning algorithms implemented in the Haystack Learning Framework are discussed in Chapter 4. This section motivates the structured and semi-structured learning frameworks and discusses the practical issues one must take into consideration when using a classifier in a real-world task.

2.4.1   Stuctured and Semi-structured Classification

One of Haystack's strengths is that it allows users to manage semi-structured data. Other information management tools force restrictive organizational schemes on users; e-mail management tools, for example, typically only allow e-mail messages to be members of one folder. Haystack provides an infrastructure and a user interface that facilitate managing information using flexible, user-defined ontologies.

Unfortunately, most machine learning algorithms are poorly suited to handle semi-structured data. Machine learning algorithms typically assume that their training documents are highly organized. Specifically, most classification systems assume that the fact that a document that is in a set of classes c implies is not a member of all other classes. The "fuzzy" algorithms in the Haystack learning framework relax this strict assumption and allow users to qualify a set of class labels with a confidence value.

Documents no longer have to be presented as strictly positive or negative examples; a document can be "definitely in class c" but "probably not in classes a and b."

2.4.2   Practical Training Issues

Training a classifier is a computationally intensive task. Depending on the classifier used, training takes anywhere from $O(n)$ to $O(n^2)$, where n is the number of documents in the training corpus. The space requirements for training can also be considerable; at best, the space requirements are $O(|C|)$, where $|C|$ is the number of classes, and at worst they are $O(n)$.

Research text classification systems are only run once; a document corpus is split into a training and a test set, a classifier is trained on the training set, and then run on the test set. Real-world text classification systems, on the other hand, must be able to deal with a continuous stream of new documents, and they must be able to learn from any classification mistakes. Both Cesium (Chapter 5), an automatic classification system for Haystack, and PorkChop (Chapter 6), a spam filter for Microsoft Outlook, constantly receive new documents and e-mail messages, and allow the user to correct any mis-classifications.

Due to their internal workings, most classifiers cannot be trained incrementally – i.e. the classifier must retrain on all documents in the training set to learn from even one additional document. Because of the considerable time and space requirements to train a classifier, it's not practical to retrain the classifier after each new message. There are a number of schemes to reduce the frequency with which a learning

algorithm has to train:

- *Scheduling.* Schedule the classifier to retrain every 2-3 hours.

- *Queue length.* If there are more than, say, 25 documents in a "to be trained" queue, then re-train the classifier.

- *Train on errors.* Train only when a classification error occurs.

The best training techniques may combine all three approaches. The goal is to re-train the classifier frequently if the corpus is changing frequently or if the classifier is inaccurate, and to reduce the training frequency in all other circumstances.

2.5   Evaluating Performance

The goal of this thesis is to develop a robust text classification system, not to break new ground and develop a new learning algorithm. As such, the performance analysis of the algorithms in this thesis is relatively unsophisticated. This section describes the data sets and methodology used to analyze classifier performance; Section 4.4 discusses actual classifier performance.

Three data sets are used to evaluate performance:

- **Reuters** The Reuters data set is one of the most widely used data sets to measure classifier performance. The data was collected by the Carnegie group from the Reuters newswire in 1987, and was compiled by Lewis [13] into a corpus of 21,450 articles that are classified into 135 topic categories. Each article can have multiple category labels. 31% of all articles have no category labels (these articles are not used), 57% of all articles are in exactly one category, and the rest, 12%, have anywhere from one to twelve class labels. The distribution of articles among the classes is very uneven.

- **Personal Spam Corpus** My personal spam corpus is derived from a collection of personal e-mail and publicly available spam. It consists of 1,747 non-spam e-mail messages and 1,613 spam e-mail messages, all from my personal Inbox.

- **Twenty Newsgroups** The Twenty Newsgroups data set is a collection 18,828 Usenet articles from twenty different newsgroups, with messages roughly evenly distributed across each category. The original Twenty Newsgroups data set contained exactly 20,000 articles, but Rennie has removed 1169 duplicate (cross-posted) articles. The classifier attempts to predict which newsgroup a message belongs in. Because each message is a member of exactly one newsgroup, the Twenty Newsgroups data set is ideal for testing multi-class classification algorithms.

All tests are performed using the same basic methodology:

- All documents are pre-processed by removing stop words, removing any words that occur only once or twice in the entire corpus, and using the Inverse Document Frequency (IDF) algorithm.

- Documents are randomly assigned to training or test sets. There are roughly equal numbers of documents in the training and test sets. The training and test splits are random, but documents are consistently assigned to either the training or test set across multiple runs of the classifier. Some corpora, such as Reuters, have standard, pre-defined training and test data splits, but these pre-defined splits are ignored.

The learning framework implements three types of classification algorithms, and each is tested differently:

2.5.1 Binary Classifiers

A binary classifier determines whether a document is in a class. Binary classifiers are tested using the Spam Corpus and selected categories of the Reuters corpus.

Joachims [10] suggests using the "acq" and "wheat" categories of the Reuters dataset to test classifiers. The "acq" category is the second most popular category, and contains articles that discuss corporate acquisitions. The "wheat" category, on the other hand, has relatively few news articles and concerns a very specific topic. A

simple classifier that assigns a document to the "wheat" category by searching for the word wheat is 99.7% accurate. The "acq" category has no such characteristic word or words; it represents a more abstract concept, and a successful classifier will have to form a more complex model.

To evaluate the performance of a binary classifier, we collect the following data:

- *The number of true positives.* A true positive occurs when the classifier predicts TRUE and the actual value is TRUE.

- *The number of false positives.* A false positive occurs when the classifier predicts TRUE, but the actual value is FALSE.

- *The number of false negatives.* A false negative occurs when the classifier predicts FALSE, but the actual value is TRUE.

- *The number of true negatives.* A true negative occurs when the classifier predicts FALSE and the actual value is FALSE.

We can represent this data in the following table:

	Actual TRUE	**Actual FALSE**
Classified Positive	True Positive (TP)	False Positive (FP)
Classified Negative	False Negative(FN)	True Negative (TN)

From this data, we can compute a number of statistics:

Statistic	**Equation**
Correct predictions	$TP + TN$
Incorrect predictions	$FN + FP$
Sensitivity	$\frac{TP}{TP+FN}$
Specificity	$\frac{TN}{FP+TN}$

The number of correct predictions is the most easily understood and commonly referenced performance metric, and it generally gives a good picture of classifier performance. However, if the test documents are unevenly distributed between classes,

then the sensitivity and specificity metrics are useful. For example, in the Reuters test set, there are only 124 positive examples of documents in the "wheat" category out of a total number of 5,041 documents in the test set. A classifier that always predicts that a document is not in "wheat" will achieve a 99.97% classification accuracy, but will have a specificity of 0.

2.5.2   Multi-class Classifiers

A multi-class classifier assigns a document exactly one class label. Multi-class classifiers are tested exclusively using the Twenty Newsgroups corpus.

To evaluate the performance of a multi-class classifier, we simply record the number of correct predictions.

2.5.3   Multi-label Classifiers

Multi-label classifier are generally constructed by using n binary classifiers – one for each category. The performance of a multi-label classifier is entirely dependent on the performance of the underlying binary classifiers.

Chapter 3

Forward Indexes and Lucene

3.1   Introduction

Lucene [16] is a fast, full-featured text search and indexing engine written in Java. It uses disk-based indexes for high performance and low memory utilization, and supports ranked searching, complex queries (such as boolean and phrase searches), and fielded searching. Lucene is currently used to store an index of all text content in Haystack, and to allow users to search that content.

A search engine like Lucene computes an inverted index – an index that is designed to support efficient retrieval of all of the documents that contain a given search term. An inverted index contains an entry for each word in the corpus; in this entry is a

Inverted Index

haystack	Doc 1 3x, Doc 2 3x
ontology	Doc 1 7x
pig	Doc 1 4x, Doc 2 2x, Doc 3 6x
cholesterol	Doc 1 2x, Doc 3 4x
farmer	Doc 2 9x
cow	Doc 2 4x
stress	Doc 3 3x
cardiology	Doc 3 1x

Figure 3-1: An example of an inverted index

list of all of the documents the given word appears in, and how many times the word appears in each specific document. Figure 3-1 provides an example of an inverted index. Inverted indices are typically used by search engines; when a search query is executed, the search engine breaks the query into its constituent words, and uses the inverted index to retrieve the documents that each word is present in. The frequency information – how often each word appeared in a given document – is typically used to implement relevance ranking; if a search word appears very frequently in a document, then that document is judged to be more relevant than a document with fewer word occurrences.

Lucene's inverted indexes are disk-based, which means that the vast majority of the index is not loaded into memory and is instead stored on disk. Because Lucene doesn't have to load the entire index into memory, Lucene can index an extremely large amount of data. Lucene's index is designed to support incremental updating – i.e. a single document can be efficiently incorporated into the index, rather than re-indexing the entire corpus to include only one new document.

3.1.1 Forward Indexes

As discussed in Chapter 2, "word frequency vectors" – histograms of the words in the document – are the foundation of most text classification algorithms. Text documents must be translated into word frequency vectors before they can be used by the machine learning system. Efficiently computing and storing these word frequency vectors is central to the efficiency of a text classification system. A text classification system must be able to efficiently retrieve the word frequency vector for a given document, but Lucene's inverted indices store exactly the opposite information.

I have leveraged Lucene's existing indexing infrastructure to store the word frequency vectors for each document. An index of word frequency vectors for documents is called a "forward index" and is the logical opposite of Lucene's inverted indices. When generating its inverted indexes, Lucene actually computes a forward index for each document as an intermediate step; I have modified Lucene to store the once-temporary forward index to disk.

Forward Index

Document 1		Document 2		Document 3	
3	haystack	9	farmer	3	stress
7	ontology	4	cow	6	pig
4	pig	2	pig	4	cholesterol
2	cholesterol	3	haystack	1	cardiology

Figure 3-2: An example of a forward index

3.2   The Modifications to Lucene

The standard Lucene distribution does not provide an efficient means of accessing the attributes of a specific document. I have modified Lucene to support efficient retrieval of a document's word frequency vector using a unique ID.

When a client adds a document to Lucene, he can specify one or more fields; typical fields might include "author," "subject," or "text." To retrieve a document via a unique ID, the unique ID must be specified in a document field. Specifically, the user must place the document's unique ID in its own field, and this field – termed the "primary field" in the rest of this chapter – is specially recognized by my Lucene modifications. I have added accessors that make retrieving a document by its primary field as easy as calling one method in Lucene's IndexReader class.

It's possible to retrieve a document by constructing a search object, restricting the search space to the primary field, and then searching for a document's unique ID. The desired document should be the first and only entry in the search results. However, looking a document up by its unique ID is a common operation for any user of the new forward indexes, and the aforementioned process involves quite a bit of code. IndexReader's accessor methods wrap this complexity and make retrieving a document by its unique ID a one-step operation.

Lucene's new index format is backwards-compatible with the old Lucene index format – users of other versions of Lucene can access indexes created by the forward-

index generating Lucene – and there is no performance impact on users of the modified Lucene library who only create an inverted index. Existing Lucene code will compile and run without modification if combined with the new Lucene library.

Like Lucene's inverted indexes, the forward indexes are disk-based and can be incrementally updated.

3.2.1 API

Lucene's interfaces are little-changed from the standard distribution. Lucene indexes are typically created via the IndexWriter class; I have created a new class, ForwardIndexWriter, that is a subclass of IndexWriter. The only public difference between ForwardIndexWriter and IndexWriter is the ForwardIndexWriter constructor, which takes a "primary field" argument. The primary field contains a document's unique ID; when documents are added to the forward index, they must store the document's unique ID in the primary field.

```
class ForwardIndexWriter extends IndexWriter
{
    ForwardIndexWriter(String primaryField, ...);
}
```

Figure 3-3: The ForwardIndexWriter class

```
IndexWriter iw = new ForwardIndexWriter("URI", ...);
Document d = new Document();
d.add(Field.Keyword("URI", "<urn:chrPQygXbyyAlupt>"));
d.add(Field.Text("text", strDocumentText));
iw.addDocument(d);
iw.close();
```

Figure 3-4: Adding a document to a forward index. The name of the document's primary field is "URI," and the contents of that field are the document's URI.

