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Machine learning inference of search engine heuristics

Part II Project

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Proforma

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Original Aims of the Project

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Special Difficulties

Declaration of Originality

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

Signed

Date

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1. Introduction

1.1. Motivation

This project is inspired by increasing importance of search engine rankings. Today major search engines given a query return web pages in an order determined by secret algorithms. Such algorithms are believed to incorporate multiple unknown factors. For instance, Google claims to have over 200 unique factors that influence a position of a webpage in the search results relative to a query [1]. Only a handful of these factors are disclosed to the webmasters in the form of very general guidelines. Moreover, the Google algorithm in particular is updated frequently. However, most of the knowledge around the area amounts to speculation. Despite the fact that it is possible to pass a vast number of queries through the black box of any existing search engine, the immensity of the search space and instability of such algorithms make them impossible to reverse engineer.

This project is concerned with application of machine learning techniques to search engines. The aim of the project, in particular, is to explore how machine learning techniques can be used effectively to infer algorithms from search engines. Even though this study does not attempt to reverse engineer any existing heuristics, the results can be applied to such an ambitious task. Moreover, such a framework is potentially more general and can be used for a range of problems.

1.2. Challenges

Machine learning is a natural approach to inferring the true algorithm from a subset of all possible observations. However, applying machine learning techniques to real search engines would be hardly effective, as the dynamic nature of the algorithms and the web as well as lack of meaningful feedback would prevent incremental improve-

[1] http://www.google.com/competition/howgooglesearchworks.html

ment: when there are as many as 200 features in question, false assumptions made by a learner may have an unpredictable effect on its performance.

More generally, there are certain ambiguities associated with machine learning, which are 'problem-specific'. For example, it proves difficult to decide how much training data is necessary, as well as and selecting it to avoid over/under-fitting[1]. Similarly, it is not straightforward which machine learning technique is best for a particular problem.

To address the limitations imposed by existing search engines, part of the task is to develop a toy search engine that allows me to control the nature and complexity of used heuristics. Such transparency addresses the problems stated above and, more importantly, allows for useful evaluation of machine learning techniques by providing meaningful feedback.

1.3. Related Work

2. Preparation

The original aims of the project were defined very broadly, so some further structuring and planning were crucial at the early stages to make sure the goals are understood and subsequently achieved.

The beginning of this chapter introduces the principles of machine learning and the particular techniques implemented during this project in order to familiarise the reader with the field and the research done at the beginning. The rest of the chapter describes the analysis undertaken before the development, in particular, formulating the goals and evaluating the relative importance of parts, as well as associated risks.

2.1. Introduction to Machine Learning

Machine learning constitutes the central part of the project. The field was completely new to me to start with, so research of different techniques was a big part of the preparation.

Machine learning is a vast field and very little is prescribed. The supervised learning approach, where the hidden function is inferred from the labelled training data, best fits our purposes for a number of reasons. Firstly, it applies well to the real-world problem of inferring the heuristics of the real search engines, as we can select training data and obtain the labels simply by querying. Secondly, supervised learning is widely used and offers a variety of flexible techniques.

An interesting known problem with machine learning in general is referred to as the Curse of Dimensionality. In the real world scenario – suppose if we were inferring an existing search engine from the observed query responses – we could not be sure about which features are and which are not relevant to the hidden algorithm. Potentially, some features we might choose to use will increase the dimensionality, but would not actually be used by the real algorithm. Gathering more features can hurt, as it makes the learner infer nonexistent dependencies. Clearly within the scope of this project we will know at each point which features are or are not used. So observations can be made as to how using more features than the search engine will affect the classifier.

Another major issue that is common to all machine learning methods is over/under-fitting. These refer to the problem of finding balance between the generalized model and the training data at hand. This is yet another source of interest to this project, as we can observe the behaviour of the learner when certain control parameters are changed.

It is generally recommended that the simplest learners are tried first[1]. Of all learners Naive Bayesian is one of the most comprehensible.This in itself is a major advantage according to the Occam's razor principle, which finds ample application in machine learning. Hence, we start with describing the principles of the two machine learning techniques used - Naive Bayes and Support Vector Machines.

2.1.1. Naive Bayes

Naive Bayes is a probabilistic classifier based on the Bayes Theorem. The posterior probability $P(C|\vec{F})$ denotes the probability that a sample page with a feature vector $\vec{F} = (F_1, F_2, \dots, F_n)$ belongs to class C. The posterior probability is computed from the observable in the training data: the prior probability $P(C)$ – the unconditional probability of a page belonging to the class C, the likelihood $P(\vec{F}|C)$ and the evidence $P(\vec{F})$:

$$P(C|\vec{F}) = \frac{P(C)P(\vec{F}|C)}{P(\vec{F})} \tag{2.1}$$

The simplicity of Bayesian approach owes to the conditional independence assumption: each F_i in $\vec{F}$ is assumed to be independent of one another to get $P(\vec{F}|C) = P(F_1|C) * P(F_2|C) * \cdots * P(F_n|C)$. This leads to a concise classifier definition:

$$\hat{C} = argmax_C P(C) \prod_{i=1}^{n} P(F_i|C) \tag{2.2}$$

where C is the result of classification of a page with feature vector $F_1, F_2, \dots, F_n$.

In practice, the crude assumption rarely holds and is likely to be violated by our data, as we expect features of pages to be interdependent. However, it has been shown that Naive Bayes performs well under zero-one loss function in presence of dependencies[2]. This has a few implications for this project, particularly, on evaluation methods

As we have seen, Naive Bayes assigns probabilities to possible classifications in the process of classifying. Even though it generally performs well in classification tasks, these probability estimates are poor [3]. However, despite poor probability estimates, there exist several frameworks, which make use of Bayesian classification and achieve decent performance in ranking. For example, Zhang [9] experimentally found that Naive Bayes is locally optimal in ranking. The paper defines a classifier as locally optimal in ranking a positive example E if there is no negative example ranked after E and vice versa for a negative exaple. A classifier is global in ranking if it is locally optimal for all examples in the example set: in other words, it is optimal in pairwise ranking. It is particularly interesting that the paper discovered that Naive Bayes is globally optimal in ranking on linear functions that have been shown as not learnable by Naive Bayes[1]. Another framework for ranking [7] is based on Placket-Luce model, which reconciles the concepts of score and rank. This framework is based on minimizing the Bayes risk over possible permutations.Existence of such frameworks suggest that Naive Bayes is an adequate choice for a prototype learner.

Although classification is a useful technique to try, it feels more natural to represent our score or rank as real numbers rather than classes. Regression is another approach to machine learning and the next learning technique we explore – Support Vector Regression – is non-probabilistic, to try something as distant from Naive Bayes as possible.

ier.

2.1.2. ϵ-Support Vector Regression

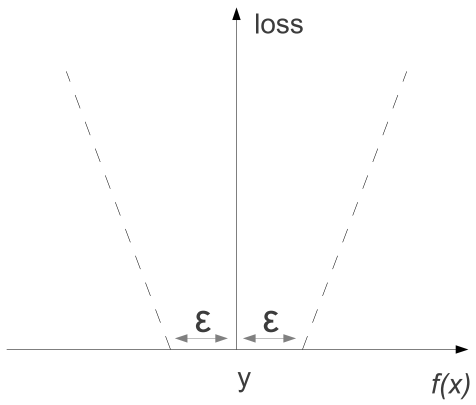
While the binary classification problem has as its goal the maximization of the margin between the classes, regression is concerned with fitting a hyperplane through the given training sequence.

A great advantage of Support Vector machines is that they can perform non-linear classification or regression by using what is referred to as the *Kernel Trick* - an implicit mapping of features into a higher dimensional space, in which the data is linearly separable. The choice of a kernel function is problem specific and the best one is usually decided by experiment.

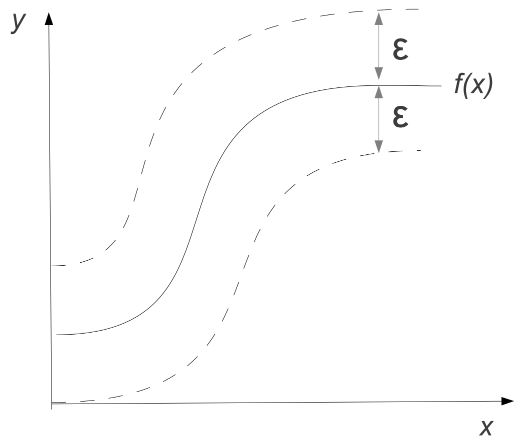
We begin with the theoretical foundations of Support Vector Regression, which were first proposed by Vapnik **??**.
Define a training sequence as a set of training points $D =$

[1] *M-of-N Concepts* and *Conjunctive Concepts* can't be learnt by Naive Bayes classifier but can be optimally ranked by it according to Zhang [9].

$\{(\mathbf{x_1}, t_1), (\mathbf{x_2}, t_2), ..., (\mathbf{x_l}, t_l)\}$ where $\mathbf{x_i} \in R^n$ is a feature vector holding features of pages and $\mathbf{t_i} \in R$ is the corresponding ranking of each page.



(a) *ϵ-insensitive loss function*



(b) *Predictions with ϵ-SVR*

In simple linear regression the aim is to minimize a regularized error function. We will be using an ϵ-insensitive error function(see Figure 2.1a (a)).

$$E_\phi(y((x) - t)) = \begin{cases} 0 & \text{if } |y(\mathbf{x}) - t)| < \epsilon \\ |y(\mathbf{x}) - t)| - \epsilon & \text{otherwise} \end{cases}$$

where $y((x) = \mathbf{w^T}\phi(\mathbf{x}) + b$ is the hyperplane equation (and so $y(\mathbf{x})$ is the predicted output) and t_n is the target (true) output.

The regression tube then contains all the points for which $y(\mathbf{x_n}) - \epsilon \leq t_n \leq y(\mathbf{x_n}) + \epsilon$ as shown in Figure 2.1a(b).

To allow variables to lie outside of the tube, slack variables $\xi_n \geq 0$and $\xi_n^* \geq 0$ are introduced. The standard formulation of the error function for support vector regression (ref Vapnik 1998) can be written as follows:

$$E = C\sum_{n=1}^{N}(\xi_n + \xi_n^*) + \frac{1}{2}\|\mathbf{w}\|^2 \tag{2.3}$$

E must be minimized subject to four constraints:

$$\xi_n \geq 0, \tag{2.4}$$
$$\xi_n^* \geq 0, \tag{2.5}$$
$$t_n \leq y(\mathbf{x_n}) + \epsilon + \xi_n, \tag{2.6}$$
$$t_n \geq y(\mathbf{x_n}) - \epsilon - \xi_n^*, \tag{2.7}$$

This constraint problem can be transformed into its dual form by introducing Lagrange multipliers $a_n \geq 0, a_n^* \geq 0$. The dual problem involves maximizing

$$L(\mathbf{a}, \mathbf{a}^*) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n - a_n^*)(a_m - a_m^*)K(\mathbf{x_n}, \mathbf{x_m}) \tag{2.8}$$

$$-\epsilon\sum_{n=1}^{N}(a_n + a_n^*) + \sum_{n=1}^{N} t_n(a_n - a_n^*)$$

where $K(x_n, x_m)$ is the kernel function, t_n is the target output,

subject to constraints

$$\sum_{n=1}^{N}(a_n - a_n^*) = 0, \tag{2.9}$$
$$0 \leq a_n,\ a_n^* \leq C, \quad n = 1, ..., l \tag{2.10}$$

I come back to these derivations again in Section 3.8 and further derivations will be constructed in order to implement the SVM.

2.2. Introduction to PageRank

The PageRank algorithm was originally described in a research paper by Page and Brin[6]. It was first introduced as a way 'to measure the relative importance of web pages'. PageRank is interesting to include in this project not only because it is a defining feature of the Google search engine, but because it is a unique feature of its type, as it depends on the link structure of the whole web as opposed to other web features such as word count and alike.

The basic idea is to capture the link structure of the web and provide a ranking of pages that is robust against manipulation. To achieve this, the importance 'flows' forward: the backlinks share their importance with the pages they link to. Such a simplified ranking of a set of pages can be expressed as an assignment

$$R(u) = c \sum_{v \in B_u} \frac{R(v)}{N_v} \tag{2.11}$$

An intuitive justification for such ranking is by analogy with a citation network, we are likely to find highly cited pages more important. The equation is recursive, so iterating until convergence results in a steady state distribution, which corresponds to the PageRank vector. Together with this intuition the paper introduces the *Random Surfer Model*: we are interested in a steady state distribution of a random walk on the Web graph. At each step the surfer either follows a random link or 'teleports' to a random page. The paper justifies the approach of ignoring the dangling links, as it doesn't have a significant affect on the ranking.

