OTIMIZANDO MODELOS DE APRENDIZADO DE RANQUEAMENTO COM BASE EM AGREGAÇÃO DE ÁRVORES DE DECISÃO

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OPTIMIZING ENSEMBLES OF BOOSTED ADDITIVE BAGGED TREES FOR LEARNING-TO-RANK

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Optimizing ensembles of boosted additive bagged trees for learning-to-rank

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"Computers aren't supposed to be creative; they're supposed to do what you tell them to. If what you tell them to do is be creative, you get machine learning."
(Pedro Domingos)

Resumo

Recuperar informação que realmente importe para o usuário é difícil quando consideramos grandes repositórios de dados como a web. Para aumentar a efetividade desta tarefa de busca de informação, sistemas têm tirado proveito da combinação automática de funções de ranqueamento por meio de métodos de aprendizado de máquina, tarefa também conhecida em recuperação de informação como aprendizado de ranqueamento. Os métodos mais efetivos de aprendizado de máquina são atualmente agregações de árvores de decisão, tais como Florestas aleatórias e/ou técnicas de impulsionamento (e.g: RankBoost, Mart, LambdaMart). Nesta dissertação, é proposta uma estrutura que combina de maneira aditiva árvores de decisão, em específico Florestas Aleatórias com Impulsionamento de maneira original para a tarefa de aprendizado de ranqueamento. Em particular, é explorado um conjunto de funções que tornam possível deduzir quais amostras do conjunto de treino são de difíceis predição em um contexto de regressão. Isso é realizado por meio da aplicação de um conjunto seletivo de abordagens de atualização da distribuição de pesos das amostras para aumentar a performance de ranqueamento do modelo de aprendizado de máquina. O modelo genérico apresentado nesta dissertação aborda algumas instâncias que consideram diferentes funções de perda e diferentes maneiras de atualizar a importância dos documentos. Nas análises experimentais, os modelos foram capazes de superar todos os algoritmos considerados do estado-da-arte em várias coleções de dados. Outra vantagem da nossa estrutura de aprendizado de máquina para ranqueamento é que ele é capaz de superar algoritmos base avaliados considerando pequenas frações de treino e com taxas de convergência superior em todas as coleções avaliadas. Isso mostra a vantagem em utilizar o nosso modelo para problemas de ranqueamento, especialmente quando consideramos a dificuldade em se obter dados de treino.

Palavras-chave: Recuperação de Informação, Aprendizado de Ranqueamento, Aprendizado de Máquina, Florestas Aleatórias, Impulsionamento.

Abstract

The task of retrieving information that really matters to the users is considered hard when taking into consideration the current and increasingly amount of available information. To improve the effectiveness of this information seeking task, systems have relied on the combination of many predictors by means of machine learning methods, a task also known as learning to rank (L2R). The most effective learning methods for this task are based on ensembles of trees (e.g., Random Forests) and/or boosting techniques (e.g., RankBoost, MART, LambdaMART). In this master degree dissertation, we propose a general framework that smoothly combines ensembles of additive trees, specifically Random Forests, with Boosting in an original way for the task of L2R. In particular, we exploit a set of functions that enable us to smartly deduce the samples that are considered hard to predict in a regression approach and apply a set of selective weight updating strategy to effectively enhance the ranking performance. We instantiate such a general framework by considering different loss functions, different ways of weighting the weak learners as well as different types of weak learners. In our experiments, our rankers were able to outperform all state-of-the-art baselines in all considered datasets with statistical significance. Another important advantage of our framework is that it is able of surpassing all baselines using just a small percentage of the original training set, with the addition of faster convergence rates in all evaluated collections. This shows the importance and potential of advantage of our approaches over the baselines since training data with graded relevance judgments is very costly and time-consuming to acquire.

Palavras-chave: Information Retrieval, Learning to Rank, Machine Learning, Random Forest, Boosting.

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Chapter 1

Introduction

Today, we live in an era of massively available information, with a never-seen-before (and increasing) rate of information production. It is not surprising that such a scenario imposes hard to tackle challenges. For example, the availability of massive amounts of data is not of great help if one is not able to effectively access the relevant content that satisfies some user needs (informational, navigational or transactional) [Broder, 2002].