Documents can have multiple fields, and the data stored in each field is kept separate from the data stored in other fields. Lucene's fields allow search engines to implement relevance ranking algorithms; i.e. if a search term occurs in the subject of a document, it can be judged more relevant than if the search term had only occurred in the body of the document.

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I use Lucene's fields to uniquely identify documents. The "primary field" specified in the ForwardIndexWriter constructor must be specified by each document, and must contain that document's unique ID. It is added to each document during indexing via the Document class's *add* method. When adding fields to a document, users can add the field using *Field.Text*, which performs tokenization on the specified text, or *Field.Keyword*, which does not perform any tokenization. Users must add the primary field to the document using *Field.Keyword*; a runtime exception will occur upon document retrieval if the document's unique ID contains more than one token. *Field.Text* should be used for regular text fields.

Accessing a forward index is accomplished by using the updated *IndexReader* class, which provides $O(1)$ retrieval and deletion of documents based on the primary field. IndexReaders can handle both old-style Lucene indexes (created with IndexWriter), and new Lucene indexes (created with ForwardIndexWriter).

```
class IndexReader
{
    Document document(Object uniqueID);
    void delete(Object uniqueID);

    // all other methods unchanged
}
```

Figure 3-5: The modified IndexReader class

The *document* method returns the Document object associated with the given *uniqueID* in $O(1)$ time. The returned Document object provides access to the document's word frequency vector. If the *uniqueID* is not found in the index, then *document* returns *null*. The *delete* method functions similarly; if the given *uniqueID* is present in the index, then it removes that document from the index.

If either the *document* or *delete* function is used on a regular Lucene index (i.e. an inverted-only index), then they will throw a ForwardUnsupportedException. Forward indices are completely backwards compatible with standard Lucene indexes; it is valid to use an IndexReader to access a Lucene index created with the standard inverted index-only IndexWriter, or the forward-index generating ForwardIndexWriter.

An accessor function, *getFrequencyMap*, has been added to the standard Lucene

Document class:

```
class Document {
    public FrequencyMap getFrequencyMap();

    // all other methods unchanged
}
```

Figure 3-6: The modified Document class

Document objects can be returned from a number of IndexReader methods. If the IndexReader that returned the Document class is accessing a forward index, then the *getFrequencyMap* function will return a FrequencyMap class, which provides easy access to the word frequency vector for a given document (see Section 2.1 and Figure 2-1 for an explanation of word frequency vectors). Otherwise, if the IndexReader is accessing an old-style Lucene index, then the *getFrequencyMap* function will return *null*.

Chapter 4

The Haystack Learning Framework

The Haystack Learning Framework module provides a robust text-learning framework with implementations of binary classifiers, multi-class classifiers, and multi-label classifiers. The Learning Framework provides two binary classification algorithms, Regularized Least Squares Classification (RLSC) and Naive Bayes, four multi-class classification algorithms, Rocchio, Error Correcting Output Codes (ECOC), Multi-class Naive Bayes, and One vs. All, and one multi-label classification algorithm, Simple Multi-Label.

Three interfaces, IBinaryClassifier, IMultiClassClassifier, and IMultiLabelClassifier, correspond to the three types of classifiers offered by the Learning Framework. The liberal use of interfaces allows users to swap-in different learning algorithms with little or no change to the client code.

4.1 Types of Classification Problems

The goal of a text classification algorithm is to assign a document a label based upon its contents. There are several different types of classification problems.

- *Binary Classification:* the classifier labels each document as positive or negative. Many powerful classifiers (Support Vector Machines, RLSC) are natively binary classifiers.

- *Multi-class Classification:* the classifier assigns exactly one of $|C|$ labels to a document. Some algorithms are natively multi-class (i.e. Rocchio), while other algorithms build upon binary classifiers.

- *Multi-label Classification:* the classifier assigns 0 to $|C|$ labels to the document. This type of classification best meshes with Haystack's flexible categorization scheme.

4.2   Binary Classification

A binary classifier takes as input a set of documents, where each document is labeled either TRUE or FALSE. The binary classifier then trains on these documents. A new test document is presented as input, and the classifier returns a TRUE or FALSE label.

Haystack implements two binary classification algorithms: Regularized Least Squares Classification and Naive Bayes.

4.2.1   API

Haystack provides a drop-in interface for binary classification via the IBinaryClassifier interface. Two binary classification algorithms are provided: Regularized Least Squares Classification and Naive Bayes. All binary classifiers implement the IBinaryClassifier interface (see figure 4-1).

```
interface IBinaryClassifier
{
    void addDocument(IDocumentFrequencyIndex dfi, boolean bClass);
    void train();
    double classify(IDocumentFrequencyIndex dfi);
}
```

Figure 4-1: The IBinaryClassifier interface

- *addDocument* The addDocument method adds a document to the binary classifier. It takes two arguments: a word frequency vector representation of the document to add, and a boolean that indicates the document's class.

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- *train* The train method trains the classifier. You cannot call addDocument after calling train, and you cannot call classify before calling train.

- *classify* The classify method applies the learned classifier to a test document. It takes one argument – a word frequency vector – and returns a floating point number. All binary classifiers center their classifier's return values around 0.0. If the floating point number returned by classify is greater than 0.0, then a document is generally labeled TRUE; otherwise, a document is labeled FALSE. The magnitude of the return value implies the classifier's degree of confidence in its prediction.

  However, the significance of the magnitude is dependent on the specific classifier. A classifier like RLSC generally places negative documents close to -1, and positive documents close to 1, while the values returned by Naive Bayes vary depending on the internal classifier state. Users of the binary classifier are free to interpret its return values however they like; by adjusting the decision threshold from 0.0, one can decrease the number of false positives at the expense of increasing false negatives, or vice versa.

Binary classifiers are given a loose specification for handling boundary conditions; their answers in boundary cases may not make sense, but the classifier must return a value (i.e. it must not crash). If Naive Bayes or RLSC is trained on a corpus where all documents are in one class, then they will predict that every document is in that class. If either binary classifier is trained on a corpus with no training documents, then its classify method will return an ambiguous answer of 0.0.

Semi-structured Binary Classification

Machine learning problems are typically well defined – a document is either a positive or negative example of a class – but real-world problems are rarely as clearly defined. A document might be "probably true" or perhaps "definitely false," and traditional binary classifiers do not model this distinction. The binary classification algorithms in this section are tailored towards "fuzzy" classification problems. Every training

document is accompanied by a confidence value that indicates the probability that the training document's label is correct.

All fuzzy binary classifiers must implement IFuzzyBinaryClassifier.

```
interface IFuzzyBinaryClassifier
{
    void addDocument(IDocumentFrequencyIndex dfi, boolean bClass, double dConfidence);
    void train();
    double classify(IDocumentFrequencyIndex dfi);
}
```

Figure 4-2: The IFuzzyBinaryClassifier interface

- *addDocument* The addDocument method adds a document to the binary classifier. It takes three arguments: a word frequency vector representation of the document to add, a boolean that indicates the document's class, and a confidence value. The confidence value is a floating point number from 0.0 to 1.0 that quantifies how confident the user is in the document's class label; a 1.0 confidence value implies absolute certainty, and values close to 0.0 imply a large degree of uncertainty. Due to internal implementation details, documents with very small confidence values − less than 0.0001 − are ignored.

- *train* The fuzzy train method functions identically to the traditional classify method.

- *classify* The fuzzy classify method functions identically to the traditional classify method.

The learning framework provides fuzzy implementations of both Naive Bayes and RLSC.

4.2.2   Naive Bayes

Naive Bayes is a relatively simple text classification model that is often utilized in text classification. Naive Bayesian classifiers run in linear time and achieve remarkable performance; Naive Bayes is generally considered to be the best linear-time classifier

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available. Naive Bayes can be used both as a binary and a multi-class classifier, but the mathematical formulations for both types of classifiers are the same and are discussed in this section.

A Naive Bayes classifier is predicated upon the fact that all attributes of the training examples are conditionally independent – i.e. all words are independent of each other given the context of their class. This assumption is known as the "Naive Bayes assumption," and while it is clearly false, Naive Bayes classifiers perform well in most real-world tasks. Because of the Naive Bayes assumption, features can be learned separately, which greatly simplifies learning, especially when there are a large number of attributes.

The Haystack Learning Framework uses the multinomial event model. Other models exist, and all models have been referred to in the literature as "Naive Bayes," which causes some confusion. McCallum and Nigam [14] give a good overview of the difference between the competing event models, and show conclusively that multinomial Naive Bayes is superior to other formulations.

A multinomial Naive Bayes classifier classifies a test document T by computing the probability that T is in each of the potential document classes. The probability for each individual class is determined by computing the probability that the words in the test document T would appear in a document of that class.

To train, a Naive Bayes classifier computes $P(w_t|c_j)$ for each word in the corpus vocabulary, V, where $|V|$ represents the total size of the corpus vocabulary, $|D_{c_j}|$ represents the total number of words in document class c_j, and $weight(w_i, c_j)$ represents the frequency with which word w_i occurs in c_j:

$$P(w|c_j) = \frac{1 + \sum_{i=1}^{|D|} weight(w_i, c_j)}{|V| + |D_{c_j}|} \tag{4.1}$$

A document is classified by computing

$$argmax_{c_j} P(c_j|d_t) \tag{4.2}$$

where

$$P(c_j|d_t) = \frac{P(c_j)P(d_t|c_j)}{P(d_t)} \tag{4.3}$$

One then computes $P(d_t|c_j)$ as follows:

$$P(d_t|c_j) = P(|d_t|)|d_t|! \prod_{w \in d_t} \frac{P(w|c_j)}{weight(w, c_j)!} \tag{4.4}$$

$P(d_t)$, $P(|d_t|)$, and $|d_t|!$ are constant across all document classes, so they can be eliminated from the calculations. Equation 4.4 is actually computed as a sum of logs to prevent a floating point precision underflow. $P(w|c_j)$ is less than one, and Equation 4.4 computes $P(w|c_j)$ for every word in the document and multiplies them all; multiplying several thousand small numbers is likely to result in a floating point precision underflow. Computing the multiplication in Equation 4.4 as a sum of logs preserves the relative values of probabilities and avoids the underflow.

The binary classifier version of Naive Bayes has only two classes – TRUE and FALSE – while the multi-class version of Naive Bayes has an arbitrary number of classes. The mathematical machinery is the same for both types of classifiers; the classifier selects the document class with the highest $P(c_j|d_t)$.

Semi-structured Naive Bayes

This section describes the modifications to Naive Bayes to enable it to process semi-structured data. In the semi-structured, or "fuzzy" model, a training document has both a class label and a confidence value. The confidence value ranges from 0.0 to 1.0, with larger confidence values implying greater confidence in the accuracy of the class label.

Recall that to train, we compute $P(w|c_j)$ for every word and class combination in the corpus. If we are given a vector, p, of the confidence values of each training point, we modify $P(w|c_j)$ as follows:

$$P(w|c_j) = \frac{1 + \sum_{i=1}^{|D|} p_i * weight(w_i, c_j)}{|V| + |D_{c_j}|} \tag{4.5}$$

In essence, we are duplicating the documents that we are the most confident in; the weights of a document with a confidence value of 1.0 are twice the weights of a document with a confidence value of 0.5.

4.2.3   Regularized Least Squares Classification

Regularized Least Squares Classification is a new method described by Ryan Rifkin in his PhD thesis [19]. It is by no means a new algorithm [3, 1], but Rifkin's thesis is the most comprehensive exploration of the problem to date. RLSC provides similar classification accuracy to Support Vector Machines, but requires less time to train. The exact time required to train a RLSC classifier (or a SVM), is a complex topic with many variables and is discussed further in Rifkin's thesis; we'll simply have to take his word that RLSC can be trained faster than a SVM.