The teleportation vector determines whether the PageRank is personalized. For the non-personalized version the teleportation vector holds equal probabilities for all pages in the Web, whereas in a personalized approach the probabilities are distributed according the knowledge of the surfer's previous activity. In this project we are only concerned with nonpersonalized ranking, which is simpler and enough for the purposes of the project.

2.3. Requirements Analysis

The original aims of the project were very high level, so explicitly defining the goals in the early stages, was central to the success of the project. The main project goals are summarized in Table 2.1.

Along with the stated requirements, it is important to note that in this project I regarded usability as a non-requirement. This decision was motivated by the fact that the project is result-oriented, therefore, quick implementation was prioritized over ease of use. The system is only meant to be used by me, hence there was no need for documentation and user interface.

Requirement description	Priority	Difficulty	Risk
Functional Requirements			
Implement a simple search engine	High	Low	Low
Ensure search engine can use both score and rank	Medium	Medium	Low
Implement two different machine learning techniques	High	High	High
Classifiers must achieve better than random results	High	Medium	High
Implement PageRank	Medium	Medium	Low
Non-Functional Requirements			
The search engine must be able to index a few thousand pages in reasonable[2] time	Medium	High	Medium
PageRank computation on a few thousand pages must complete in reasonable time	Medium	High	Medium
Machine learning modules must learn and classify within reasonable time	High	High	High

Table 2.1.: *Project objecives*

To effectively plan the development, I also evaluated the dependencies of the core modules of the project. Figure 2.1 shows the major dependencies present in the project. It can be seen that there was a lot of freedom as to the order of implementation. Another observation that was revealed during the dependencies evaluation relates the integration. All the parts of the project come together in the evaluation, and so it was important to make sure the input formats of machine learners match with the output of the parser and so on. It also became obvious that due to the apparent convergence of the modules integration would be a complex exercise. Therefore, a prototype had to be implemented very early on to see the design at work and to avoid surprises at the end.

2.4. Choice of Tools

2.4.1. Data Gathering

Data gathering is of major importance, as data decisions have tremendous impact on the rest of the implementation and the success of the project. The rest of the system assumes the existence of a pool of web pages available offline for fast indexing and parsing. Ideally the corpus of web pages would be 'representative' of the whole web, to make generalisations more accurate. Originally, I was hoping to get such collec-

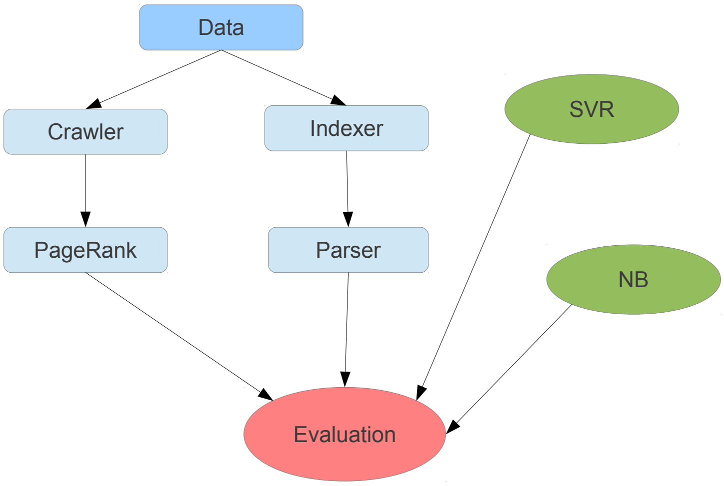


Figure 2.1.: *Summary of Main Dependencies*

tion from a resource, namely, the web corpus of the *Text Retrieval Conference* (TREC). However, such data is not easily available, so I had to retrieve pages using *Wget*. To approach the similarity to the web, I restricted the corpus to one semantic area by only downloading websites related to construction materials[3]. This limitation of topic has certain advantages: relatively few pages need to be downloaded before the pages appear sufficiently interlinked, so the corpus has a distinct structure (as web pages similar in the field link to each other). All the links were converted, so that the link structure was preserved offline.

As for the size of the training data, Domingos [1] suggests that a primitive learner given more data performs better than a more complex one with less data. This, of course, is under certain assumptions of data quality, namely the assumption that the training data is a representative subset of all the possible data. Intuitively, provided there is no bias in data gathering, more data implies better generality. I have started with a training set spanning an order of a few thousands of pages, however, in practice, I found that there is no particular improvement beyond a thousand pages.

To conform with machine learning guidelines I separated data for Test and Training at the very beginning. Different seed pages were used and the web pages were downloaded into different directories. Each directory was estimated at around 3000 pages. In addition to this, I have taken the further precaution of setting aside small Development

[3] There is no particular reason to choose this topic, except that it had been used by the external project originator in his experiment trying to infer Google's ranking factors. This is described in the Proposal in more detail.

and Verification corpora to be used only while development to ensure no bias towards training data at the implementation stage. Also, its comparatively small size meant faster development.

2.4.2. Search Engine

Next important decision regarded the search engine. Originally, I considered using open source existing engines, in particular, *Lucene*. Even though I could freely modify it for the purposes of the project, the complexity of it was superfluous. I saw writing a simple search engine as a more beneficial exercise, as developing it in the first place potentially gives an insight into the problem.

Functionally, the search engine is a black box that takes a set of web pages and a set of queries and outputs an order. The order is determined by the features of the page, which together make up a score. The score is the function that needs to be inferred using the ranking assigned by the search engine, however, we are only given the order as evidence. For most of this project I have assumed an existence of conversion between rank and score, and so the machine learners interact directly with scores. I have looked in more detail at the issue of score and rank, however, I decided that implementation would be beyond the scope of the project due to time limitations.

In general, there are two aspects of information retrieval that have to be accounted for: precision and recall.

Precision	– *the fraction of retrieved pages that are relevant to the query.*
Recall	– *the fraction of relevant documents that are retrieved.*

Even though both are important to make a good search engine, in practice, the web is very large, and so precision, or even *precision at n*[4]) has become more prominent in defining a good search engine: very rarely the user actually browses returns that are not in the top few tens of returned pages. As a result, modern search engines tend to focus on high precision at the expense of recall [5]. Therefore, I will concentrate primarily on precision when designing a search engine.

2.4.3. Prograzomming Language

When choosing a programming language, main considerations reduced to library availability and simplicity. The project imposes no special requirements on the language,

[4]'Precision at n' only evaluates precision with respect to n topmost returned pages.

apart from, perhaps, library infrastructure for parsing web pages, maths and natural language processing. Python is a rapid development language with extensive library support. As for efficiency, all the mathematical operations in this project rely on python math libraries, which are implemented in C. I have not programmed in Python before the project, so a slight overhead was caused by having to learn a new language.

2.4.4. Libraries

The project makes extensive use of libraries, Figure 2.2 shows an abstract diagram of the main libraries. As I mentioned earlier, library support was a major criterion when choosing a language and a lot of time was spent searching for and getting familiar with the relevant libraries. This section discusses some core libraries used in this project.

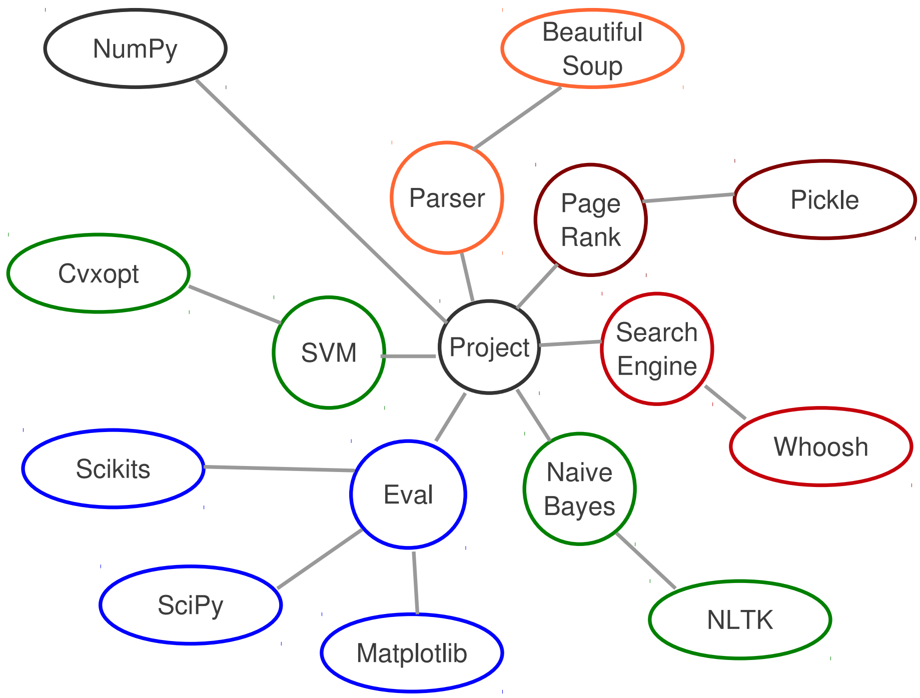


Figure 2.2.: *Libraries required in the project*

HTML parsing

Parsing HTML pages is crucial to the project and relies entirely on the library. I have chosen to use the **BeautifulSoup** library to build and navigate the parse tree. There are some simpler tools available for python, however, they do not have such a diverse functionality. For example, among the requirements were tag filtering and a variety of underlying parsers. The library was mainly used by the parsing module when constructing feature sets, as well as by the indexer.

Maths

NumPy is the most popular scientific Python library and was used throughout the project for various purposes including linear algebra, array and matrix manipulation, random number generation and many others.

A library providing a Quadratic Programming Solver, required in order to implement the SVM, was the hardest to find. The **CvxOpt** library was one of very few with such functionality.

Other maths libraries, such as **SciPy** and **Scikits**, were of secondary importance to the project and were needed primarily during evaluation for tasks like curve fitting and statistical bootstrapping.

Plotting

Adequate plotting capabilities were essential to the implementation and evaluation of the machine learners. **Matplotlib** is the de facto standard for plotting in Python. It has a simple API and importantly supports 3D plots, which were used extensively for visual verification of SVM and Bayes.

Indexing

The choice of indexer was driven primarily by the ease of customisation. The **Whoosh** library is a powerful open source indexer with a purely Pythonic API and plentiful capabilities, a lot of which are highly customisable.

Object Serialization

This functionality was required mainly to allow for precomputing of the PageRank vector and other static page features. **Marshal** and **Pickle** were the two alternatives considered in this project. **Pickle** has proved more robust and portable, and so was preferred.

Naive Bayes

A Bayesian classifier is not hard to implement, so after some consideration I decided to use a library implementation, as a fast solution was desirable for the first prototype. There were surprisingly many implementations available, among which I chose the **Natural Language Toolkit Library (NLTK)**, as it had a concise and clear implementation as well as a simple input format.

2.4.5. Development Environment

All of the development was carried out on my personal machine running Ubuntu Linux 12.04. Code was written primarily in the *Vim* editor in concert with the Python shell for interactive development. Vim is a powerful editor which provides syntax highlighting, fast text navigation and manipulation as well as shell integration. I used the extended IPython shell due to its stored history and autocompletion features.

2.4.6. Version Control and Backup

I chose to use the Mercurial source control management tool for both version control and remote backup. The choice was motivated by its ease of use, simple setup and my own familiarity with it. In addition, it is integrated with the online repository hosting service BitBucket.

The backup of the code was twofold: every time a substantial change was made the remote repository was updated to hold the newest version. Regularly both the code and the data used and obtained during evaluation were also backed up onto an external hard drive.

2.5. Software Engineering Techniques

2.5.1. Iterative Development

While the set up of Part II projects encourages waterfall-like development model, the nature of this project motivated an iterative approach. The first iteration rendered a prototype: a primitive search engine with a Naive Bayesian baseline classifier. The next iteration modified each part of the system towards a more complex solution. Testing and debugging was performed at each iteration to ensure the system was improved. Main advantage of iterative development to this project was the ability to verify validity of the proposed design early on by means of the first working prototype.

2.5.2. Incremental Build Model

Within each iteration the development followed the evolved waterfall model – the incremental build model. The system was split into components ('builds'), such that each represents a functionally separate unit of the system: a search engine, a learner, a parser and an assessment module. Increments were developed sequentially and were tested separately before integration at the end of the iteration. This approach allowed to decompose a complex system into manageable chunks, which eased the development.

2.6. Summary

In this chapter I have outlined the research and planning completed prior to the implementation stage. In particular, the chapter provided brief introductions to the machine learning techniques and the PageRank algorithm as well as shaping more detailed aims of the project. I also touched upon the development strategy followed during the project as well as the libraries used.

3. Implementation

This chapter describes the implementation of the system that was implemented in this project. The outline of the overall architecture is followed by more detailed descriptions of the individual components.

All components were implemented successfully and together form a working system.