RLSC and SVM's belong to a general class of problems called Tikhonov regularization problems. While a thorough discussion of the mathematics behind Tikhonov regularization problems is beyond the scope of this thesis, the concept is simple. A Tikhonov regularization problem tries to derive a function, f, that accurately predicts an answer, y, given an input x. The accuracy of f is measured using a loss function, $V(y_i, f(x_i))$, and one attempts to find the f that minimizes the total loss. We can state this formally as follows:

$$\min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} V(y_i, f(x_i)) + \lambda ||f||_K^2 \tag{4.6}$$

In the case of text classification, y_i represents the binary label of a training case x_i, and f is the decision function that we're trying to derive. The norm expression $||f||_K^2$ and the λ parameter quantify our willingness to trade off training set error for the risk of overtraining. A Tikhonov regularization problem can be used to describe both Regularized Least Squares Classification and Support Vector Machines; by using the hinge loss function $V(f(x, y)) = (1 - yf(x))_+$, one can re-derive a Support Vector Machine (Chapter 2 of Rifkin's thesis). Replacing the hinge loss function with the square loss function, $V(f(x, y)) = (y - f(x))^2$, Rifkin arrives at his Regularized Least

Squares algorithm. Because the square loss function is differentiable everywhere, the mathematics for RLSC are much simpler than the mathematics for Support Vector Machines. Substituting the square loss function in to Equation 4.6, the problem becomes:

$$\min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} (y_i - f(x_i))^2 + \lambda ||f||_K^2 \tag{4.7}$$

The goal of our classifier is to arrive at a decision function, f, that classifies a training set with minimum error. Using the Representer Theorem, which is described in Rifkin's thesis and [22], one can show that the decision function, f^*, must take the form:

$$f^*(x) = \sum_{i=1}^{\ell} c_i K(x, x_i) \tag{4.8}$$

K represents a kernel matrix which is derived from the training data (its derivation will be explained later). After we substitute Equation 4.8 into Equation 4.7 and convert to matrix notation, we arrive at:

$$\min_{c \in \mathcal{R}} \frac{1}{\ell} (y - Kc)^T (y - Kc) + \lambda c^T K c \tag{4.9}$$

Now that the decision function, f, has a well-defined form, the problem begins to take shape. In the above equation, ℓ represents the number of documents, K is a kernel function that is derived from the training data in an as-yet-undefined manner, and y represents the true values of the training examples. c is a ℓ dimensional vector of coefficients for the decision function; to properly train our classifier, we must try to find the c that minimizes the training error. Because RLSC uses a square loss function, which is differentiable everywhere, and the kernel matrix K positive definite, we can minimize Equation 4.9 by differentiating it and setting the equation equal to zero. After differentiation and simplification, we find that the optimal c vector can be found by solving the following equation:

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$$(K + \lambda \ell I)c = y \tag{4.10}$$

In the above equation, I denotes an appropriately sized identity matrix, ℓ is the number of training documents, and λ is a regularization parameter that quantifies how willing we are to increase training set error but decrease the risk of overtraining.

A Tikhonov regularization problem requires an $\ell \times \ell$ kernel matrix K. However, our training data is provided in an $\ell \times w$ matrix A that corresponds to the training text (there are ℓ rows, one for each document, and w columns, one for each unique word). Because text classification is typically assumed to be a linear problem (see Section 2.1), we can use a linear kernel K, which we compute simply by $K = AA^T$. Thus training our RLSC classifier becomes:

$$(AA^T + \lambda \ell I)c = y \tag{4.11}$$

Because $(AA^T + \lambda \ell I)$ is positive definite and therefore invertible, a straightforward way to solve this problem is to compute:

$$c = (AA^T + \lambda \ell I)^{-1}y \tag{4.12}$$

Unfortunately, solving this equation directly using a method like Gaussian elimination is intractable for large matrices. Methods like Conjugate Gradient (discussed in Section 4.2.3) can solve this equation efficiently.

Once we have solved Equation 4.11 and discovered the appropriate c constants, we have all parameters of our decision function, f. Recall from Equation 4.8 that decision function, f, takes the following form:

$$f(x) = \sum_{i=1}^{\ell} c_i K(x, x_i) \tag{4.13}$$

Because the kernel, K, is linear and $K = AA^T$, we can simplify the above equation to:

$$f(x) = (cA^T)x \tag{4.14}$$

To classify a new data point, x, we compute (cA') and multiply by x.

Semi-structured RLSC

This section describes the necessary modifications to RLSC to enable it to handle semi-structured data. In the semi-structured, or "fuzzy" model, a training document has both a class label and a confidence value. The confidence value ranges from 0.0 to 1.0, with larger confidence values implying greater confidence in the accuracy of the class label.

Equation 4.7 presents the RLSC minimization problem. Recall that the goal of RLSC is to determine a function f that minimizes error, where the error is quantified by summing $(y_i - f(x_i))^2$ over a training corpus. Given an array of confidence values p for each document, we can modify RLSC as follows:

$$\min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} p_i (y_i - f(x_i))^2 + \lambda ||f||_K^2 \tag{4.15}$$

The loss associated with a specific training document is multiplied by the confidence value for that document, p_i. If we minimize the above equation by differentiating and simplifying, we arrive at:

$$(AA^T + \frac{\lambda \ell}{p} I)c = y \tag{4.16}$$

It is easy to see why the IFuzzyBinaryClassifier interface specifies that all documents with a confidence value of less than 0.0001 are ignored; dividing the right side of the sum with a very small confidence value will result in a very large number, which might cause in a floating point overflow.

Conjugate Gradient

The Conjugate Gradient method is an efficient means of computing the solution to systems of linear equations of the form $Ax = b$. Conjugate Gradient is an iterative algorithm; it begins with a candidate solution x', and iteratively refines the solution until Ax' approaches b. The number of iterations required to converge on a specific solution is variable and depends on A and b, though conjugate gradient generally converges very quickly. Traditional algorithms like Gaussian elimination run in a fixed amount of time, and operate directly on the matrix A.

Iterative algorithms like conjugate gradient are well-suited for problems such as text classification, which involve large, sparse matrices. In a typical text classification problem, A has anywhere from several hundred to several thousand rows (one for each training document), and tens of thousands of columns (one for each distinct word in the corpus), though only several hundred of the columns in each row will be non-zero. It is easy to compute Ax' if A is a sparse matrix. Gaussian elimination, on the other hand, performs row operations, which are exceedingly slow on large, sparse matrices.

Jonathan Richard Shewchuk's paper "An Introduction to the Conjugate Gradient Method Without the Agonizing Pain" [23] is an excellent introduction to the conjugate gradient method.

4.2.4 Alternative Binary Classification Algorithms

Support Vector Machines

Support Vector Machines are currently regarded as the most capable binary classification algorithm available. Broadly speaking, a SVM attempts to find a hyperplane that maximizes the margin between positive and negative training examples, while simultaneously minimizing training set misclassifications. SVMs are universal learners; by plugging in the appropriate kernel function, SVMs can learn linear threshold functions, polynomial classifiers, radial basic function networks, and three-layered sigmoid neural networks [11].

While SVMs are powerful, they do require approximately $O(n^2)$ time to train

(Joachims [11] estimates between $O(n^{1.7})$ and $O(n^{2.1})$). This makes them infeasible for large datasets (i.e. a million data points). The quadratic running time of Support Vector Machines is their major downfall, and there have been a number of attempts to overcome this problem:

- *Subsampling:* Subsampling involves training on only a subset of the total training data. By removing data from the training set, one loses a lot of information and classifier performance suffers [17].

- *Bundled SVM:* A bundled SVM [24] reduces the number of training points presented to a SVM learner by concatenating randomly chosen datapoints in the same class. By tuning a s parameter that determines how many data points to combine, one can achieve a tradeoff between accuracy and speed (between $O(n)$ and the typical SVM $O(n^2)$). The bundled SVM implementation described in [24] achieves the current record for a ROC breakeven point on Reuters-21578, though there is little theoretical justification for this result. Bundled SVMs show a good deal of promise; even when the s parameter is tuned so the bundled SVM runs in $O(n)$, the bundled SVM implementation still performs significantly better than a benchmark Naive Bayes implementation.

Other Algorithms

- *Neural Networks:* A neural network is a type of classification algorithm patterned off the physical neurons in brains. The network consists of groups of nodes connected together in various patterns, with adaptive weights associated with each connection. By varying the pattern of the nodes and adjusting the function applied by the nodes, one can construct both linear and nonlinear classifiers. Neural networks are generally slow to train, theoretically inelegant (i.e. there are more direct ways to express a nonlinear classifier), and perform relatively poorly [28].

- *k-Nearest Neighbors:* The k-Nearest Neighbor algorithm is simple in concept; given a test document, the system finds the k-nearest neighbors to the document

according to a similarity measure (generally the same cosine metric used in the Rocchio algorithm – see Equation 4.21). The neighbors are grouped according to their category, and weighted according to their similarity scores. Training a k-Nearest Neighbor classifier is simple (just record each document in the training set), but given a m document training set and an n document test set, classification takes $O(mn)$ time.

4.3 Multi-class and Multi-Label Classification Algorithms

There are three broad types of classification algorithms: binary classifiers, multi-label classifiers, and multi-class classifiers. Binary classifiers have been discussed already in Section 4.2. Multi-label classifiers can assign a document 0 to $|C|$ document labels, while multi-class classifiers assign a document exactly one label.

This section describes four multi-class algorithms – One vs. All, Error Correcting Output Codes (ECOC), Naive Bayes, and Rocchio – and one multi-label algorithm – Simple Multi-Label. One can group these algorithms into two categories:

- Naturally multi-label or multi-class classifiers.

- Composite classifiers that build upon binary classifiers and decompose the classification task into any number of binary problems.

Algorithms like Rocchio and Naive Bayes are naturally multi-class, though both can be used as binary classification algorithms. A binary classifier version of Naive Bayes is described in Section 4.2.2. While Rocchio can also be converted to a binary classifier, Joachims [10] has shown conclusively that Naive Bayes performs better than Rocchio; Rocchio was not converted to be a binary classifier.

The most sophisticated algorithms – Support Vector Machines and RLSC – are natively binary classifiers. While there has been some research regarding adapting SVM and RLSC to be natively multi-class, the best results have been achieved by

combining binary classifiers to form a multi-class classifier [19]. Algorithms like Simple Multi-Label, One vs. All, and Error Correcting Output Codes construct multi-class or multi-label classifiers from arbitrary binary classifiers.

The learning architecture provides five multi-class or multi-label classification algorithms:

- *Simple Multi-Label.* The simple multi-label algorithm trains $|C|$ different binary classifiers. To classify a document, the algorithm iterates through the $|C|$ binary classifiers; those that return TRUE are labeled with that class.

- *Error Correcting Output Codes.* Error Correcting Output Codes split the training data among $O(|C|)$ classifiers in a pattern that provides some error-correcting properties.

- *One vs. All.* The One vs. All algorithm is a multi-class adaptation of the Simple Multi-Label algorithm. It can be expressed via the matrix framework used by ECOC classifiers.

- *Naive Bayes.* Naive Bayes is a popular and powerful linear-time inherently multi-class classification algorithm.

- *Rocchio.* Rocchio is a natively multi-class algorithm that was implemented primarily for debugging purposes. Naive Bayes is also linear-time and consistently outperforms Rocchio.

4.3.1   API

Multi-Label Classification

The learning framework provides simple interfaces to multi-label and multi-class classification. A multi-label classifier must implement the IMultiLabelClassifier interface.