3.1. System Architecture

To achieve the goal of the project, a machine learning techniques comparison framework was necessary. In the Introduction Chapter I mentioned the benefit of having a transparent system as an object of learning. To further justify this decision, it is worth mentioning that generalisation using machine learning is different from most optimization problems in that the function that is being optimized is out of our reach, and all that is visible to the machine learner is the training error. Because the goal of the project is not the correct classification of real data, but identifying the means to correct classification, it is important that informed choices were made towards the improvement of the learner. Taking this into account, knowing the function to be learned and having direct control over it, guided the improvement of the search engine.

Following this argument, a system in three parts was designed: a search engine, a machine learner and a parser to mediate between the two. Figure 3.1 illustrates the proposed learning system for the classifier case.

The Training Data is the web pages gathered as described in Section **??** and set aside at the beginning specifically for the training purposes. The Queries are implicitly part of the Training Data, as they determine which pages are returned by the search engine. The pages in the Training directory are first indexed and the PageRank is computed for them. The queries are passed to the search engine, which outputs the returned pages and the order of importance. The parser computes feature sets for all the pages in the training directory and assigns a category to each page depending on the query and the

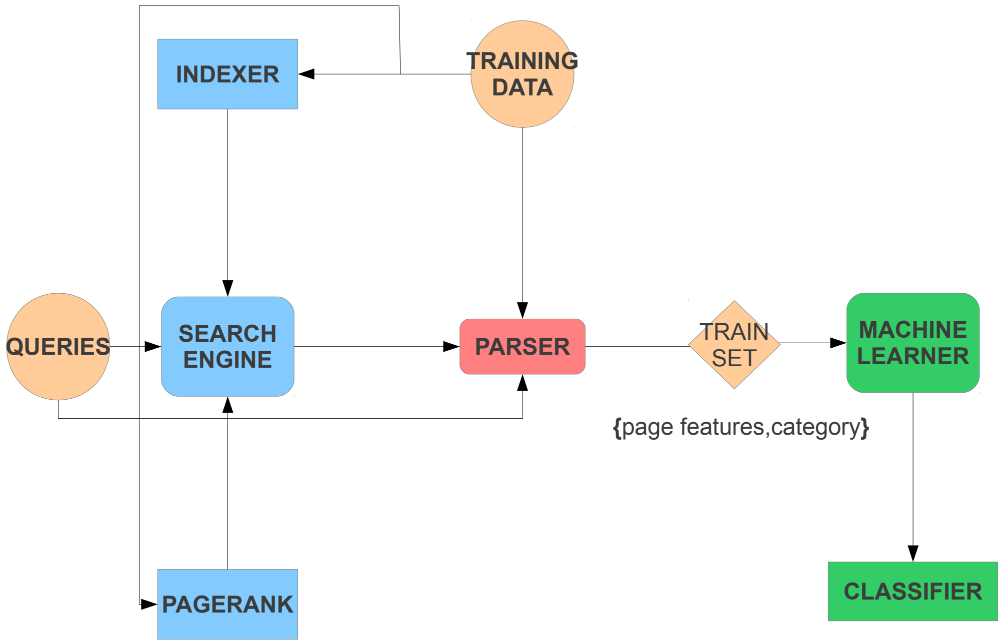


Figure 3.1.: *Overview of the system. Three major parts from left to right are search engine, parser and machine learner. The colour coding indicates belonging to the same component: green for the learner, blue for the search engine, pink for the parser and peach for the data.*

output from the search engine. The feature sets are then used to train the learner. The trained classifier is the output of the whole system.

In the course of this project two distinct machine learning algorithms have been used. Apart from speed and informal correctness, another important aspect of the design was the non-interference between the data gathering modules (search engine and parser) and the machine learners to avoid biased results. In addition, these parts had to be sufficiently decoupled for the purposes of scalability and code reuse: both machine learners must communicate with the system via the same interface.

Evaluation module is also an essential part of the developed system, as it facilitates the feedback loop that would help assess the performance of the classifiers. Figure 3.2 shows a high level diagram of th evaluation process for a classifier. The categorizer is a part of the parser that assigns true categories to the input pages. The search engine and the categorizer together are used to output the correct classification. This is then compared with the classifier's output. The classifier evaluation is further described in

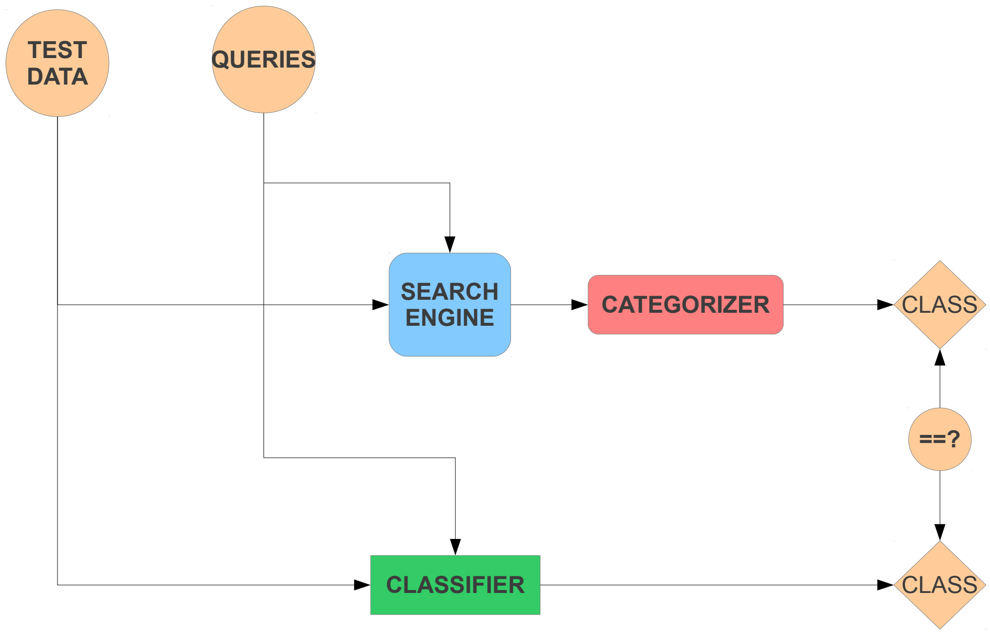


Figure 3.2.: *Evaluation process.*

Section 4.2 as well as the methodology adopted.

The rest of this chapter outlines the implementation of the core parts of the system, the challenges faced and the optimizations conducted.

3.2. Search Engine

The existence of the search engine had twofold significance in the project: firstly, it gave me an insight into how search engines work and secondly, it was a way of gathering data for the machine learners. The first prototype of the system was heavily reliant on the engine ranking the pages. In the following iterations, however, its importance was diminishing: scores were computed for all pages, making the queries irrelevant (see Section **??**).

Because I had decided to concentrate on precision, as discussed in Section **??** of the Preparation chapter, it was assumed for simplicity that all relevant documents were returned by the searcher. This assumption also emphasizes secondary importance of the search engine to the project: evaluation of the search engine itself could be ignored. The project swiftly moved on from the specifics of web pages towards the more general goal, which is concerned a lot more with the nature of the hidden score function than the features themselves.

Even though the search engine capabilities were not used to the extent I had envisaged, this section will elaborate further on the implementation of the indexer, as it helped me gain a useful insight into the field.

3.2.1. Indexer and Searcher

The module requirements featured flexibility, speed of indexing and retrieval as well as simplicity and usability. The *Whoosh* python library provides all of these – it is an open source indexing library, so I had the option of modifying any part of it. It is built in pure Python, so it has a clean pythonic API. Its primary advantage is fast indexing and retrieval, although we are mostly concerned with retrieval speed, as indexing is done rarely. The predecessors of Whoosh have served as the basis of well-known browsers such as *Lucene*, so it is also a powerful indexing tool, should I have needed more sophistication.

I have defined a very simple indexing schema. Perhaps, one notable detail is that Whoosh can store timestamps with the index, which enabled me to provide both clean and incremental index methods. The incremental indexing relies on the time stamp stored with the index and compares it to the last-modified time provided by the file system. The user can specify whether indexing has to be done from scratch or updated to accommodate some document changes or document addition/deletion. Even though I haven't originally expected to need an incremental indexing capability, throughout the project it has permitted for a significant speedup.

In the first prototype of the system, the search engine output the pages in the order of non-increasing PageRank. Subsequently, the sorting has been decoupled from retrieval and incorporated into the Parser module, which is described later in detail.

3.3. Computing PageRank

Section **??** of the Preparation chapter explains the principles of the PageRank algorithm. In this section the PageRank algorithm is implemented using matrix inversion. This is the simplest method to compute PageRank for a few thousands of pages and turned out to be reasonably fast. All matrix operations were performed using *Numpy* – the Python numerical library. The implementation is derived in the rest of the section.

First, a few variables need to be defined:

t	the teleportation probability
s	the probability of following a random link
E	the teleportation matrix
G	the matrix holding the link structure of the data

Matrix G can be defined as follows:

$$G_i, j = \begin{cases} 1/L & \text{there is a link from i to j and L = number of links from i} \\ 0 & \text{there is no link from i to j} \end{cases}$$

G is computed by traversing the data, which is described in more detail in the next section. E is chosen to be:

$$E_i, j = 1/N,$$

which corresponds to a non-personalised PageRank computation: the teleportation probabilities are identical for all surfers and all transitions are equiprobable. Both G and E are stochastic matrices: their entries are non-negative and their columns sum to one.

Probabilities s and t=1-s are customizable and represent the willingness of the surfer to follow links as opposed to jump onto a random page. I used the values proposed in the original paper[**?**] with s=0.85.

I defined a stochastic matrix M representing the web surfer activity, such that M_i, j is the probability of going from page i to page j,

$$M = s * G + t * E \tag{3.1}$$

In one step the new location of the surfer is described by the distribution Mp. The objective is to find a stationary distribution p, so by definition p is unchanged by surfer's activity:

$$p = M * p \tag{3.2}$$

Substituting 3.1 into 3.2

$$p = (s * G + t * E) * p = s * G * p + t * E * p \tag{3.3}$$

Rearranging equation 3.3 gives

$$p * (I - s * G) = t * E * p \tag{3.4}$$

where I is the identity matrix.

Because members of p must sum to one, E*p can be expressed as P:

$$P = [\overbrace{1/N, 1/N, \ldots, 1/N}^{N}].T$$

where T denoted matrix transpose operation. So computing PageRank amounts to

$$p = t * (I - s * G)^{-1} * P \tag{3.5}$$

where $(I - s * G)^{-1}$ denotes a matrix inverse operation.

This solution is simple at the expense of speed. Although computing inverse of a matrix is computationally expensive, the project does not require the computation to scale beyond a few thousands of pages. The resultant performance was surprisingly pleasing, the time spent computing PageRank was insignificantly small in comparison to the time spent crawling the directory.

The PageRank vector computation happens within the `Pagerank` class. The whole `Pagerank` object is written to memory using the Python object serialization module `Pickle`. This allows the PageRank vector to be precomputed and stored for each directory. The `load` class method is defined on the `PageRank` class to retrieve the relevant object for a given directory. The class is instantiated with an instance of the `Crawler` class, which embodies the link structure of a directory and is described in the next section.

3.4. Crawler

The `Crawler` abstracts away the underlying data directories and computes their link structures as matrices. The matrix G, used for the PageRank computation, represents random link following activity. To obtain such a link structure each page has to be parsed, and all links recorded. Because the training and test data are obtained from a single source page by recursive link following, every page in a directory is guaranteed to be discovered by a spider.

The `Crawler` class recursively traverses the pages depth first starting with the seed page, the same as the seed page used for recursively downloading the pages from the

Page	A
A	0
B	1/2
C	1/2
D	0

Table 3.1.: *Illustration of non-dangling pages: B and C share A's 'importance' equally.*

web. To make sure each page is only explored once, a dictionary is used to hold pairs of absolute path, which uniquely identifies the page, and a numerical value corresponding to the time stamp when the page has been first discovered.

Although every page has a unique path, the links to other pages are relative. Such links need to be normalized to maintain consistency. A page object is used to encapsulate path complexity: all link paths are converted to absolute paths before addition to the dictionary. All outbound links are stored with the page in a Set data structure, such that no link is added more than once.

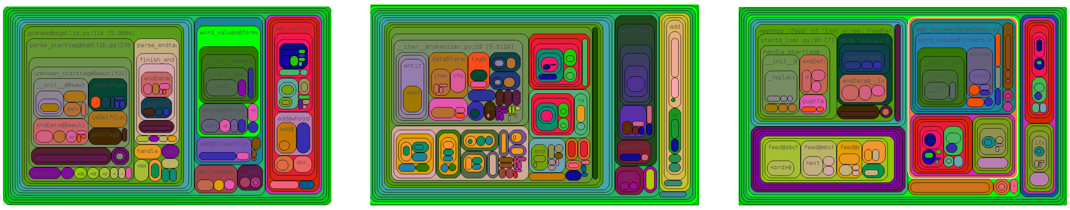
To produce the stochastic matrix G, an empty NxN matrix is initialised, where N is the total number of pages. I also assume that whenever a surfer encounters a dangling page – a page that has no outbound links – a teleportation step occurs. Therefore, every dangling page links to every page in the pool including itself with equal probability 1/N. For non-dangling pages, all links are assumed equiprobable and all pages that are not linked to have probability of 0. So if page A links to pages B and C, but not itself or D, its row in G is described by the Table 3.1.

3.5. Optimizations

One characteristic peripheral requirement for the system implemented in this project is speed. Even though it is not our direct goal to produce efficient implementations, optimization could not be overlooked, because significant amount of time is spent processing large quantities of data: indexing, PageRank and feature set computations all must complete in 'feasible' time, i.e. in the final implementation the longest computation takes order of minutes and processes a few thousand pages. Various optimizations have been used to achieve this.

Both PageRank vector and the index are precomputed and kept in persistent storage. Incremental indexing feature allows us to edit parts of the index as opposed to recomputing the whole index from scratch. These precomputations provide certain speedups, but were not enough. Because the system is fairly complex and a lot of library code is used in places, it was hard to determine which code most affects the speed. 'Blind' attempts at optimization did not work well, which motivated the use of a profiling tool.

Profiling the first prototype of the complete system revealed a surprising fact: most time was spent in the library code parsing pages. To mitigate this issue I have tried using custom parsers instead. Apart from speed, robustness was another important consideration, as a failure of a parser increases compute time. Two of the most renowned python parsers are*html5lib* and *lxml*. Figure 3.3 below shows visual representation of time profiling of 3 different runs obtained using the *RunSnakeRun*, each exploiting a different parser. Despite *html5lib* being quoted as the most robust/lenient, *lxml* was sufficiently faster to be preferable.



(a) *Default* (b) *html5lib* (c) *lxml*

Figure 3.3.: *Visual profiles of three parsers from left to right: default python html parser, html5lib and lxml. The internal boxes are sized in proportion to the time spent in each function. In all profiles three distinct major compartments can be seen, the leftmost being the compartment of interest: time spent in parsing. Taking into consideration that the other modules are unaffected by changing the parser implementation, it can be observed that lxml (rightmost) is the fastest and html5lib is the slowest.*

Another useful limitation was discovered due to profiling. The PageRank vector was loaded into memory every time a page was parsed: once for each page. This clearly is undesirable. I used caching to ensure that each of the two possible PageRank vectors (corresponding to the test and train directories) is loaded from memory exactly once. This is achieved via a double singleton class, which loads the vectors lazily.

3.6. Parser

So far we have looked at the search engine. This section describes the parser – a functional unit, which provides an interface from the search engine to the machine learners. The search engine simply retrieves pages in response to a query and the machine learner expects as its input a set of labelled features for training and unlabelled features for classification/regression. The Parser, therefore, must hide the nature of the data we are dealing with by translating it into the universal language of machine learners. Hence, the primary function of the Parser is to compute feature vectors for pages. However, it is easy to outsource search engine heuristics into the Parser, too, as they require page parsing.

To accomplish these multiple goals, I have taken an object oriented approach to the design of the module. What I refer to as the Parser is a few classes, which together perform a series of tasks related to page parsing. The module operates in two modes: rank and score and handles both classification and regression. The high level specification two objects are created: a `TestFeatureSetCollection` and a `LabelFeatureSetCollection`. These objects encapsulate all the data, so can be passed around to the machine learners, as well as evaluation and plotting modules. These objects each operate within their own directories, to keep training and testing sufficiently separate.

Both category and rank are treated as page features and hence are part of the `LabeledFeatureSet` class state. The `LabeledFeatureSetCollection` class generates training sets from queries, whereas the `TestFeatureSetCollection` class computes predicted category given an instance of a classifier. Both, however, need to generate feature sets, one for the Training data and the other for the Test data. This common functionality is embodied in their abstract base class, `FeatureSetCollection`. Figure 3.4 shows a UML class diagram illustrating the main structure of the module.

The rest of this section talks about the specifics of the implementation, in particular, the features used and how HTML parsing is done.

3.6.1. Rank and Score

Conceptually a `FeatureSetCollection` is a dictionary of `LabeledFeatureSet` objects indexed by both path to page and query term. After initialisation, all the features are computed and 'filled up' per query term per page. In the original prototype the search engine used to output ranks (the ordinal representing the position of the page

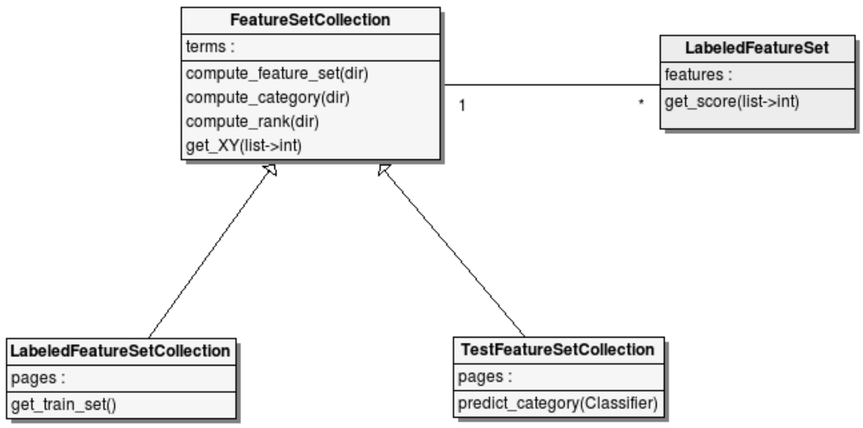


Figure 3.4.: *A UML class diagram describing operation of the Parser.*

in returns) as the target value for the machine learners to infer. This was fine for a prototype, however, there was an obvious flaw in this approach: the rank depends on the other web pages, which makes it impossible to infer from the features of a single page.

The later prototype assumed the existence of conversion between rank and score and passed scores directly to the machine learners. The score function was implemented as a class method on the `LabelledFeatureSet`, so that the scores could be computed ad hoc for a variety of heuristics.

3.6.2. Features

The requirements analysis does not prescribe the use of any particular features. However, it states that both dynamic (query dependent) and static(query independent) features must be used. PageRank is a dynamic feature that has quite special place among others: it takes into account all the pages in the pool and reflects on the structural hierarchy of the web pages. The parser loads the pre-computed PageRank vector indexed by page name to extract the PageRank of any particular page.

An example of a dynamic feature used in the project is query term count: the number of times the query term occurs on the page. This is obtained directly from the html files using the BeautifulSoup library, just like for the link parsing in the crawler. The html is parsed into clean text and the count is computed on the string.

A related but different feature – stem count – is the number of times the stem of the word occurs in the text. This is obtained using the `PorterStemmer` module in NLTK library.

Boolean features are a slightly different variety of feature, so was worth putting in. An example of this is a presence of an image on the page, compliance of the page to an existing HTML standard or presence of advertisements.

The features have been added incrementally as the project progressed. All other features are similar to the ones described above and are obtained using the same methods.

3.7. Naive Bayes

In Section **??** it has been shown that Naive Bayesian is a good learner to implement for the first prototype, so a very quick implementation was preferable to make sure the system can potentially function as intended. Due to its simplicity and popularity, Naive Bayesian is widely available in the libraries. Because the implementation of this module is straightforward, not central to the project, I decided to use one of many existing python implementations.

The *NLTK* library implementation was particularly appealing as it offers a very concise interface. A classifier object is initialised by the `train` method on the `NaiveBayesClassifier` class. The format of the training set is defined as a list of tuples of featuresets and labels, e.g.

$$[(featureset_1, label_1), \cdots, (featureset_N, label_N)]$$

The `train` method simply computes the prior – the probability distribution over labels P(label) and the likelihood – the conditional probability P($featureset = f|label$) by simply counting and recording the relevant instances. The method outputs a `NaiveBayesClassifier` instance parametrized by the two probability distributions. P(features) is not computed explicitly, instead, a normalizing denominator **??** is used.

$$\sum_{l \in labels} (P(l)P(featureset_1|l) \cdots P(featureset_N|l)) \tag{3.6}$$

The `classify` method on the `NaiveBayesClassifier` object takes exactly one featureset and returns a label which maximizes the posterior probability P(label|featureset) over all labels. Previously unseen features are ignored by the classifier, so that to avoid assigning zero probability to everything.

The only tangible difficulty with the implementation was the framework in which classification is done. This task is, however, achieved by the Parser. To batch classify everything in the test directory, the classifier object is passed to the Parser, where the featuresets for the test directories are computed, classified and recorded for the evaluation stage later. The particulars of this process is described in section **??**.

3.8. Support Vector Regression

In Section 2.1.2 I have introduced the theory of support vector machines. This section starts off with the implementation, which builds on the theory described in Section 2.1.2 and explains further transformations, which made up the essential part of the implementation. The section goes on to introduce some kernel functions and finishes off by explaining how hyperparameters might be tuned.

3.8.1. Implementation

To implement a support vector machine one must solve a problem of optimizing a quadratic function subject to linear constraints – usually referred to as the *Quadratic Programming* (QP) problem. Therefore, the first implementation task was to convert our existing optimization problem into a generic QP form to make use of the available solvers.

The maximization problem 2.8 can be trivially expressed as a minimization problem (equation 3.7).

$$min_{\boldsymbol{\alpha},\boldsymbol{\alpha}^*} \frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T P(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) + \epsilon \sum_{i=1}^{l}(\alpha_i + \alpha_i^*) - \sum_{i=1}^{l} t_i(\alpha_i - \alpha_i^*) \tag{3.7}$$

subject to constraints 3.8 and 3.9 below.

$$\mathbf{e}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*) = 0 \tag{3.8}$$

$$0 \le \alpha_i, \alpha_i^* \le C, \ i = 1, ..., l \tag{3.9}$$

where $\mathbf{e} = [1, ..., 1], \ P_{ij} = K(x_i, x_j), \ t_i$ is the target output, $C > 0$ and $\epsilon > 0$.

At this point in the implementation, for the first time, Python did not seem like the ideal choice fo programming language. *Cvxopt* is one of the few Python libraries that implements a QP solver. The specification to the QP function is as follows: `cvxopt.solvers.qp(P,q,G,h,A,b)` solves a pair of primal and dual convex quadratic programs

$$\min \frac{1}{2} x^T P x + q^T x \tag{3.10}$$

subject to

$$Gx \le h \tag{3.11}$$

$$Ax = b \tag{3.12}$$

Described in the next few pages are the transformations I devised to reconcile the minimization problem 3.7 and the library specification 3.10 and their respective constraints. We take x to encode both $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}^*$ simultaneously, treating the upper half of x as $\boldsymbol{\alpha}$ and the lower half as $\boldsymbol{\alpha}^*$:

$$x = \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^* \end{bmatrix}$$

We will see later how this representation allows for elegant representation of the problem (3.7).

First, we express the first term in 3.10 to hold $(\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)^T P (\boldsymbol{\alpha} - \boldsymbol{\alpha}^*)$. Take matrix P in equation 3.10 as

$$P = \begin{bmatrix} K & -K \\ -K & K \end{bmatrix}$$

where $K_{ij} = K(x_i, x_j)$ is the kernel.
Observe that now

$$x^T P x = \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^* \end{bmatrix} \begin{bmatrix} K & -K \\ -K & K \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^* \end{bmatrix}$$

is equivalent to the first term of equation (2.8)

$$\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n - a_n^*)(a_m - a_m^*)K(x_n, x_m)$$

Now expressing the remaining two terms of 3.7 by taking

$$q = \begin{bmatrix} \epsilon * \mathbf{e} - t_0 \\ \vdots \\ \epsilon * \mathbf{e} - t_{N-1} \\ \epsilon * \mathbf{e} + t_0 \\ \vdots \\ \epsilon * \mathbf{e} + t_{N-1} \end{bmatrix}$$

to achieve

$$q^T x = \epsilon \sum_{i=1}^{l}(\alpha_i + \alpha_i^*) - \sum_{i=1}^{l} t_i(\alpha_i - \alpha_i^*)$$

To encode constraint 3.9 consider the following pair of G and h.

$$G = \begin{array}{cc} \begin{array}{cc} \overbrace{\qquad\qquad\qquad}^{\text{N}} & \overbrace{\qquad\qquad\qquad}^{\text{N}} \end{array} & \\ \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \ddots & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \ddots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \ddots & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \ddots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} & \begin{array}{l} \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\end{matrix}}\right\}\text{2N} \\ \left.\vphantom{\begin{matrix}0\\0\\0\\0\\0\\0\end{matrix}}\right\}\text{2N} \end{array} \end{array}$$

$$h = [\overbrace{0\dots0}^{2N} \,|\, \overbrace{C\dots C}^{2N}]^T$$

The final constraint 3.8 is trivial to adapt by simply taking

$$A = [\overbrace{1, \ldots, 1}^{N}, \overbrace{-1, \ldots, -1}^{N}]$$

and

$$b = 0$$

Having worked out all the matrices, the rest of the implementation dealt simply with coding the matrices up. The *Cvxopt* library has its own matrix constructor, however, has generally limited functionality when it comes to matrix operations, so *Numpy* was used a lot for matrix manipulations.