The SimpleMultiLabelClassifier is currently the only multi-label classifier implemented in the Haystack Learning Framework. The interface to multi-label classifiers is fairly straightforward:

```
interface IMultiLabelClassifier
{
    void addDocument(IDocumentFrequencyIndex dfi, Set classes);
    void train();
    Set classify(IDocumentFrequencyIndex dfi);
}
```

Figure 4-3: The IMultiLabelClassifier interface

- *addDocument* The addDocument method is used to add a document to the classifier. It takes two arguments: a word frequency vector that represents the document, and a Set containing all of the document's labels. This classifier assumes that a document is a member of all labels specified in the *classes* parameter, and is not a member of all other classes in the corpus. If the document to add has multiple labels, you should pass all of those labels in the second argument to addDocument. Calling addDocument multiple times with the same document but with different class labels will add the document multiple times and will produce incorrect behavior.

- *train* The train method trains the classifier. You cannot call addDocument after calling train, and you cannot call classify before calling train.

- *classify* The classify method applies the learned classifier to a test document. It takes one argument – a word frequency vector – and returns a Set that represents the document's labels.

Semi-Structured Multi-Label Classification

The traditional multi-label classifier assumes that the classification problem is well defined, and makes very strong assumptions about the underlying categorization ontology. Specifically, it assumes that if a document is a member of a set of classes, then it is not a member of every other class in the corpus. Realistically, this is often not the case, especially when dealing with semi-structured data.

To accurately capture complex and poorly defined category structure, we introduce the concept of "fuzzy membership." Documents might be "probably members of classes a and b," but "definitely not members of classes c and d." We expand on the

existing multi-label classification interface by adding separate methods to separately add positive and negative examples, and allow users to associate a confidence value with each set of classes. The confidence value is a floating point number from 0.0 to 1.0 that quantifies how sure we are that a given document is or is not a member of a set of classes. A confidence value of 1.0 represents the maximum amount of certainty, and 0.0 represents the minimum amount of certainty. Practically, due to implementation details, documents with confidence values less than 0.0001 are ignored – their confidence value is too low to affect the classifier model.

All fuzzy multi-label classifiers must implement IFuzzyMultiLabelClassifier.

```
class FuzzyMultiLabelClassifyResult
{
    public double value;
    public Object cls;
}

interface IFuzzyMultiLabelClassifier
{
    void addPositiveDocument(IDocumentFrequencyIndex dfi, Set classes, double dConfidence);
    void addNegativeDocument(IDocumentFrequencyIndex dfi, Set classes, double dConfidence);
    void train();
    Set classify(IDocumentFrequencyIndex dfi);
}
```

Figure 4-4: The IFuzzyMultiLabelClassifier interface

- *addPositiveDocument* The addPositiveDocument method is used to present a document *dfi* as a positive example for the set of classes *classes*. The confidence value indicates how certain the user is that *dfi* is in *classes*. One can call addPositiveDocument or addNegativeDocument multiple times, but only for orthogonal sets of classes; if a document is added to a class multiple times, the classifier will most likely function incorrectly.

- *addNegativeDocument* The addNegativeDocument functions identically to addPositiveDocument, except that it adds the given document as a negative example of *classes*.

- *train* The train method trains the classifier. You cannot call addDocument after calling train, and you cannot call classify before calling train.

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- *classify* The classify method applies the learned classifier to a test document. It takes one argument – a word frequency vector – and returns a Set of Fuzzy-MultiLabelClassifyResults. The classifier will return one FuzzyMultiLabelClassifyResult for each unique document label in the classifier. The *value* attribute of FuzzyMultiLabelClassifyResult implies how confident the classifier is in its prediction. *value* is not constrained to a specific range, but the larger *value* is, the more confident the classifier is that the test document is a member of class *cls*.

Multi-Class Classification

A multi-class classifiers labels a document with exactly one category. A multi-class classifier must implement the IMultiClassClassifier interface.

```
interface IMultiClassClassifier
{
    void addDocument(IDocumentFrequencyIndex dfi, Object cls);
    void train();
    Object classify(IDocumentFrequencyIndex dfi);
}
```

Figure 4-5: The IMultiClassClassifier interface

- *addDocument* The addDocument method takes two arguments: a word frequency vector, and the document's class. addDocument may be called only once for each document; if the same document is passed to addDocument twice, the classifier may function improperly.

- *train* The train method functions identically to IMultiLabelClassifier.train.

- *classify* The classify method takes one argument – a word frequency vector – and returns the predicted class of the test document.

There are currently four multi-class classifiers: Rocchio, Naive Bayes, One vs. All, and Error Correcting Output Codes.

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The Classifier Constructors

Implementors of IMultiClassClassifier or IMultiLabelClassifier differ only in their constructors. Composite algorithms that build upon binary classifiers take an IBinaryClassFactory in their constructor, which the multi-class or multi-label classifier uses to instantiate different binary classifiers.

For example:

```
// Two composite classifiers
IMultiClassifier imc = new OneVsAllClassifier(new RLSCBinaryClassifierFactory());
IMultiLabelClassifier iml = new SimpleMultiLabelClassifier(new NaiveBayesBinaryClassifierFactory());

// A natively multi-class classifier
IMultiClassifier imc2 = new NaiveBayesMultiClassClassifier();
```

Figure 4-6: Instantiations of various classifiers

RLSCBinaryClassifierFactory and NaiveBayesBinaryClassifierFactory implements the IBinaryClassifierFactory interface. By using the power of Java's polymorphism, we are able to provide a generic plug-in interface for binary classifiers. Different binary classifiers can be swapped in and out of the same multi-class or multi-label classifier. Composite multi-class or multi-label classifiers must be passed an argument to a binary classifier factory, but natively multi-class algorithms like Naive Bayes can be constructed without any arguments.

4.3.2 Simple Multi-label

The Simple Multi-Label classifier, as its name implies, is a fairly straightforward algorithm. It is a composite algorithm that requires a plug-in binary classifier. A multi-label classifier's training documents can be labeled with anywhere from 0 to $|C|$ categories, and, likewise, the classify method of the Simple Multi-Label classifier can label a test document with anywhere from 0 to $|C|$ categories.

To do this, the classifier constructs $|C|$ binary classifiers, one for each class. To train a document d with class labels c, d is presented as a positive example to the set of c classifiers, and as a negative example to the set of $C - c$ classifiers. To classify a document, one runs all $|C|$ binary classifiers. According to the convention established

by the binary classification interface (see Section 4.2.1), a document is labeled with a class if the binary classifier for that class returns a value of more than 0.0.

While most organizational systems (i.e. filesystems, personal information managers such as Outlook), only allow documents to be members of one class, Haystack frees the user from this restrictive ontology. Multi-label classification, which allows a document to be a member of an arbitrary number of classes, is best suited to Haystack's loose notion of categories.

Fuzzy Multi-label

The Fuzzy Multi-label classifier relaxes the strong assumptions made in the Simple Multi-label classifier – namely that if a document is a positive example of a set of categories, then it is a negative example of all other categories. It still constructs $|C|$ binary classifiers, but users can manually specify the set of classes that a document is in or not in, and can associate these class labels with a confidence value that quantifies how certain the user is in these class labels.

4.3.3   Code Matrix Approaches: ECOC and One vs. All

The One vs. All classifier and the Error Correcting Output Codes (ECOC) classifier are subclasses of a generic matrix-based classifier which assigns documents to classifiers based upon the pattern in a characteristic matrix. One vs. All and ECOC can be expressed by running the general matrix multi-class classifier on different characteristic matrices.

One vs. All

One vs. All is a very simplistic algorithm for performing multi-class classification, but it is also one of the most effective multi-class classification algorithms. A One vs. All classifier builds $|C|$ classifiers, one for each class. A document that is a member of one class, c, is presented as a positive example to the classifier for c, and a negative example for all other $C - c$ classifiers.

Rifkin [19] provides a fairly convincing argument that One vs. All is an excellent multi-class classification algorithm, eclipsed – and only slightly - by ECOC.

Error Correcting Output Codes

Error Correcting Output Codes are an approach to building composite multi-class classifiers developed by Dietterich and Bakiri [2]. Like other composite multi-class and multi-label classifiers, it reduces the classification problem to a set of F binary classifiers, where F is generally on the same order of magnitude as the number of classes.

An ECOC classifier defines a $\{+1, -1\}$-valued code matrix, R, that determines how the training data is split among the F binary classifiers. R is a $|C| \times F$ matrix, where the i-th row of R defines the code for class i, and the j-th column of R defines how the training documents are split among classifier j. R_{ij} therefore refers to a document in class i and binary classifier j.

To train the classifier on a document d with class label i, one iterates through all F classifiers ($j \in \{0 \ldots F - 1\}$). If $R_{ij} = +1$, then a document in class i will be presented as a positive example to binary classifier j; similarly, if $R_{ij} = -1$, then a document in class i will be presented as a negative example to binary classifier j.

The structure of R determines the characteristics of the ECOC classifier. One vs. All can be constructed by placing $+1$ on the diagonal of a $|C| \times |C|$ matrix, and -1 elsewhere (Equation 4.17).

$$\text{One vs. All Matrix} = \begin{bmatrix} +1 & -1 & -1 \\ -1 & +1 & -1 \\ -1 & -1 & +1 \end{bmatrix} \tag{4.17}$$

Dietterich and Bakari fill their code matrix with BCH codes, which are constructed to have error-correcting properties. Their thesis is that if the minimum Hamming distance between any two rows of R is m, then the resulting multi-class classifier will be able to correct $\left\lfloor \frac{m-1}{2} \right\rfloor$ errors [2]. Columns define how the training data is split among the F classifiers; if two columns of the matrix R are identical (or the opposite of each

other), then they will make identical errors. Comparing Dietterich and Bakari's BCH codes to the One vs. All matrix, we note that the One vs. All matrix has independent columns, but its rows have no error correcting properties. Dietterich and Bakari provide their BCH error correcting codes at http://www-2.cs.cmu.edu/~rayid/ecoc/.

To classify a document d', one computes $\{f_0(d'), \ldots, f_{F-1}(d')\}$, where $f_j(d')$ is the result of running binary classifier j on a training document d'. Then, the document class is determined by finding which row of R is most similar to the matrix row represented by $\{f_0(d'), \ldots, f_{F-1}(d')\}$:

$$argmin_{i \in C} \sum_{j=0}^{F-1} \left(\frac{1 - sign(R_{ij} f_j(x))}{2} \right) \qquad (4.18)$$

This equation computes the Hamming distance between row i of the code matrix R and the classifier output, $\{f_0(d'), \ldots, f_{F-1}(d')\}$, and selects the row with the minimum Hamming distance.

From the existing literature [2, 19], it appears that Error Correcting Output Codes provide slightly better performance than a One vs. All classifier. However, it should be noted that the difference is generally small, and that the simplicity of implementing a One vs. All classifier probably outweighs any slight gain in accuracy that could be obtained by using an ECOC classifier.

4.3.4 Other Composite Multi-Class and Multi-Label Classifiers

There are a number of other composite multi-label and multi-class classifiers, but while One vs. All and ECOC train $O(|C|)$ binary classifiers, many of the alternative classifiers require training orders of magnitude more classifiers.

All vs. All, for example, trains $\frac{|C|(|C|-1)}{2}$ pairwise classifiers, each separating a pair of classes. It performs about as well as One vs. All [19], but at a huge cost.

4.3.5 Naive Bayes

Naive Bayes is a powerful, linear-time classifier described in Section 4.2.2. The mathematical machinery for both the binary classifier and multi-class classifier versions of Naive Bayes are identical; the binary classifier version of Naive Bayes only computes class probabilities for two classes, while the multi-class version operates on an arbitrary number of classes.

4.3.6 Rocchio

The Rocchio classifier [21] is one of the most widely used learning algorithms. While it was originally designed for optimizing queries from relevance feedback, the algorithm can be adapted to text categorization problems. The algorithm is fairly intuitive, is easy to implement, and yields acceptable results on a broad range of classification tasks. The Rocchio classifier was implemented mostly for debugging and development purposes; Naive Bayes (Section 4.3.5) is also linear-time, and performs much better on common classification tasks [10], so there is little reason for production systems to use Rocchio.