During the first implementation attempt, the solver gave mostly unintelligible error messages, so for the prototype of the SVM I actually used `Matlab`. Matlab's `quadprog` function had an identical specification to the Python solver I intended to use. Matrices in Matlab are a lot more straightforward to manipulate, which was also a good reason to use it to check the correctness of my matrices before porting the code to Python.

3.8.2. SVM Kernel Functions

The kernel functions offer SVMs great flexibility, however, it can be difficult to pick an appropriate one. If the expected pattern is well-defined, kernel selection might be intuitive. For example, a linear kernel is perfect for linear heuristics and the problem is reduced to fitting a hyperplane. Similarly, Radial Basis Kernel picks out hyperspheres and so on. However, when we have no expectation of data, we need a most general kernel.

In this section I examine a few kernels with various score functions: both intuitive and not to observe how performance of each degrades as we use less The kernels used in this section have been tuned as described in Section 3.8.3.

Kernel functions are the central component of support vector machines, and its choice is highly dependent on the application. I have considered a variety of kernel functions and experimented with their combinations to see how the performance differs. Table 3.2 shows the kernel functions I have used.

The simplest kernel function is the Linear kernel. It is simply a dot product of two vectors. Its generalized version is the Polynomial kernel, which takes degree as a parameter. Intuitively, the polynomial kernel is a lot more flexible than linear, but the larger the degree, the less 'smooth' it becomes, so it might overfit the training data.

Name	$\boldsymbol{K(\vec{x},\vec{y})}$
Linear	$ax \cdot y^T + c$
Gaussian	$\exp^{-\gamma\|\|x-y\|\|^2}$
Sigmoid	$\tanh(ax \cdot y^T + c)$
Polynomial	$a(x \cdot y^T)^d$
Weighted Sum	`a*Gaussian(x,y,`γ`)+(1-a)*Linear(x,y)`
Product	`Linear(x,y)*Gaussian(x,y,`γ`)`

Table 3.2.: *Kernel Functions*

The Gaussian kernel is an example of a family of the Radial Basis Function kernels, which are most popular in Support Vector Machines. $||x - y||$ denotes the Euclidean distance of the two feature vectors. The γ parameter is equivalent to $\frac{1}{2\sigma^2}$. The choice of γ has a major effect on the performance of the kernel and represents a trade off between over- and underfitting.

The Sigmoid kernel is commonly used in neural networks and in combination with an SVM classifier forms a two layer perceptron network, where the scale parameter a is usually set to 1/N, where N is the number of dimensions (features)[4]. This kernel is different from the rest described here, as it only satisfies Mercer conditions[1] for some values of its parameters, which means SVM can be constructed only for those values[8].

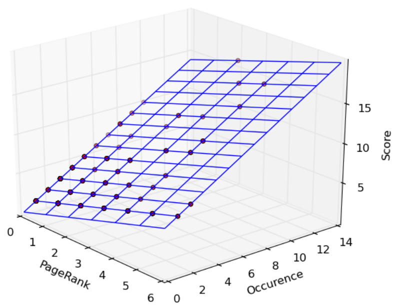
The Sum and Product kernels are both an example of combination kernels, in this case a combination of the linear and Gaussian kernels. I found that in many situations combining kernels in various scenarious where just one kernel does not perform well.

Figure 3.5 shows four different kernels applied to their native two dimensional heuristics. Clearly, the first three fits seem effortless, but fitting the step function with an RBF kernel was a lot more tricky. The γ parameter was chosen by tuning described in the next section.

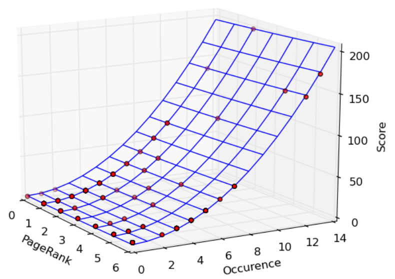
3.8.3. SVM Hyperparameter Tuning

In comparison to Naive Bayes, the SVM has a lot of degrees of freedom. Kernel functions is one such degree of freedom and each kernel has more adjustable parameters. Selecting a kernel itself is discussed in more detail in the next section. This section illustrates how kernel parameters might be tuned.

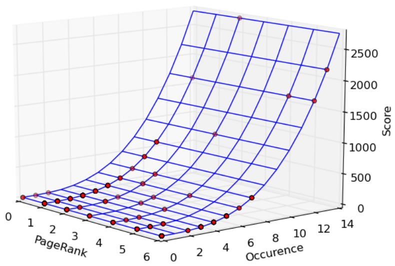
[1]



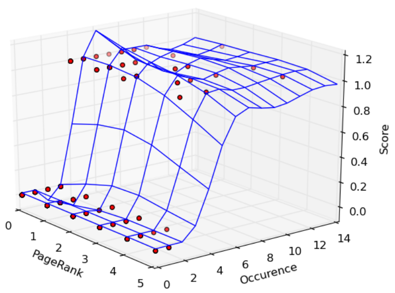
(a) *Linear*



(b) *Quadratic*



(c) *Cubic*



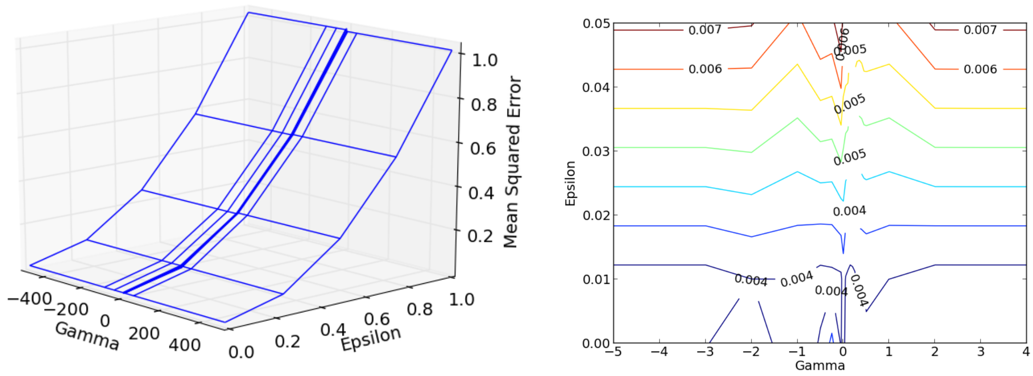
(d) *Step*

Figure 3.5.: *Four different two dimensional heuristic functions are fitted by SVR with four corresponding kernels: linear, polynomial degree 2, polynomial degree 3 and Gaussian.*

There are several ways of adjusting parameters of which Grid search is the simplest. In grid search we specify a range of parameters and note down the Mean Squared Errors for each value (or combination of values). To chose the domain successfully, the analysis has to happen at different scales, starting from coarser (wider spread) parameter values, each time only choosing the best for finer tuning, so the algorithm works in a tournament fashion. Essentially, it is hill climbing and does not scale beyond a few variables.

As an example a combined product kernel will be used. The data used is deliberately noisy and non-injective. We want to find out how perturbing the plane with Gaussian can provide a better fit. Given a positive sigma, the Gaussian component varies between one and zero. Varying gamma determines the contribution of the linear the fit as well as overfitting. Varying the epsilon also controls overfitting.

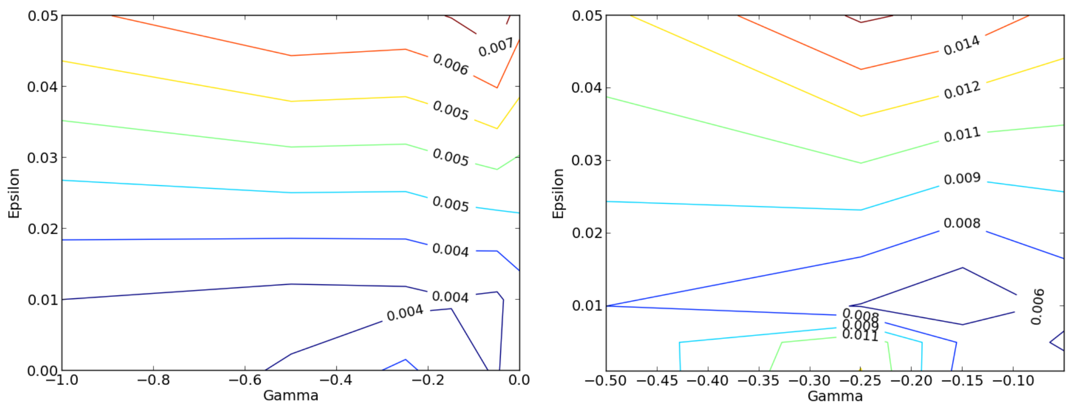
Figure 3.6 shows analysis at different scales on the training data: the coarsest and the finest. First it is found that the contribution of the ϵ affects the error a lot more in comparison to γ. As the problem is symmetric, further analyses are only performed with positive gamma. Looking further, it eventually becomes visible that the minima lie where γ is small.



(a) *Coarse analysis* (b) *Fine analysis*

Figure 3.6.: *It is clear from (a), that increasing epsilon affects the fitting of the test data so greatly, that changing gamma is insignificant in comparison. However, on the finer scale contour map (b), the minima can be found.*

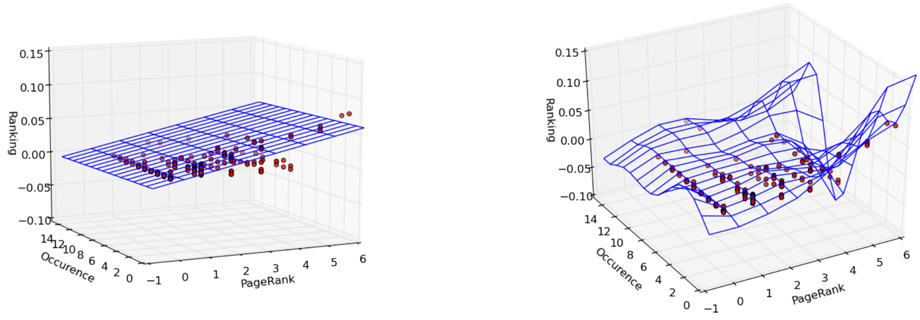
Figure 3.7 demonstrates the effects of overfitting: the minima for training and test data do not coincide. Whereas the training data is best fit with the epsilon approaching zero, as might be expected, the test data is fit better when the error is non-zero.



(a) *Training Data* (b) *Test Data*

Figure 3.7.: *Effects of overfitting: non-zero epsilon allows for better fit of the test data.*

Now having found the best Gaussian and error parameters, the two different fittings are plotted in Figure 3.8



(a) *Linear kernel fit* (b) *Combined Product kernel fit*

Figure 3.8.: *Linear fit is improved by Gaussian: when gamma is tuned, the hyperplane is perturbed to provide the best fit.*

Hyperparameter tuning was, perhaps, the hardest part of SVM, which required both very good understanding of the kernel functions, as well as data at hand. Though in this section I described a primitive way of tuning, I would consider more advanced automated tuning schemes, perhaps, even using machine learning techniques to determine parameters.

3.9. Summary

In this chapter I have taken the reader from system architecture through the design and implementation of the various components which included the search engine, the parser as well as two machine learning modules.

Work was split between theoretical and pure software engineering. The theoretical work included derivations of the PageRank algorithm and support vector regression, whereas the software engineering – in assembling libraries and classes as well as optimizing throughout the various components.

4. Evaluation

This chapter presents an overview of the results of the work undertaken for the project and a comparison of these results to the initial goals. The results include both the evaluation of methods implemented as well as qualitative and quantitative assessment of the implementation itself. Furthermore, the chapter describes the measures undertaken to ensure a correct implementation.

4.1. Overall Results

The original success criteria for the project stated in the Proposal (see Appendix A) are summarized below:

Criterion 1: *Implemented classifier can identify the importance of PageRank factor in the heuristic.*

The goal has been achieved as described in Section 4.2. Both classifiers were evaluated with PageRank being one of the features. Although PageRank is indistinguishable from any other feature as far as machine learning is concerned, it has been implemented as described in Section 3.3.

Criterion 2: *Various heuristics have been tried with different machine learners.*

This criterion constitutes the core part of the project and the evidence for it can be found in Sections 3.8.2, 3.6 and 4.2.

To achieve the original criteria the following modules have been implemented:

1. Search Engine
2. PageRank vector computation

3. Support Vector Regression and various kernels
4. Naive Bayes Classifier
5. Parser with a data structure supporting various heuristics

The project has been successful in achieving the goals stated in the original proposal. The result of the development is an extensible framework for classifier evaluation that can be used for further evaluation and analysis of machine learning techniques in general.

4.2. Classifier Evaluation

Two machine learning techniques explored in this project – regression and classification – are different in principle. The challenge in the evaluation is, therefore, to obtain results that can be compared despite the differences in implementation. To satisfy the comparability requirement, both SVM and Naive Bayes are run in the score mode: heuristic functions are used to output the score and the classifiers must predict the score. The regression case is straightforward, however, there are obvious difficulties in the case of the classifier.

Classes can be used to approximate the score as shown in Figure 4.1. Suppose there are two classes separated by a threshold value T. Then for training all the scores are trivially mapped to the right class depending whether they are greater or smaller than the threshold T. During evaluation the conversion has to be from the class to the score. Because information is lost during the quantization stage, the every example classified into Class 1 is mapped to the median value of the scores – M1 in the hope to minimize the error due to quantization.

The section starts by describing general methodology used throughout the evaluation. The rest is structured in the form of hypotheses and evaluation.

4.2.1. Methodology

Evaluation and comparison of classifiers is largely unprescribed: there is no method that applies well to every case. A lot of ambiguity is due to the fact that results obtained are ultimately dependent on the data used for training and testing. There are, however, generic guidelines to ensure adequate evaluation and comparison where possible. This

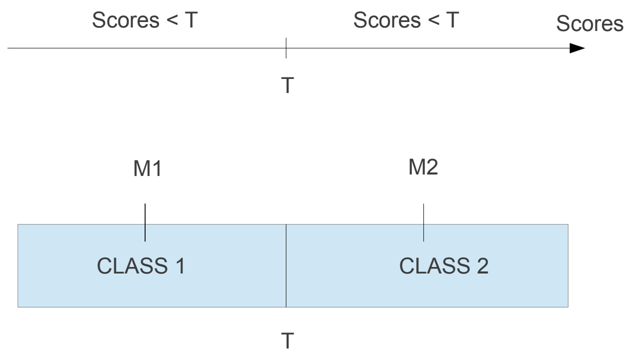


Figure 4.1.: *Quantization into two classes*

section highlights several such aspects, which are then applied throughout the whole chapter.

Classification and Quantization Error

To compare classification and regression effectively, the error incurred in quantizing scores is tracked. In a two-class scenario there is one threshold score value that separates the two classes. This score value is computed as a median to have adequate class representation. When Bayes assigns a class to a feature set, it is perceived as assigning the mean value of the scores present in the class.

Data

To avoid biased results Development corpus was used during development, which is disjoint from the real Test corpus and is of smaller size. The development corpus is further subdivided into the Training corpus and the Validation corpus to mirror the Training and the Test corpora, which are used to obtain all the results presented in this chapter. The evaluation was performed after the development of the whole system was complete and validated on the Development corpus.

Mean Squared Error (MSE)

As a measure of classifier performance I have chosen to use mean squared error. It is computed as

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(Actual_i - Predicted_i)^2$$

where $Actual$ is an array of true values of size $|Actual|$ and $Predicted$ is the corresponding array of predictions made by the classifier. MSE is the second moment of the error and hence, incorporates both variance and bias of it. Squaring penalizes large errors heavily, but small errors vanish, therefore MSE is sensitive to outliers as opposed to Mean Absolute Error (MAE). On the other hand, MAE is more sensitive to noise, which we expect when predicting continuous scores. Altogether, MSE provides a good measure that is easily visualised.

Tolerance intervals

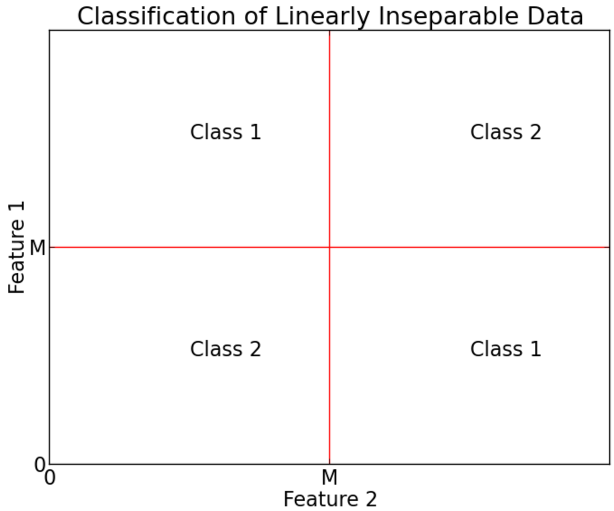
As MSE already captures the variance of the squared error, computing error bars to be the standard deviation of the squared error would offer no new information. In contrast, tolerance interval of the mean error itself is a good visualisation of how spread the error is. In the best case, the interval is tight, indicating the stability of the seen error. If the error is spread, the classifier is making inconsistent mistakes. It is particularly important to include these in our evaluation due to the presence of quantization error. The mean error of the ceiling and its spread is a good indicator of the mean and variance introduced by quantization.

To compute confidence intervals one could repeat the measurement on different data subsets. The number of subsets would have to be around 20 or more for the Central Limit Theorem to apply. In practice, the data is scarce and recomputing the errors is time consuming, so a way to compute the intervals with just one error measurement is desirable. Bootstrapping achieves exactly that by sampling randomly from the array of squared errors to recompute a new mean error. Even though bootstrapping might be less reliable, it provides a simple way to check the stability of the results. 95% confidence intervals are used throughout this chapter to compute error bars.

4.2.2. Linear and non-linear classification

Hypothesis: Naive Bayes performs better with linearly separable data.

Naive Bayes is a linear classifier and, therefore, linear separability of data is a premise of successful classification. To test this hypothesis, two minimal two-dimensional examples are constructed as shown in figures 4.2 and 4.3 below. Example 4.2 cannot be solved by fitting a separating line between the classes, so Bayes is expected to fail in this case. Example 4.3 illustrates a 'cut-off sum' function and is trivially separable. Such a linear heuristic should be easy for Bayes to pick up on.



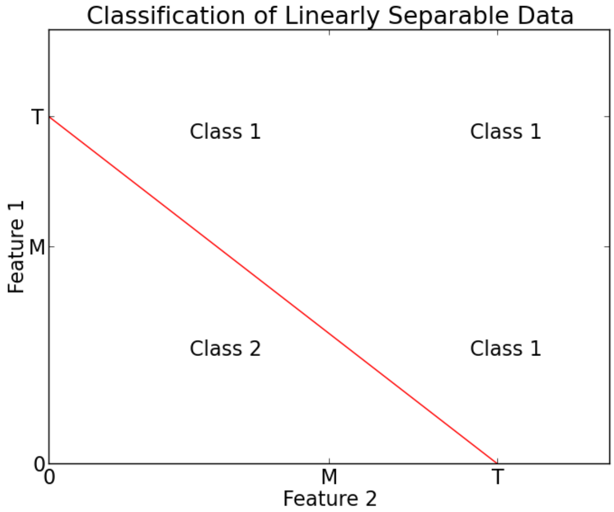

```
def score_inseparable:

    if f1 > M(f1):
        if f2 > M(f2):
            return class2
        else: return class1
    elif f2 > M(f2):
        return class1
    else: return class2
```

Figure 4.2.: *An example of inseparable data. M represents median points for corresponding features. The red lines visualize the boundaries between the classes, separating four distinct quadrants. The M value is chosen to be a median, so that adequate number of training examples was available for all quadrants.*

To evaluate the real Bayes behaviour the programs described above are ran with class 1 score equal to 1 and class 2 score equal to 50. Mean squared errors are computed for both cases. Figures 4.4a and 4.4b show the mean squared errors within their corresponding confidence intervals. Along with the actual Bayes classification error (denoted as 'Actual' on the y axes) the Baseline and Ceiling errors are plotted for comparison. The Baseline performance is evaluated by randomly assigning classes, whereas the Ceiling error illustrates the contribution of quantization error, inherent in classification of non-discrete scores.

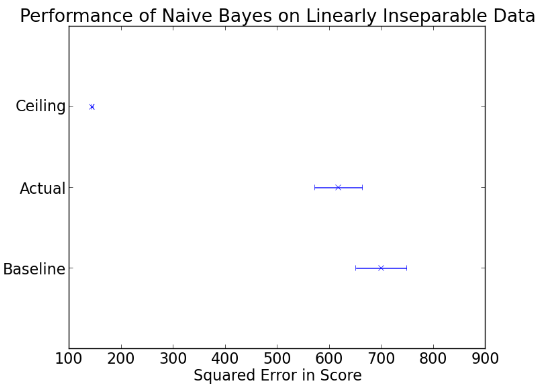
The mean squared error in the inseparable case is significantly larger: in fact, its confidence interval overlaps with the one of the error in random classification (the Baseline



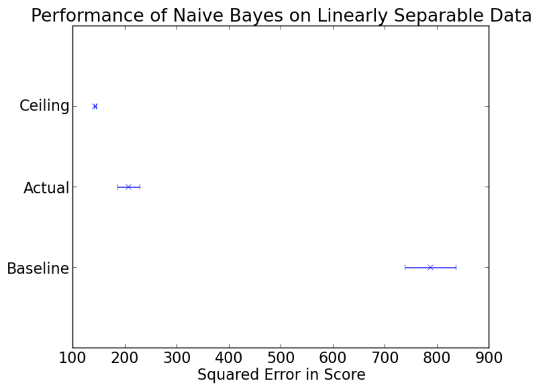

```
def score_separable:

    if f1 +f2 > T:
        return class1
    else:
        return class2
```

Figure 4.3.: *An example of separable data. On the red line the sum of features is equal to the threshold value T. As before, T is chosen to be the median of the sum f1+f2 to supply equally many training examples on either side of the line.*



(a) *The mean error is near the baseline performance with similarly wide spread.*



(b) *The mean error is distinctly better than the baseline and approaches the goal performance.*

error). Similarly, the standard deviation of the error is similar in width to the Baseline. This is due to the fact that the classifier is making mistakes as frequently. In contrast, the separable data case shows a convincing improvement in classification error, however, the classifier is still not perfect. This might be a result of insufficient or unbalanced training data. In this particular case and in general, adding more training data improves the error up to a point when overfitting occurs. Nonetheless, it is rarely possible to gather a subset of training data that will have enough points very near to the class boundary to allow for perfect classification. Therefore, the result is consistent with the proposed hypothesis.

Hypothesis: SVM with linear kernel performs well for linear heuristics, but becomes unusable for non-linear ones.

For comparison, SVM with a linear kernel is tested for linearly separable and non-separable data. In this particular experiment the number of features used is fixed at 2 and the heuristics used are shown in the table 4.1 below.

Name	Function
Linear	$x + y$
Quadratic	$x^2 + y$
Cubic	$x^3 + y$
Exponential	$exp(x) + y$

Table 4.1.: *Heuristic functions used to evaluate the performance of linear kernel.*

The SVM with Linear Kernel is run with each of the heuristics shown above. The error parameter is tuned as described in Section **??**. The error that produces the best result is used in each case, for example, the error is zero in the case of a linear heuristic. The baseline performance is a hyperplane fitted through the mean score. The ceiling performance is computed as a least squares solution of an equation which has the form of the particular heuristic used. *Numpy* provides a *lstsq* function which finds the coefficients of a particular heuristic such that the squared error is minimimal.

Figure **??** shows a failure of the linear kernel to fit non-linear data. The ceiling error due to numerical error in computation: this explains why the ceiling error in the exponential case is the largest of all.

Clearly, as in the Bayes case, the degradation is rapid. In the cubic and exponential cases the SVM seems to perform worse than the baseline, which can be explained by overfitting.

4.2.3. Bayes: Effects of Quantization

Hypothesis: Bayes classifies better when fewer classes are present.