Rocchio is natively a multi-class classification algorithm; classification is accomplished by computing the similarity of a test document and $|C|$ vectors representing each class. The test document is assigned the class that it is closest to. The positive and negative examples for each class are weighted and then combined into one class vector.

To train a Rocchio classifier, one must compute a word frequency vector, d, from a training document. Rocchio is typically paired with IDF; the IDF algorithm (Section 2.2.3) is generally run on the training corpus, which produces an updated word frequency vector, d_{idf}. Finally, each document vector may be normalized by the length of the document so that the classifier is not biased towards longer documents:

$$d_{norm} = \frac{d_{idf}}{||d||} \tag{4.19}$$

Training a Rocchio classifier is simple; the word frequency vectors of each docu-

ment are combined to form a word frequency vector that represents an entire class. A class's characteristic vector is computed as follows:

$$C_j = \alpha \frac{1}{|C_j|} \sum_{d \in C_j} d_{norm} - \beta \frac{1}{|D - Cj|} \sum_{d \in D - C_j} d_{norm} \tag{4.20}$$

C_j represents the characteristic vector for class j. D is the set of all documents. α and β are constants that specify the relative weights of positive and negative words (i.e. how many negative words it takes to cancel out a positive word). As recommended by [10] we use $\alpha = 16$ and $\beta = 4$. To classify a new document, d', one compares d' to all classifiers C_j using a similarity measure. The document is assigned the class that it is most similar to. The similarity measure used is the cosine of the angle between two vectors, which is easily computed as follows:

$$\cos(d', C_j) = \frac{d' \cdot C_j}{||d'|| * ||C_j||} \tag{4.21}$$

To classify a document d', we compute

$$argmax \sum_{j=1}^{|C|} cos(d', C_j) \tag{4.22}$$

4.4 Classifier Performance

This section describes performance evaluations of the classifiers in the Haystack Learning Framework. The goal of this thesis is to develop a robust learning framework, not to develop a new classifier and perform extensive benchmarking and analysis on this classifier. As such, the performance metrics used to evaluate the classifiers are relatively unsophisticated; we simply want to ensure that the classifiers are working as advertised, and are not buggy.

Section 2.5 describes the methodology used to evaluate classifier performance. This section contains the results of testing Haystack's classifiers using the previously defined methodology.

RLSC Parameter Tuning

Rifkin's thesis [19] states that the RLSC algorithm is relatively unaffected by parameter tuning, but I found that this to be far from the case. RLSC has a single parameter, $\ell\lambda$, that quantifies one's willingness to trade off error on the training set with the risk of overtraining. When run with the $\ell\lambda$ parameter equal to 1, as recommended in Rifkin's thesis, binary classification performance was dismal. Empirical testing with different values of $\ell\lambda$ showed that the best performance was achieved with a much larger value of $\ell\lambda = 2000$.

4.4.1 Binary Classifiers

Binary classifiers are tested using my Personal Spam Corpus and the "acq" and "wheat" categories of the Reuters corpus.

Spam Corpus

The Spam Corpus contains 3,360 total messages, 1,613 of which are spam and 1,747 of which are not spam. There were 1,694 messages in the test set.

RLSC

	Actual TRUE	Actual FALSE
Classified Positive	772	33
Classified Negative	49	840

Statistic	Value
Correct predictions	95.1%
Incorrect predictions	4.8%
Sensitivity	0.940
Specificity	0.962

Naive Bayes

	Actual TRUE	Actual FALSE
Classified Positive	721	21
Classified Negative	100	852

Statistic	Value
Correct predictions	92.8%
Incorrect predictions	7.1%
Sensitivity	0.878
Specificity	0.975

Reuters "acq"

The Reuters corpus was split into training and test sets, with 5,082 news articles in the test set, 1,103 of which are in the "acq" category.

Joachims [10] achieves accuracy rates of around 90% using Naive Bayes on the Reuters "acq" category.

RLSC

	Actual TRUE	Actual FALSE
Classified Positive	883	94
Classified Negative	220	3885

Statistic	Value
Correct predictions	93.8%
Incorrect predictions	6.2%
Sensitivity	0.800
Specificity	0.976

Naive Bayes

	Actual TRUE	Actual FALSE
Classified Positive	931	185
Classified Negative	172	3794

Statistic	Value
Correct predictions	92.9%
Incorrect predictions	7.1%
Sensitivity	0.844
Specificity	0.953

Reuters "wheat"

The Reuters corpus was split into training and test sets, with 5,082 news articles in the test set, 125 of which are in the "acq" category.

Joachims [10] achieves accuracy rates of around 95% using Naive Bayes on the Reuters "acq" category.

RLSC

	Actual TRUE	Actual FALSE
Classified Positive	84	10
Classified Negative	41	4947

Statistic	Value
Correct predictions	98.9%
Incorrect predictions	1.1%
Sensitivity	0.672
Specificity	0.997

Naive Bayes

	Actual TRUE	Actual FALSE
Classified Positive	102	124
Classified Negative	23	4833

Statistic	Value
Correct predictions	97.1%
Incorrect predictions	2.8%
Sensitivity	0.816
Specificity	0.974

4.4.2   Multi-Class Classifiers

Multi-class classifiers are tested using the Twenty Newsgroups dataset. There are a total of 18,826 newsgroup messages distributed roughly evenly across twenty newsgroup categories. There are 9,410 messages in the test set.

Rocchio and Naive Bayes are natively multi-class classifiers, while the One vs. All and ECOC classifiers are composite classifiers that build upon binary classifiers. We test One vs. All and ECOC with both Naive Bayes and RLSC as the underlying binary classifier.

The ECOC classifiers use the code matrices provided by Dietterich and Bakari at http://www-2.cs.cmu.edu/~rayid/ecoc/. The 63-classifier, 20-category BCH matrix was used to perform the Twenty Newsgroups classification task.

Classifier	% Correct	Previous Results
Rocchio	83.2%	≈80% (Joachims [10])
Naive Bayes	85.3% ≈84%	(Joachims [10])
One vs. All (Naive Bayes)	75.2%	*n/a*
One vs. All (RLSC)	79.4%	86.9% (Rifkin [19])
ECOC (Naive Bayes and BCH-63)	87.6%	*n/a*
ECOC (RLSC and BCH-63)	85.1%	87.5% (Rifkin [19])

Rifkin also used the BCH-63 matrix, so the results are directly comparable.

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Chapter 5

Haystack

This chapter describes the design and implementation of Cesium, an auto-classification agent for Haystack, and Haystack's first real autonomous agent.

Cesium's job is to learn a model from a Haystack categorization scheme, and to apply this model to any new documents in a collection. Cesium produces a set of predicted class labels for a document, and annotates the document with its predictions. These annotations are distinct from the document's manually assigned categories, and while the classifier's predictions are displayed in the UI, the predicted categories do not affect any other aspect of UI operation; the rest of the Haystack UI is still keyed-off of the manually assigned category. The classifier's predictions are an unobtrusive but valuable addition to the categorization UI.

Cesium is backed by the learning framework's Fuzzy Simple Multi-label classifier, which is described in Section 4.3.1. The aforementioned "fuzziness" allows Cesium to assert facts about documents with varying degrees of confidence, and is discussed below in Section 5.2. The fuzziness extends beyond training, and encompasses the classifier's predictions as well; the classifier does not make a simple binary decision regarding class membership – a document is not simply in or out of a class – but, instead, the classifier produces a list of potential categories, ranked by their likelihood according to the classification model.

5.1 Problem Specification

An auto-classification agent should have the following characteristics:

- *The classifier must be able to place documents in more than one category.* Some types of classifiers assume that documents are only a member of exactly one class. While these classifiers might be appropriate for a traditional e-mail handling program, where an e-mail is located in exactly one folder, Haystack's flexible categorization scheme requires the flexibility of a multi-label classifier, which can label a document with any number of categories.

- *The classifier must be kept fresh.* Training a classifier is a time-consuming process, and cannot be done incrementally. The auto-classification agent must conserve system resources (i.e. re-training every time a document is added is most likely not an option) but maintain a relatively fresh corpus.

- *The user must be able to specify arbitrary "training" and "test" sets.* While the notion of a training and set set has little meaning on a real-world classification system – it is mostly an artificial distinction made in research classifiers – the user must be able to tell the classifier to learn from a set of documents and to apply its model and classify another set of documents.

- *The classifier must not train over its own predictions, even if its "training" and "test" sets refer to overlapping collections of documents.* The job of a classifier is to predict new categories for a document, but these predictions may not be accurate, and the user may not correct all mis-classifications. If the classifier trains using its predicted data, classification performance will suffer; there must be a mechanism for distinguishing the predicted categories from the actual, manually-specified categories.

- *The user must be able to correct mis-classifications.* The classifier should learn from its mis-classifications, and it must remember all corrections.

5.2 Fuzzy Categorization

One of the chief benefits of Haystack is its ability to manage semi-structured information. Haystack provides a powerful infrastructure for storing semi-structured information, and allows users to easily navigate this semi-structured information. Unfortunately, machine learning problems are typically highly structured. Most machine learning algorithms have an absolute and exclusive definition of categories; if a document is a member of a category, then it is definitely not a member of any other category.

Haystack's flexible, semi-structured ontology is at odds with the restrictive assumptions commonly made in machine learning systems. A typical Haystack might contain a few manually categorized documents that are known to be in specific categories, a few manually categorized documents that have no category labels, but are known to not be in specific categories, and a large body of uncategorized documents. Additionally, unlike in a typical e-mail program, where the fact that an e-mail message is located in the Inbox implies that the e-mail message is not located in any other folder, in Haystack, the fact that a document is marked as a member of a category does not preclude it from being a member of another category.

In order to model the uncertainty inherent in a semi-structured data model, the machine learning algorithms have been augmented to handle "fuzzy" categories. Fuzzy categorization is accomplished by annotating each document presented to the classifier with a confidence value that quantifies how certain one is about a set of category labels. Further details are provided in Chapter 4.

Cesium, in its current incarnation, uses fuzzy categorization in a very simplistic way to model only one type of categorization uncertainty, described in Section 5.4.2.

5.3 A Cesium Agent's Properties

A Cesium agent has a number of properties that govern how it works:

- *The set of training documents.* Haystack lets the user define arbitrary cate-

Figure 5-1: Cesium Properties. The "Sharing," "Access Control," and "Locate additional information" property headings are provided by Haystack, and are not relevant to this thesis.

gorization schemes, and an arbitrary number of these categorization schemes define the training data for Cesium's classifier. A categorization scheme, an example of which is shown in Figure 5-2, is defined by a set of possible categories, and the documents in the Haystack that have these categories. As such, documents that have no category are not considered part of a categorization scheme, and are not considered by the classifier.

New categorization schemes can be added by dragging and dropping them on the appropriate place in the Cesium properties page (see Figure 5-1).

- *The set of test documents.* An Cesium agent can have any number of test sets, or "autoclassify collections." The Cesium agent monitors these autoclassify collections, and when new documents appear, it annotates them with its predictions.

  An agent's autoclassify collections are the collections where the classifier will apply its model. Cesium monitors the autoclassify collections for changes, and when a new document is added, it runs the classifier and annotates that document with its predictions. A collection can be added to an agent's list of autoclassify collections by dragging and dropping the collection in the appropriate place in the Cesium properties page (see Figure 5-1).

- *Training Schedule.* Training is a resource-intensive process, and cannot be done incrementally. The Cesium agent retrains itself every hour, by default, though this time period can be adjusted. There are other training schemes, some of which are documented in Section 2.4.2, but Cesium simply re-trains itself on an interval.