It is intuitive that at a large number of classes, the more classes we introduce, the more precise the classifier has to be to perform equally well. However, taking into account the

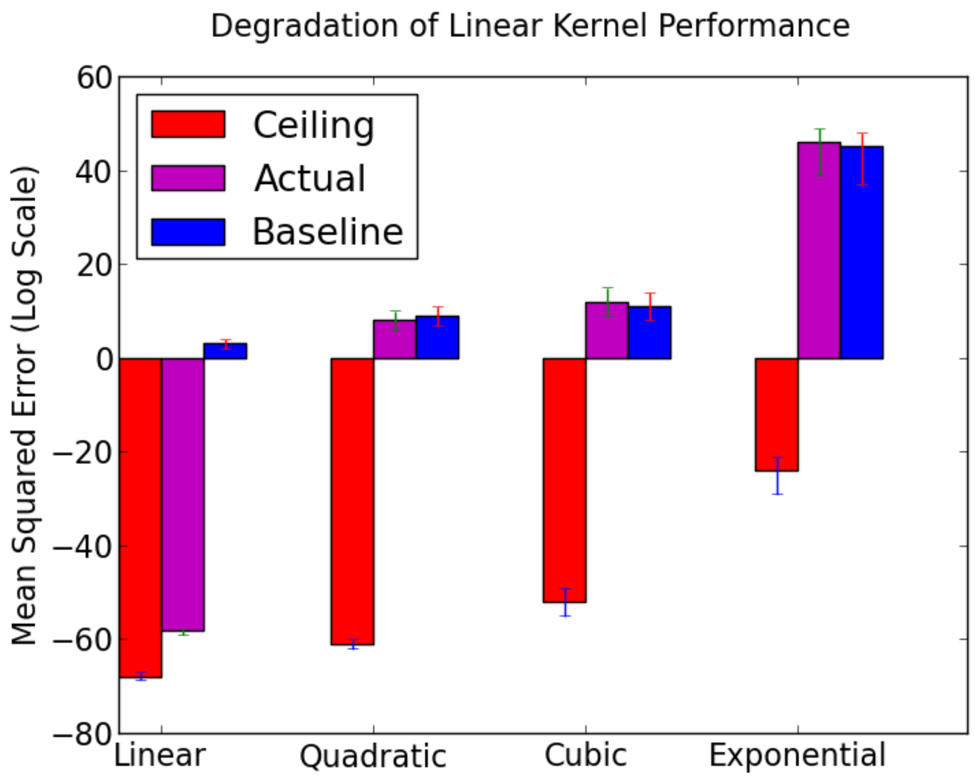


Figure 4.4.: *SVM with a linear kernel is evaluated against four different heuristics (x axis). Note than the MSE is in log scale. The error in the linear case is negligibly small, but is similar to the baseline case for all other heuristics.*

quantization error, non-linear behaviour might be expected: performance will improve due to the quantization error decreasing faster than precision up to a certain point. This experiment aims to determine the number of classes that minimizes the overall error of the classifier. In some sense, quantization is akin to a hyperparameter: the results are specific to the heuristic and the data used.

In this experiment, a linear heuristic is used with two features as before. The number of classes is varied starting with two classes. Classes are added until the maximum possible number is reached – the number of distinct scores.

Figure 4.5 shows a result inconsistent with the proposed hypothesis: the error is diminishing as rapidly as the quantization error (ceiling). It is visible from figure 4.6 that the data remains separable (as expected) independently of the number of classes. Clearly, Bayes is very effective at classification with the given heuristic. It is worth noting, that the actual performance is still worse than the ceiling and does not converge to zero as

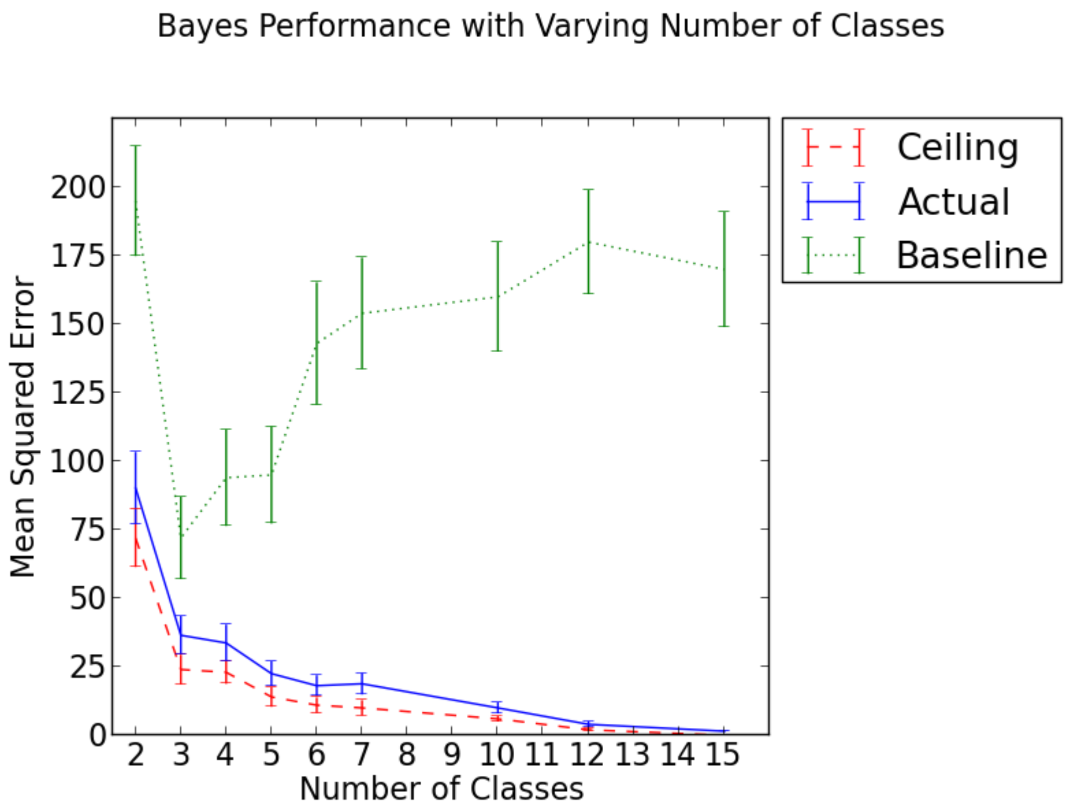
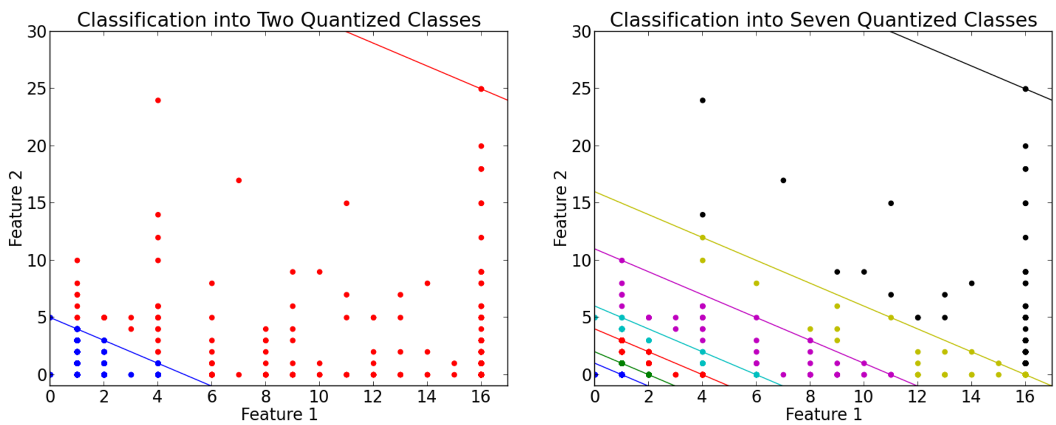


Figure 4.5.: *Error response to varying number of classes.*

opposed to quantization error. It is possible that Bayes consistently misclassified a few particular examples, which lead to a gap in the plot.



(a) *Two classes*

(b) *Seven classes*

Figure 4.6.: *Classification with different number of classes. The data is consistently separable.*

The example chosen does not verify the hypothesis and proves the intuition wrong: the Bayes erformance depends solely on whether the data is separable or not.

4.2.4. Curse of Dimensionality

Hypothesis: Bayes performance degrades rapidly as the number of features grows.

So far I have explored two dimensional cases where only two features were used for convenience of visualization. Dimensionality curse is one of the well-known issues with classification: when new features are added, the size of the training set has to grow exponentially to cover all the new dimensions. Naive Bayes, however, lessens this problem a little due to the assumption of conditional independence. It is interesting to see how rapidly its performance degrades when more features are added while the training data is unchanged. It is important that all the features used are conditionally independent, as otherwise, the results would not be valid.

The number of classes is fixed at a value of 7, at which the performance is reasonable but still has some quantization error. This is done to prevent the effects of the extremes of performance. We are only interested in relative performance, so it should not matter how many classes are used, however, it is important that the number of classes used produces a significantly better result than the baseline, to make sure a random guess could not produce a good result.

The result for a few linearly separable functions is computed and the average errors are plotted in figure 4.7. The actual classification diverges from the ceiling when the number of features is about 6. The rapid growth of the random classification curve is explained by the curse of dimensionality: degrees of freedom grow exponentially. The exponential growth is plotted in black for comparison: initially the baseline growth is near exponential, but less steep subsequently. This is due to the quality of training and test data: as the number of features grows, the number of training examples for each class is reduced, influencing the overall performance.

The ceiling and the actual curves are growing almost monotonously, as is expected. The flat regions at 5-6 and 7-8 are explained by the data specifics: the particular features added at those point appeared insignificant in the scores as they occurred infrequently and had small values.

It has proven hard to pick many conditionally independent features. Among the ones

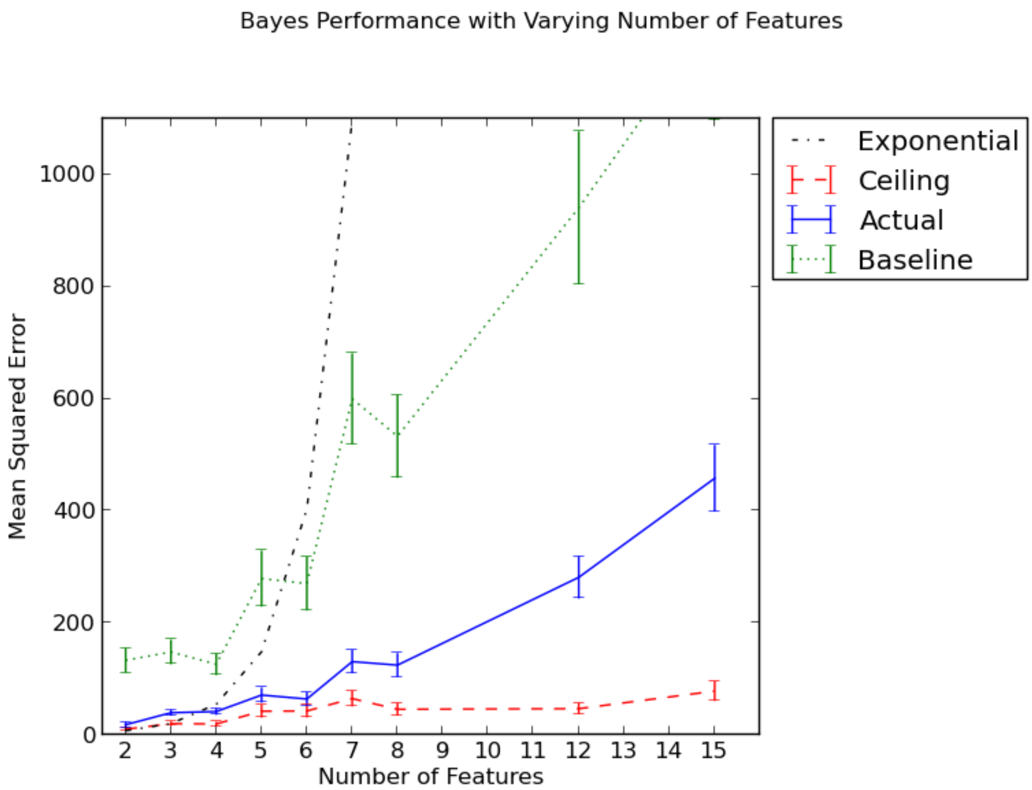


Figure 4.7.: *Error response with varying number of features.*

used were pagerank, image count, word count, frequency of search term occurrence, quality of html, price information availability and alike.

The hypothesis is verified: the error grows as the number of features is increased. The growth, however, depends also on the quality of features – how much the addition of a new feature alters the classification, as well as on the training set – how many training examples are supplied.

Hypothesis: SVM performance does not degrade as the number of features grows.

As before, linear kernel is used in combination with a linear heuristic. Figure 4.8 supports the hypothesis: the error looks almost constant even in logarithmic scale. Hyperplane fitting is more resilient to more dimensions in the presence of linear heuristics.