5.4   Classification and Correction

Classification occurs automatically when new documents appear in a Cesium agent's "autoclassify collections." The predictions of the classifier are distinct from the manually generated labels. This is done for two reasons:

- *Classifier inaccuracy.* The classifiers discussed in this thesis perform well, but an 80-90% classification accuracy is far from perfect. The UI is currently keyed off of a document's manually specified labels – all navigation and organization UI components use the manually specified labels. The classifier's recommendations are displayed as just that – tentative recommendations – and accomplishing this requires that the manually generated labels be distinct from the classifier's predictions.

- *The classifier must not train off of its own predictions.* The classifier only trains off of manually labeled categories; classifier performance would suffer if the classifier trained off of its predicted labels.

5.4.1 The Data Model

A document's category or predicted category is represented by annotating that object with one of three possible types of annotations:

- *memberOf.* This assertion is used when a user manually assigns a document to a category.

- *notMemberOf.* This assertion is used when a user manually indicates that a document is not a member of a category.

- *predictedMemberOf.* This assertion is used by the classifier to predict a document's category.

A Belief Engine

This data model is inelegant in that it introduces a new type of memberOf assertion, predictedMemberOf, that represents a specialized form of membership asserted by a single agent, Cesium. While this is an acceptable short-term fix, if every type of agent made its own, specialized assertions about class membership, the data model would quickly become cluttered.

The elegant way to implement predictedMemberOf is to use a belief system. A belief system takes the disparate memberOf assertions provided by each agent, determines how much we trust each of the assertion's creators, and filters the results accordingly. A belief system obviates the need for separate types of memberOf assertions such as predictedMemberOf.

5.4.2 Training a Fuzzy Classifier

Much ado has been made about the "fuzziness" of some of the classification algorithms in Chapter 4. A traditional multi-label classifier makes the assumption that if a document is in set of categories, then it is not in all other categories. While this assumption is an inaccurate description of Haystack's categorization ontology, it does have the benefit of generating a large number of negative training examples. Haystack does provide a mechanism for users to assert that a document is not a member of certain categories, but it's unlikely that users will manually negatively label many documents. Documents will most likely be assigned negative labels only when the classifier mis-predicts an item's category and the user corrects this prediction; we estimate that there will be significantly fewer negative examples than positive examples.

It's likely that there wouldn't be sufficient data to build a robust model if the classifier trained only on the user's explicit categorizations. We use the traditional categorization assumption – that a document that is a member of a set of classes is not a member of all other classes – to generate additional negative training examples, but we tell the classifier that these examples are "weak."

Fuzzy classifiers associate each set of document's labels with a confidence value that quantifies how certain we are about the document's categorization. We are absolutely certain about manually classified documents, and they are presented to the classifier with a confidence value of 1.0. Documents generated by the traditional categorization assumption are presented to the classifier with a much smaller confidence value.

To summarize:

Figure 5-2: Haystack's Organize Pane

- *Assertions made by the user are presented as concrete examples.* If the user manually labels a document as either a positive or negative example of a category, then the document and its label are presented to the classifier with a confidence value of 1.0.

- *Negative examples generated by the traditional categorization assumption are given weak confidence values.* Machine-learning problems typically assume that if a document is a positive example for a set of classes, then it must be a negative example for all other classes. This assumption is generally not true in Haystack, but without this assumption there wouldn't be sufficient numbers of negative examples in each class for most learning algorithms to generate an effective model. Class labels generated by this assumption are presented to the classifier with a weak confidence value.

5.4.3 The Classification User Interface

A good user interface for classification must have the following capabilities:

- *The UI must be able to denote that a document is in a category, is not in a category, or that a document's category is unknown.*

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- *The classifier's predictions must be displayed in a unobtrusive way.* The classifier will be incorrect frequently enough that the classifier's recommendations should not significantly alter the UI – i.e. the classifier's predictions should not be used for navigation.

- *Users must be able to correct and validate predictions.* If the classifier's prediction is correct, then the user must be able to validate this prediction. Similarly, if the classifier's prediction is incorrect, then the user must be able to correct this mis-classification.

- *Different predictions have different strengths.* Not all predictions are created equal; the classifier might be very confident about one prediction, but uncertain about another. The user interface should differentiate between the different prediction strengths.

Cesium's categorization user interface is simple and easy to use, but contains a lot of functionality and renders a lot of information. The centerpiece of the categorization UI is the "Organize" pane, which is displayed in Figure 5-2.

The most important job of a categorization UI is to display membership – i.e. whether a document is or is not in a category. This is accomplished by a series of check boxes adjacent to the category names. If a document is in a category – if there is a memberOf assertion connecting the document with a category – then a check appears in the check box adjacent to the category. The absence of a check implies that either the user has not labeled the document, or that the document is not in that category. The user cannot distinguish between the two cases, but they are represented differently in the underlying data model, and are used differently by the classifier. Documents that are not in a category have have a notMemberOf assertion connecting the document and the category, while an unknown category has either a memberOf or a notMemberOf assertion. To the classifier, documents that are definitely not members of a category are regarded as concrete negative examples, while documents with unknown labels are passed on to the classifier as "weak" negative examples of those categories.

Predictions are displayed in the user interface via a light bulb – if a light bulb appears next to a category, then the classifier has predicted that the current document is in the category. The intensity of the color of the light bulb indicates the strength of the prediction – a deep yellow light bulb indicates that the classifier is fairly confident in its prediction, while a light yellow light bulb indicates that the classifier is relatively uncertain of its prediction.

The classifier's predictions can be validated by clicking on the light bulb – clicking the light bulb will change the tentative predictedMemberOf assertion to a concrete memberOf assertion, will remove the light bulb from the user interface, and will place a check next to the category. To correct a classification, a user clicks on a light bulb and then unchecks the category.

5.5 Oscar

Cesium is the name of a general type of auto-categorization agent backed by a Simple Multi-Label classifier that learns from a categorization scheme and applies its model to a collection. To set the machine learning machinery in motion, you must create an instantiation of a Cesium agent, and configure the Cesium agent's properties. Oscar is currently the only Cesium agent in Haystack. By default, Oscar trains on any indexable document, and automatically classifies items in the Haystack Inbox.

Oscar trains over all Haystack content, but new instantiations of Cesium should probably specialize on a specific type of information. For example, a new classification agent, Einstein, could be created to categorize research papers.

Chapter 6

PorkChop: An Outlook Plugin for Spam Filtering

This section describes the implementation of a spam-filtering Microsoft Outlook plugin using the learning algorithms described in Chapter 4. Outlook was chosen because it has a dominant market share, and because its API is much more flexible than the plug-in APIs of other competing programs like Eudora.

Spam Filtering Tools

There are a large number of spam filtering programs out there. A search of download.com for "spam filter" yields over 100 Windows programs – and this excludes the UNIX universe. This section discusses, in-depth, several popular spam-filtering programs and techniques.

Spam filtering programs, in general, are far from state of the art. The most common spam filters these days use rules-based filtering; only recently have naive bayesian filters started appearing in popular spam detection packages.

Blacklists

Blacklists were the earliest means of spam filtering. A blacklist is a simple concept – various groups like MAPS, SPEWS, and Spamhaus [26, 27, 25] respond to complaints

from users and compile a list of originating domains that are used to send spam. ISPs that subscribe to the blacklist then block all e-mail messages (or even all network traffic) from these domains. Early blacklists were met with open arms – blacklists were viewed by ISPs as a way to reduce the network traffic associated with spam and therefore lower their costs, all while pleasing their customers [5].

However, spammers have adapted well to the challenge posed by blacklists. They often hop from SMTP server to SMTP server, operating one step ahead of the blacklists. An article in Network World [4] references a study that found that the MAPS RBL, one of the most popular blacklists, blocked only 24% of actual spam messages, but blocked 34% of legitimate messages. Such results are absolutely abysmal and even the most unsophisticated content-based filters can easily accomplish better classification performance.

Additionally, the spam blacklist maintainers have made many enemies by adopting a "shoot first and ask questions later" blacklisting policy. In one rather exceptional case [4], one customer of the iBill electronic billing service complained to MAPS about unsolicited e-mail from one of iBill's clients. The e-mail was not even sent from iBill itself – it was sent by one of iBill's thousands of customers. MAPS not only placed the accused spammer on their Realtime Blacklist (RBL), but they placed all of iBill's IP addresses on the blacklist as well. iBill received no warning – only complaints from customers confused by the blackout – and lost over $400,000 during the four-day blackout. The blacklist maintainers' heavy-handed tactics have won them few fans among IS managers at blacklisted companies – "There's no appeals process once you're blacklisted. The MAPS folks were arrogant and pompous to deal with. They're out of control."

CRM114

The CRM114 "Controllable Regex Mutilator" is a system to process large data streams, and has been used to build a Naive Bayes e-mail filtering system. The author makes impressive claims about the accuracy of the software – it is over 99% accurate on a corpus of 5,800 messages – but his results have not been independently

and rigorously verified.

While most machine learning systems generally try to reduce the number of features, both to reduce computational requirements and to decrease the potential for over training, the CRM114 system tries to generate as many features as possible by moving a 5-word sliding window over the incoming text and generating subphrases from this 5 word window. See Section 2.1.1 for more information on CRM114's phrase expansion algorithm.

Spam Assassin

Spam Assassin is a framework for combining disparate spam detection techniques. Rather than use one technique – Naive Bayes statistics or rules-based detection algorithms – Spam Assassin provides a framework to combine any number of heuristics. SpamAssassin maintains a table of different spam detection techniques. Each entry in the table has two components: 1) code to calculate the specific metric, and 2) the weight of the metric. Most of the metrics are typical rules-based metrics, but one of the metrics is the Naive Bayes classification of the e-mail message. To classify a message, Spam Assassin runs each metric in the table, and adds up the weights of the triggered metrics; if they exceed a specified threshold, then the message is marked as spam. Spam Assassin runs a genetic algorithm on the spam detection table, altering the weights of each classification technique until it maximizes the classifier's efficiency.

There are a number of possible ways to combine traditional rules-based systems and Naive Bayes classifiers, and the Spam Assasin designers believe that they have found the best way to combine the power of the two respective approaches. It's easy to write a rule to detect a malformed e-mail message header (indicative of spam), but it's much more difficult to, for example, determine a numerical measure of how malformed a header is, and then use that measure as a feature in a message's word frequency vector.

The Spam Assasin team experimented with using Naive Bayes to learn different measures of "spammishness" in the text (i.e. the number of ALL CAPS words), but found this to be ineffective. Most spam metrics are positive – i.e. they are designed

to identify spam, rather than identify non-spam – but machine learning algorithms work best when the feature vectors contain both positive and negative metrics. The rule table used in Spam Assassin is additive, which is better suited for positive spam metrics; if a rule is triggered, then the weight associated with that rule is added to the spam metric. Naive Bayes is implemented as a single entry in the rule table, though the genetic algorithm usually gives a high weight to the output of the Naive Bayes classifier.

6.1   PorkChop Implementation

The Outlook spam filter plugin uses the learning framework provided in Chapter 4. The Outlook filter uses the binary classification algorithms provided by the learning architecture – specifically the Regularized Least Squares Classification algorithm – to classify spam.

When PorkChop is first installed, it must be initialized with e-mail messages from the user's Inbox; PorkChop does not come pre-programmed with a spam database. When new messages are downloaded from the e-mail server, PorkChop runs these messages through the learning framework and produces a predicted classification for each message. Messages that are suspected to be spam are invisibly marked as such via an Outlook CustomProperty, and are moved by Outlook's filtering mechanisms to a special Spam folder. New buttons in the Outlook interface are provided to handle mis-classified e-mail.

Training the classifier is a resource-intensive process, and cannot be done incrementally. The classifier can be trained on demand, but it is automatically run when there are more than 100 new messages in the "to be trained" queue, or when there is a message in the queue that has been around for more than eight hours.

In addition to the binary classifier, PorkChop uses whitelists to properly classify e-mail. The whitelists are manually maintained – users must add e-mail addresses. Messages from users on the whitelist are not run through the classifier; whitelists reduce both false positives and total total computation time.

The Haystack Learning Framework is written in Java, but it takes a substantial amount of work to bridge the gap between Microsoft Outlook and Java. Microsoft Outlook provides a very robust scripting interface via Visual Basic for Applications (VBA). While VBA is well-suited for GUIs and other lightweight tasks, more heavy-duty tasks are often offloaded onto COM modules. COM stands for Component Object Model, and is Microsoft's distributed object system. Java modules can export COM interfaces, but, unfortunately, Java support for COM ties you to a specific VM; Microsoft provides support for COM interfaces in its VM, while Sun's VM supports COM interfaces via JavaBeans. SWT provides VM-independent COM interface support, but then you're tied to the SWT library; the SWT library comprises about a megabyte – not exactly lightweight.

Ironically, the easiest way to interface the Java machine learning code with Outlook's VBA is to use C++. Microsoft Visual C++ has excellent support for COM development, and JNI allows C++ functions to call Java code. Because there were only a few functions (addDocument, train, and classify), it was easy to write a C++ COM wrapper for the Java learning functions. When an action needs to be performed in Outlook (i.e. a message must be classified), Outlook VBA code calls C++ COM code, which uses JNI to invoke the Haystack Learning Framework.

6.2 Performance

PorkChop uses whitelists and the RLSC algorithm to filter spam messages from Outlook. The performance metrics in Section 4.4 show that RLSC can distinguish spam with roughly 95% accuracy. This is impressive, but there are better frameworks for spam detection.

SpamAssassin, described in Section 6, uses a combination of static rules and dynamic machine learning algorithms (Naive Bayes) to detect spam. While machine learning algorithms perform extraordinarily well by themselves, some attributes of spam are extremely difficult to quantify and present as a feature to a machine learning algorithm. For example, spam e-mails often have malformed e-mail headers; it's
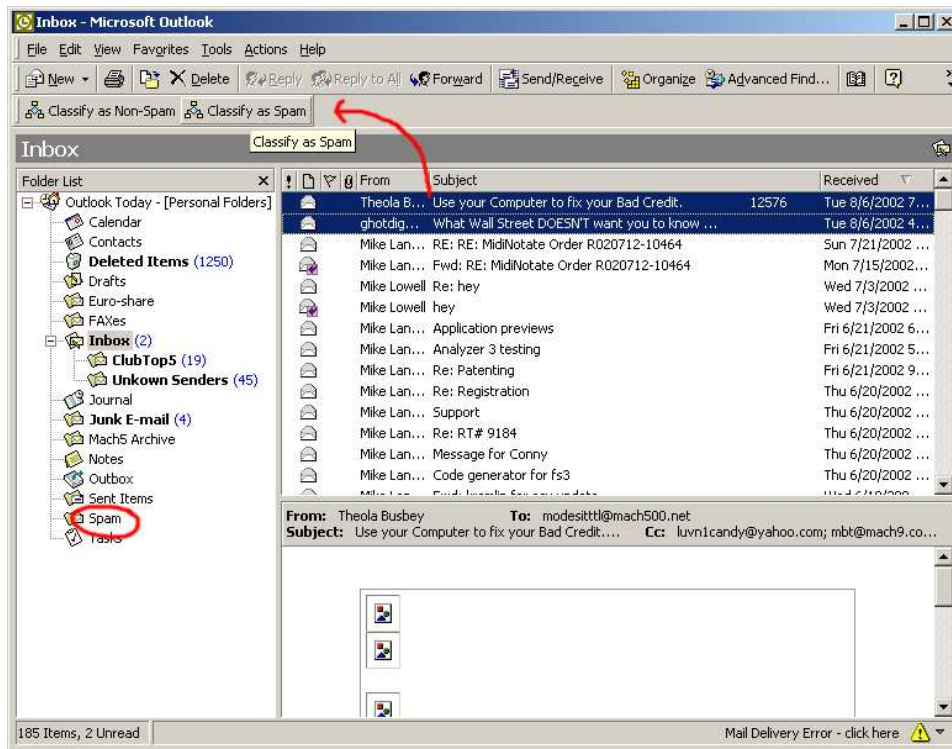
Figure 6-1: PorkChop in action

difficult to make a machine learning algorithm learn whether a header is well-formed or malformed, but it's easy to write a rule that determines the validity of an e-mail header.

SpamAssassin's hybrid approach to spam detection is more robust than Pork-Chop's machine-learning only spam detection algorithms. Were I to write PorkChop again, I would not code it as a stand-alone application; I would incorporate it into the SpamAssassin codebase.

Chapter 7

Cholesterol

7.1   Introduction

Resource Description Framework, or RDF, forms the backbone of Haystack; all data in Haystack is stored in RDF. Haystack's RDF store is called Cholesterol, and because of RDF's central role in Haystack, the design, features, and performance of Cholesterol have a major effect on Haystack. RDF statements are triples – a subject, predicate, and object, and Cholesterol is a database that is purpose-build to store these RDF triples.

Because Cholesterol is the backbone of Haystack, it is placed under a very high query load. For Haystack to be sufficiently responsive to user interface commands, Cholesterol must be able to execute thousands of queries per second over a typically 80-120 megabyte corpus. Cholesterol bears little resemblance to the common notion of a database – i.e. one that supports transactions, tables, and can be manipulated using SQL. Clients interface with Cholesterol using a Java API; the overhead of creating a connection and parsing the SQL query is too great to achieve the kind of performance expected by Cholesterol. Unlike SQL, which has a rich query syntax, Cholesterol's query interface is very minimalistic; the only tools one has to work with are wildcards and joins.

As of the writing of this thesis, there are three versions of Cholesterol. Cholesterol1 is the first incarnation of the Cholesterol database, and was a hasty C++ port of a

Java database. Cholesterol1 indexed its RDF triples with an eye toward the common case; as long as the predicate of a query is not a wildcard, Cholesterol1 can execute the query fairly quickly. However, because Cholesterol1 was quickly written, its code was not very readable, and the complexity of the code led to a number of nagging, virtually unsolvable bugs. Cholesterol2 uses the same architecture as Cholesterol1, but is completely rewritten with the goal of improving code readability. Unfortunately, due to memory copying overhead in the query execution code, Cholesterol2 is only half as fast as Cholesterol1. Cholesterol3 is a completely new take on the Cholesterol database that manages its own memory and indexes all fields.

7.2   Cholesterol API

This section discusses the Cholesterol API that is implemented by all Cholesterol databases. The Java interface IRDFStore defines the Java interface that must be implemented by an RDF Store, but because of the need for speed, all three Cholesterol databases are written in C++. The CholesterolRDFStore implements IRDFStore, and specifies that the following JNI native interfaces must be provided by a C++ Cholesterol database.

```
class CholesterolRDFStore
    native void doNativeInit(String basePath);
    native void doNativeKill();

    native boolean add(String subj, String pred, String obj, String id);
    native boolean addAuthored(String subj, String pred, String obj, String id, Object [] authors);
    native void remove(String ticket, Statement s, Resource[] existentials) throws ServiceException;

    native Set query(String ticket, Statement[] query, Resource[] variables, Resource[] existential)
        throws ServiceException;
    native Set queryMulti(String ticket, Statement[] query, Resource[] variables,
        Resource[] existential, RDFNode [][] hints) throws ServiceException;

    native boolean contains(String subj, String pred, String obj);
    native RDFNode extract(String ticket, Resource subject, Resource predicate, RDFNode object)
        throws ServiceException;

    native Resource[] getAuthors(String ticket, Resource id) throws ServiceException;
    native Resource[] getAuthoredStatementIDs(String ticket, Resource author) throws ServiceException;
    native Statement getStatement(String ticket, Resource id) throws ServiceException;
}
```

Figure 7-1: The native interface provided by each C++ Cholesterol database

- *doNativeInit.* The doNativeInit function initializes the Cholesterol database.

- *doNativeKill.* The doNativeKill function indicates to Cholesterol that Haystack is shutting down, and that Cholesterol can begin to free up its internal data structures. However, practically, queries continue to be issued to Cholesterol even after the doNativeKill function is called. Implementations of doNativeKill should flush any buffers to ensure that Cholesterol's state is written to disk, but doNativeKill should not delete any data structures because Cholesterol must handle queries even after doNativeKill is called.

- *add.* The add method adds an RDF triple, plus a unique identifier, to the Cholesterol database. After the add function is called, subsequent calls to query must reflect the updated database state. However, Cholesterol is not a transactional database; after a crash, Cholesterol does not have to recover the exact pre-crash state, which allows for faster add performance. Adds are written to a log (more details in Section 7.4.3).

- *addAuthored.* The addAuthored method has the same interface as add, except that it takes an additional argument that represents the authors of a specific statement. The *authors* parameter is an array of Object classes, whose toString() values are stored in the database and are used to answer queries to the getAuthors and getAuthoredStatementID methods, which are part of the belief layer described in M. Zhurakhinskaya's thesis [29].

- *remove.* The remove function removes the given RDF triple from the database. The RDF triple may be fully specified (i.e. no wildcards), or it may include wildcards. The wildcard matching scheme is implemented in the same manner as in the query method. C++ implementors of remove must make a JNI call to the CholesterolRDFStore.addToRemoveQueue method, which is used to implement triggering. Removes are written to a log (more details in Section 7.4.3).

- *query.* The query method queries the Cholesterol database. The query method

takes an arbitrary number of RDF triples that may contain wildcards. If a query has more than one RDF triple, then Cholesterol performs a join across the triples. Section 7.3 discusses Cholesterol queries in detail. The *existential* argument to query contains an array of RDFNodes which represent the existentials used in the query. The *variables* argument contains an array of Resources that must be a subset of the Resources in the *existential* argument.

The query method returns a Set that contains all of the possible existential bindings. Each element of the Set is an array of RDFNodes, and the existentials in the RDFNode array are stored in the same order as the existentials were specified in the *variables* array. For example, if the first element of *variables* is the existential `?x`, then the first element of every RDFNode array corresponds to the value of the existential `?x`.

- *queryMulti.* The queryMulti method has the same interface as query, with the addition of a *hint* parameter. This parameter provides data that restricts the values of some variables in the query. The data in the n-th row of the *hint* parameter represents the set of all allowed values for the n-th existential in the existential parameter. If data is present for an existential (i.e. the row is not null), then that existential is constrained to one of the given values. The *hint* parameter is used to optimize federation, which is an inter-database join.

- *contains.* The contains method takes as an argument a single RDF triple (no wildcards allowed), and returns true if that triple exists in the database.

- *extract.* The extract method is a specialized form of query. Exactly one of the arguments to extract must be null, which implies a wildcard in that position. The extract method will then execute the query defined by the RDF triple and return one of the possible values of that existential. If there are many values for the existential, then extract is free to return any possible value.

- *getAuthors.* The getAuthors method returns all authors of a given statement ID (or null if the statement has no authors). The getAuthors method is used

to implement authoring, which is described in M. Zhurakhinskaya's thesis [29].

- *getAuthoredStatementIDs.* The getAuthoredStatementIDs returns the statement IDs created by a given author. A statement ID uniquely identifies a statement, and is specified in calls to the add or addAuthored methods. The getAuthoredStatementIDs method is used to implement authoring, which is described in M. Zhurakhinskaya's thesis [29].

- *getStatement.* The getStatement method returns the RDF triple associated with the given statement ID. The statement ID uniquely identifies a statement, and is specified in calls to the add or addAuthored methods.

Cholesterol may be called from within multi-threaded client programs, and must, therefore, be thread-safe.

7.3   Queries

This section describes how to query a Cholesterol database. The following database is used in all subsequent examples.