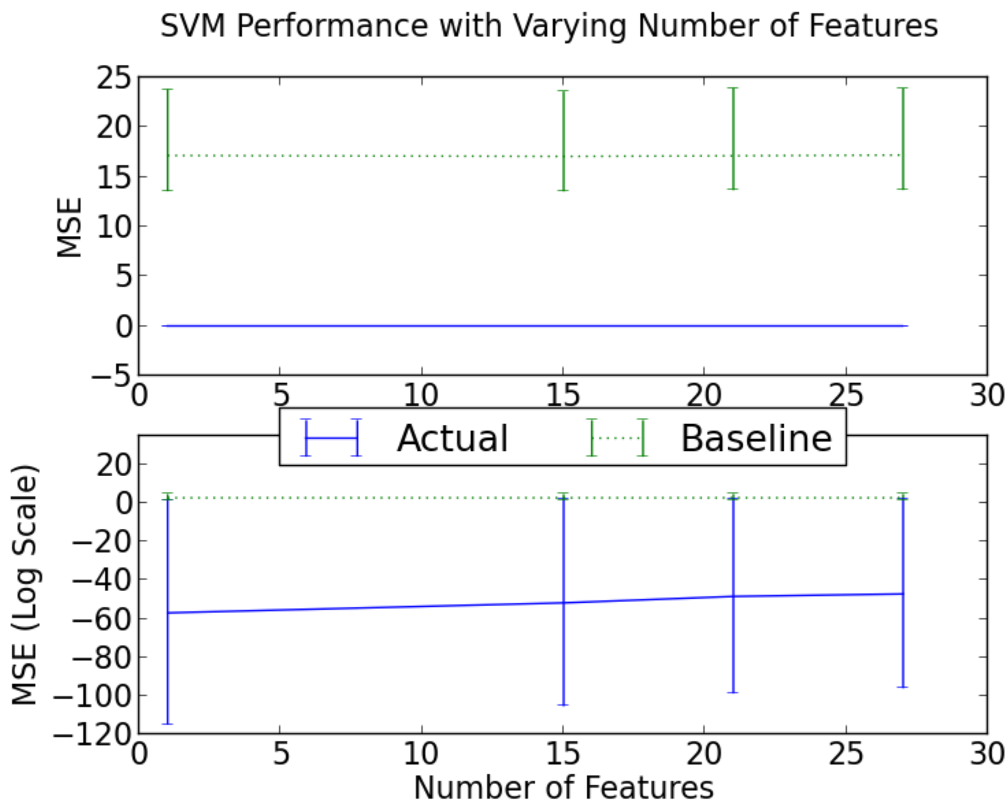


Figure 4.8.: *Both normal (upper figure) and logarithmic (lower figure) scales are shown. The error grows too slow for the growth to be noticeable without the logarithmic scale.*

4.3. Performance Evaluation

As stated in the Preparation, the project does not have any hard timing requirements. PageRank computation, indexing and learning were envisaged as most time consuming. In the end, the time taken in learning and classifying was negligible and same can be said about parsing. Throughout the implementation, it has become obvious that the most time was spent in indexing and PageRank computation. Therefore, in this section, I am looking in more detail in the timings and scalability of the two modules.

The plots were generated using a benchmark suite, which makes repeated measurements and calculates means and confidence intervals. I have configured the suite to take a hundred repeat measurements for a range of page numbers. The 95% confidence intervals are represented by the error bars on the plots.

The benchmarks were performed on my personal computer with the following specifications:

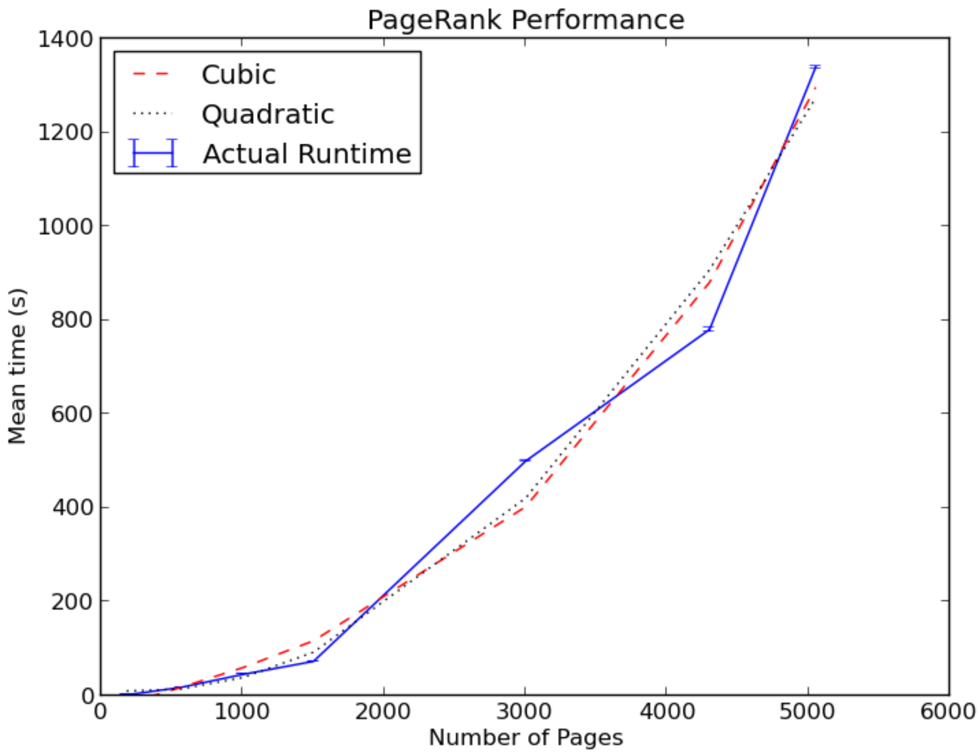


Figure 4.9.: *Time taken in computing PageRank for a growing set of pages. For convenience of comparison, a cubic and a quadratic curves are fitted.*

Memory	1.7 GB
Cache Size	3072 KB
CPU	IntelCore2 Duo CPU
CPU Clock Frequency	2.26 GHz

Both plots also display fitted cubic and quadratic curves. The curves are fitted using the *Scipy* library curve fitting function, which uses Levenburg-Marquardt algorithm[1]. Figure 4.9 shows how the performance of the PageRank computation degrades with the number of pages. Although neither cubic nor quadratic curve fits well, it can be said that up to around 5000 pages the growth is bound by $O(n^2)$. The average number of pages used in the project was around 3000 for each directory, which means it took around seven minutes to crawl and generate the PageRank vector. However, it is expected that the growth is more rapid beyond the limit of 5000 pages. If dealing with more pages was within the scope of the project, the PageRank computation would have

[1]Also known as Damped Least Squares method, the Levenburg-Marquardt algorithm works by minimizing a function over the space of its parameters.

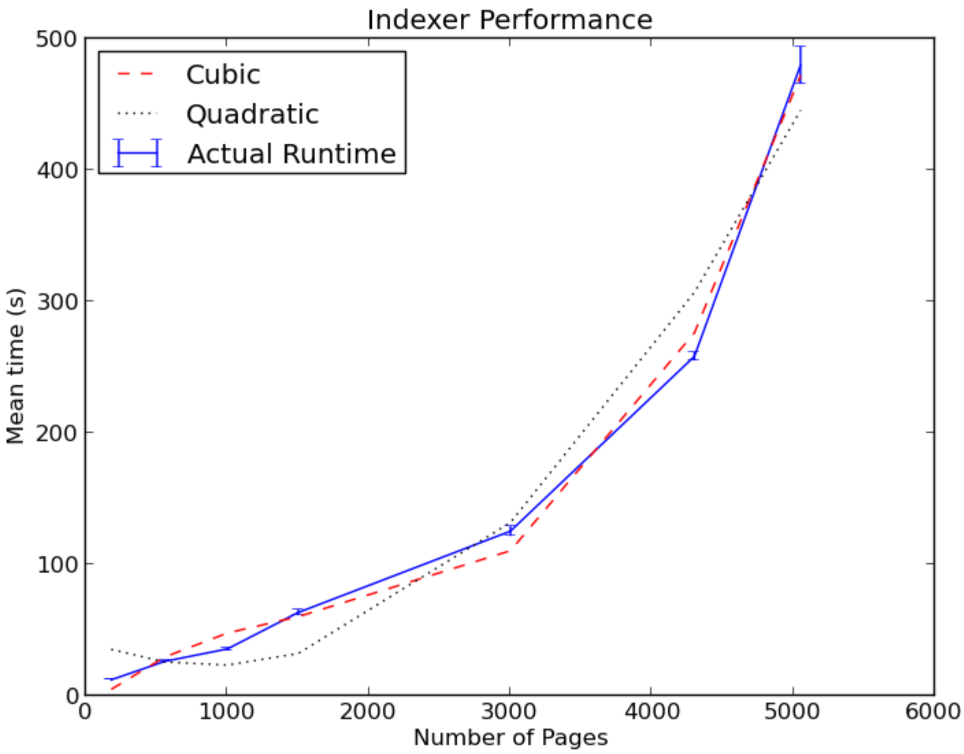


Figure 4.10.: *Time taken in indexing for a growing set of pages. For convenience of comparison, a cubic and a quadratic curves are fitted.*

to be optimized further, as matrix inversion does not scale for a problem bigger than a few thousand pages.

Indexing shows similar behaviour, although it seems a lot smoother and unambiguously exhibits cubic behaviour. Indexing 300 pages takes around two minutes, which is satisfactory considering that speed was not the primary objective of the project.

Altogether, both modules could potentially become a bottleneck. However, as development was carried out on a comparatively small development corpus (only around 500 pages), and the verified program was then run on the actual data only once, which means the time loss was infrequent. Both the index and the PageRank vector were stored and reused to avoid expensive recomputation. All things considered, it was not worth further optimizing the modules in question, as speed of implementation was prioritized over the speed of computation due to its apparent infrequency.

4.4. Testing

Formal correctness proofs are neither within the aims of the project, nor would they be feasible in the time given. Therefore, the main purpose of the testing is to gain a degree of certainty in the correctness of the program. The system developed is in a sense a prototype: it only gets used one time in order to obtain certain results. Therefore, tests do not need to be run as often as for a system that would be used in production. In addition, human analysis was often required to assess the quality of the programs. These aspects of the system motivate the decision to use manual testing, which is described further in this section.

4.4.1. High Level Test Plan

Table 4.2 summarizes the test plan used for manual testing. Each of these tests was conducted at the end of module development and whenever a substantial change occurred that could potentially change the behaviour in the cases described.

Module	Test Objectives
Crawler	The output matrix accurately reflects the link structure of the pages
PageRank	The PageRank vector accurately reflects the hierarchy of the web pages
Indexer	Clean indexing overwrites existent index
Indexer	Incremental indexing adds/removes relevant index changes to reflect the changed web pages
Parser	Parser is robust in the face of bad formatting and encodings
Naive Bayes	Classification is better than random for separable data
SVM	The hyperplanes fit the data and change with the data to provide better fitting

Table 4.2.: *Summary of Test Objectives*

4.4.2. Example Test Cases

Crawler and PageRank

Both Crawler and PageRank were tested on artificially engineered small examples of link structure to verify the test objectives have been achieved.

Indexer

Indexing is heavily reliant on the library, so only the implemented parts required extensive testing – incremental and clean indexing capabilities. These were tested on the verification corpus. To test incremental indexing, pages were added, removed and altered and the relevant queries executed to verify that the changes have taken effect. The clean index was build both without an existent index – in which case a new index was created – and with an existent index – to verify that the old index is replaced by the new one.

Parser

The objective of the Parser testing was mainly its resilience to failure: examples of malformatted html and pages with special characters in the address were used to verify the robustness.

SVM and Bayes

Machine Learning modules both were tested with the visual aid of plotting in the two- and three-dimensional cases. The data was plotted alongside the hyperplane (SVM) or the separating line (Naive Bayes). The data was altered to provoke change in the hyperplane/separator and the subsequent change was verified.

4.5. Summary

In this chapter I assessed the performance of classifiers with different heuristics and drew some comparisons between them with the means of hypotheses. I also illustrated the testing strategies adopted in this project and evaluated the quality of implementation of the slowest modules.

5. Conclusions

The exploratory nature of the project allowed me to learn a lot both in the field of information retrieval and machine learning. I have started with very little insight in either field and thoroughly enjoyed the discoveries I made throughout.

5.1. Lessons Learnt

The main lesson I have learnt from this project is that the importance of design cannot be underestimated. At the beginning I expected the programming to be the hardest part and, perhaps, rushed into implementation without having spent adequate time planning what should be done and how best to do it. This resulted in some redundant work that could have been avoided. If I were to do this project again, I would allocate a lot more time to design at the beginning.

Another important observation that I am taking away is in tune with the previous point: writing loosely coupled and modular code pays off eventually. As code grew, refactoring often became unavoidable, but could have been made easier, had I programmed with reusability in mind.

5.2. Future Work

Although the implementation is complete in the sense that it fulfills the success criteria for the project, the greater goal of project is open ended. The framework developed can be used to further explore the machine learning techniques considered as well as to integrate the data from the real existing search engines. The machine learners can be used for a variety of different purposes unrelated to search engines.

The implementation can be enhanced by a user interface and made available on the internet for anyone to download, use and improve.

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A. Project Proposal