Subject	Predicate	Object
mark	likes	melanie
mark	likes	robert
melanie	likes	joe
beth	likes	joe
mark	hates	kim
melanie	likes	steve

Cholesterol supports a very minimalist query interface. A query is composed of an arbitrary number of RDF statements, which may or may not contain wildcards. A wildcard – also called an existential – will match any possible row. For example `mark likes ?x` matches:

?x
melanie
robert

Existentials, by convention, are prefixed with ?, but practically, an existential is any value specified in the *existential* parameter of the *query* or *queryMulti* methods. A query may contains any number of existentials – `?x ?y ?z` matches all rows in the database.

A query consists of an arbitrary number of statements. If there is more than one statement in a query, then the results of querying the database for each individual statement are combined using a join. A join combines values with similar existentials. For example, `mark likes ?x, ?x likes ?y` matches:

?x	?y
melanie	joe
melanie	steve

If the statements in a query do not share any common existentials, Cholesterol joins the statements by computing their Cartesian product. For example, `mark likes ?x, melanie likes ?y` produces:

?x	?y
melanie	joe
melanie	steve
robert	joe
robert	steve

7.4   Cholesterol1 and Cholesterol2

This section describes the architecture of Cholesterol1 and Cholesterol2. Cholesterol2 uses the same architecture as Cholesterol1, but the Cholesterol2 code is vastly more readable than the Cholesterol1 code. Cholesterol1 was written quickly, and its code is difficult to maintain; there are several nagging bugs in the query code of Cholesterol1

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have proven to be nearly impossible to fix. Cholesterol2 is a ground-up rewrite of Cholesterol1 that fixes the query bugs and has a much more elegant design. Unfortunately, due to not-clearly-understood causes – most likely memory copying overhead in the query code – Cholesterol2 is about twice as slow as Cholesterol1.

Because Cholesterol1 and and Cholesterol2 have the same architecture, they are discussed together.

7.4.1 Indexing

Conceptually, the RDF store can be viewed as a flat table of RDF triples. Queries are composed of any number of statements, with an arbitrary number of wildcards in each statements. While each RDF triple may have an arbitrary wildcard pattern, some types of queries are performed much more frequently than other types of queries. Specifically, most queries do not have an existential predicate, and Cholesterol1 and Cholesterol1 optimize for this common case.

Predicate Table for "likes"

Subject -> Object		Object -> Subject	
mark	melanie, robert	melanie	melanie, robert
melanie	joe, steve	robert	joe, steve
beth	joe	joe	joe
		kim	melanie, robert
		steve	joe, steve

Figure 7-2: A predicate table for the predicate "likes"

The triples in a database are organized into "tables," where each unique predicate has its own table. The mapping between predicates and their tables is stored in a hash table; given a literal predicate, it is very efficient to retrieve its table. However,

if the predicate in a query is an existential, then Cholesterol must iterate through every predicate in the database to execute the query.

Within each table, there are two indexes; one that associates subjects with objects, and one that associates objects with subjects. The indexes are implemented as hash tables, which allows for efficient lookup of subject and object data. Given a literal subject, it's very efficient to retrieve the object parameter of all triples in the database with that subject. Similarly, given a literal object, the other index can be used to efficiently retrieve the subject parameter of all triples in the database with that literal object.

This indexing structure means that the following queries can be executed quickly: `?x predicate object`, `subject predicate ?x`, and `?x predicate ?y`.

7.4.2 Joins

In Cholesterol's simple query interface, joins and wildcards are the only way to extract data from the database. Joins are used commonly and must be very efficient. A join occurs when a Cholesterol query consists of more than one RDF statement; Cholesterol executes each RDF statement separately, and combines the results of each single-statement query using a join.

Queries are implemented internally via executing one statement at a time; the database knows how to query itself using a single statement with any pattern of wildcards. A higher-level join engine combines the results of separate single-statement queries. Figure 7-3 is a listing of the Cholesterol2 join code and shows the modularity of the query execution engine.

The statements that compose each query could be executed individually, and after every statement has been processed, combined by the join engine. However, this is inefficient; once you have executed one statement that contains one existential, you have constrained the value of that existential. Subsequent queries and joins can only reduce the total set of possible values for that existential.

Once Cholesterol has executed a query involving at least one existential, it stores a list of all possible values for that existential. Ensuing queries that involve that exis-

```
CResultSet *CCholesterolDatabase::doQuery(const CStatementArray &statementArray)
{
    if (statementArray.NumStatements() == 0)
        return NULL;
    else if (statementArray.NumStatements() == 1)
        return doSingleStatementQuery(statementArray.GetStatement(0));
    else
    {
        CResultSet *pAllResults = new CResultSet(statementArray.GetNumExistentials());
        CResultSet *r = doSingleStatementQuery(statementArray.GetStatement(0));
        if (r == NULL) return NULL;
        pAllResults->Append(r);
        delete r;

        for (int q=1;q<statementArray.NumStatements();q++)
        {
            CQueryRestriction qr(pAllResults);
            CResultSet *nr = doSingleStatementQuery(statementArray.GetStatement(q), &qr);
            if (nr == NULL) return NULL;
            pAllResults->Join(nr);
            delete nr;
        }

        return pAllResults;
    }
}
```

Figure 7-3: The Cholesterol2 Join Code

tential, rather than examining all possible values for the existential, can examine only the known values for the existential. One can illustrate the usefulness of constraining an existential using the example database defined in Table 7.3 and the example query mark likes ?x, ?x likes ?y.

After the first statement has been executed, the ?x variable is constrained to either melanie or robert. If ?x likes ?y were to be executed independently, it would return 5 rows (nearly all of the rows in the database). However, because of the constraints on ?x, ?x likes ?y can be executed as melanie likes ?y and robert likes ?y. The more constrained the existentials in a statement are, the faster subsequent single-statement queries will execute.

7.4.3 Logging

Cholesterol1 and Cholesterol2 serialize the contents of their database using a log. The log is relatively simple; it is a sequential record of every add or remove that has been performed on the database. To load the database, all adds and removes in the log are simply re-played. There is currently no optimization to remove redundant log lines;

rows that are added and then removed still exist in the log.

Cholesterol1 and Cholesterol2 originally enforced a strict coherency model; after an add or remove successfully executed, the database was required to recover to the exact same pre-crash state and had to reflect every successfully executed add or remove operation. However, this restriction requires writing to disk after every add or remove, which severely impacts Cholesterol's performance.

This strict coherency requirement has been relaxed, and writes to the log are now cached in memory, and are flushed to disk only when the cache becomes full. This means that if Cholesterol crashes abruptly, the most recent database modifications may be lost. However, this is an acceptable price to pay for the nearly 2x performance improvement that accompanies cached log writes.

7.4.4   Locking

Cholesterol is called simultaneously from different threads in Haystack; to prevent race conditions and data corruption, it must place locks around its data structures.

Some testing was performed, and locks in both Windows and Linux are very inexpensive; there is virtually no overhead to obtain a lock. As such, Cholesterol uses very fine-grained locks. There is a lock for nearly every individual data structure, and locks are held as briefly as possible – only over accesses to a single data structure. If locks were expensive to obtain, more coarsely-grained locking would be used; i.e. there would be a single lock across the entire add function.

Cholesterol does not use typical critical sections or mutexes; it uses custom read-write locks. These read-write locks allow multiple threads to read from the same data structure, but if a thread wishes to write to a data structure, it must have exclusive access.

7.4.5   Resource IDs

Cholesterol implements a basic form of compression to reduce total memory consumption and to make some internal computation more efficient. Strings are represented

internally as integer resource IDs. At all entry points – i.e. the add or query method – strings are translated into integer resource IDs. The reverse occurs at all exit points; for example, when the query method returns, all of the internal resource IDs are translated to strings. Not only does this reduce memory consumption – a string exists only once in memory, even if it exists multiple times in the database – it also speeds up internal computation. It is much more efficient to compare two integral resource IDs than it is to compare two null-terminated strings.

The downside of using resource IDs is that there is a central bottleneck that all methods must access before they execute, but profiling has found that resource ID translation takes up a negligible amount of time. The majority of the time is spent inside of the query and add functions, where all computation is done using the integer resource IDs.

7.5   Cholesterol3

Cholesterol3 uses a dramatically different architecture than Cholesterol1 or Cholesterol2. Older versions of Cholesterol were fairly fast, but they had a large memory footprint, and, unfortunately, the primary assumption of the index structure – that most query predicates are not existential – is not true a significant portion of the time.

Cholesterol1 and Cholesterol2 load the entire database into memory. Theoretically, the operating system should efficiently send unused portions of memory out to disk and load them back in if they are needed, but, empirical testing has shown that Cholesterol generates an abnormally large number of page faults, even on systems that should have enough physical memory to store the entire database. Cholesterol3 implements its own custom memory management system.

While all versions of Cholesterol support queries with arbitrary patterns of wildcards, Cholesterol1 and Cholesterol2 optimize for what is a common case – the predicates of each query are literal. While this is true the majority of the time, queries with existential predicates execute very slowly. Cholesterol3 has a more robust indexing

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system.

7.5.1   Memory Management

An average Haystack store contains about 500,000 RDF triples that comprise 80 to 120 megabytes of data. This should, theoretically, not be a problem for a modern operating system's virtual memory facilities. The operating system is supposed to send unused portions of memory out to disk – to a page file – and load them back into memory on demand. Unfortunately, empirical testing has shown that the operating system makes poor decisions about which portions of memory to unload; even on systems with much more physical memory than the 80-120 megabyte Cholesterol footprint, Cholesterol has an abnormally large number of page faults. The OS's own memory management algorithms are, unfortunately, inadequate for applications such as Cholesterol, which deal with large data sets and are highly dependent on memory access speeds.

Cholesterol implements its own memory manager. The basic block of the Cholesterol memory manager is the node, which contains a value and a number of indexes that contain triples with that value. For example, a predicate node contains the predicate itself, and then hash tables that index the subjects and object parameters of triples with that specific predicate. A predicate node looks much like the table described in Figure 7-2.

Cholesterol starts a watcher thread which monitors the total number of nodes loaded into memory. If there are too many nodes in memory, the watcher thread locks the database and then writes nodes to disk. Cholesterol decides which nodes to write to disk using the least recently used (LRU) algorithm – each node remembers its last access time, and the oldest nodes are written to disk. If the nodes are requested – i.e. they are needed for a query – then they are loaded back in from disk.

The paging implementation is far from complete. If a node is paged to disk and then loaded back in, the next time it is paged to disk, it will be written to in a new location. Thus, given a database which contains more nodes than the maximum number of nodes allowable in memory at a single time, the total disk space consumed

by Cholesterol will grow as queries are performed. When a query is executed, it may touch old pages, which must be loaded into memory. As new queries are executed, these pages will become old again and will be paged out to disk again, but in a new location. Even if no new nodes are added, the disk footprint of the database will increase.

Cholesterol3 makes extensive use of memory mapped files; rather than allocating internal memory using malloc, most data is stored in a memory mapped file.

7.5.2 Indexing

All versions of Cholesterol support arbitrary queries, but Cholesterol1 and Cholesterol2 optimize for common-case queries. Specifically, queries with existential predicates may take a long time to execute, as Cholesterol1 and Cholesterol2 must traverse every unique predicate in the database.

Cholesterol3 improves upon the older indexing schemes by indexing on every field, rather than just on predicate. In Cholesterol1 and Cholesterol2, there is a table for every unique predicate, and a hash table makes it efficient to retrieve the table associated with each predicate. Within each table, there are separate hash tables that index the subject and object parameters of triples with the specified predicate. This table structure is discussed in Section 7.4.1 and Figure 7-2.

Cholesterol3 uses the same table abstraction, but stores a table for the subject, predicate, and object. A subject table, for example, is keyed on the subject of a RDF triple, and contains indexes of the predicate and object. This means that all queries with identical numbers of existentials are executed in the same manner, regardless of the position of the existentials.

This index structure duplicates the database many times over, and thus consumes a large amount of memory. Cholesterol3 allows you to revert back to the old-style indexes; the new index structure consumes too much memory for most machines.

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