The problem arises when trying to make assertions of document relevance (importance of web pages) to each individual user. This is quite difficult since the concept of relevance is user dependent and therefore the same set of terms might have different meanings when posed in comparison of two distinct users. This difficulty is mainly attributed to the ambiguity of the query (e.g., "bond" may refer to the secret agent James Bond, Original Electric String Quartet or a concept commonly used in finances) [Santos et al., 2015] or simply due to the fact that the user may not express their needs using the "best set of terms". Another issue is that modifying the query length by stretching or shrinking it to key terms does not assist the search engine in solving the retrieval problem since it is known that every query, independent of its length, can be considered ambiguous or ill-specified [Song et al., 2007].

Therefore, to answer this problem the main question that arises is: *How to obtain the "best rank" amongst all possible permutations of retrieved documents containing the most relevant documents on top and non-relevant on the bottom?*. The answer to this specific question has become of extreme importance in the new era of mobile devices with smaller screens, in which the need to focus **only** on the top most relevant results is key [Pass et al., 2006, Granka et al., 2004]. This is even more important nowadays when relevance depends on many other factors: location, timing, device capabilities and many other conditions captured by wearables (smart watches).

Retrieval systems, such as search engines, question and answer (Q&A) forums,

and expert search systems serve exactly this purpose: given an information need, expressed in the form of a query (normally between 2 to 3 terms [Silverstein et al., 1999]) and a set of possible information units (e.g.: documents, web pages, images), the main goal is to provide an ordered list of information units according to their relevance with relation to the query [Manning et al., 2008]. The desideratum is to increase the likelihood of satisfying a user's information need in an effective manner by optimizing some retrieval metric, which translates into pushing the truly relevant results on top of the less relevant ones.

One of the key aspects that influence retrieval systems is how they determine the relative relevance of candidate results in order to produce a ranked list containing the most representative documents on top, and the least ones in the bottom. The quality of those rankings is of primary importance in order to guarantee efficient and effective access to relevant information (and, hopefully, the satisfaction of the user's information needs). Several approaches to generate such ranked lists do exist, being traditionally performed by the specification of a function that is able to relate some user's query to the set of known (indexed) information units. Usually, ranking functions consider several features, such as those that rely on the relatedness between query and possible results by capturing the correlation of the list of documents and the searched subject (e.g.: TF-IDF, BM25, edit distance, similarities in vector space models) or on link analysis information that captures the "relative importance" of the document (e.g., PageRank, TrustRank) in some context (e.g., Web link structure) [Liu, 2011].

Unfortunately, to specify and fine-tune ranking functions turns out to be a major problem, since it is known that most of them have sensitive parameters to the subtle differences of the input space, what makes the learning process extremely expensive and time-consuming to obtain. Moreover, improving ranking effectiveness is even more difficult, since it requires to effectively combine the individual features [Gao and Yang, 2014], which increases the complexity of the problem as the number of features grows with non-trivial interactions amongst them.

1.1 Motivation

This difficulty in effectively combining the best pieces of evidence in order to boost ranking effectiveness motivates the use of Machine Learning (ML) algorithms to devise such combinations. It is known that ML is capable of finding and combining several pieces of evidence (predictors or features) in a non-trivial way (e.g., non-linearly) towards optimizing some goal (a.k.a: loss functions) [Liu, 2011]. This is a field of study

in information retrieval known as "Learning to Rank (L2R)", whose primary goal is to learn a model that is capable of automatically deriving the relevance score of unseen documents.

More specifically, based on a set of {query ⫞, documents} pairs with known relevance judgments, the goal is to learn a function $f(q, d)$ that is capable of accurately devise the relevance prediction for a document d, with respect to a query q. Due to ML importance in the information retrieval context, several approaches for L2R have been proposed in the literature. As a matter of fact, ensemble methods based on boosting such as RankBoost [Freund et al., 2003] or AdaRank [Xu and Li, 2007] and bagged additive decision trees such as Random Forests [Breiman, 2001] or its variations such as [Geurts and Louppe, 2011]), are deemed to be the techniques of choice for L2R, achieving higher effectiveness in published benchmarks when compared to other algorithms [Geurts and Louppe, 2011, Canuto et al., 2013].

Normally, ensemble strategies based on boosting are used as a wrapper iterative meta-algorithm that combines a series of weak learners (normally decision trees or neural networks) [Drucker, 1997] in order to come up with an improved final learner, focusing on hard-to-classify regions of the input space as the iterations increase [Schapire and Freund, 2012]. Each weak learner is a predictor with generalization capabilities better than random guessing and its concept is interchangeable with the strong learnability concept since it is possible to transform a weak learner into a improved strong learner [Schapire, 1990]. The ensemble strategies based on Random Forest rely on the combination of several decision trees, learned with bagging (**b**ootstrap **agg**regati**o**n) of samples in the training set with additional randomization procedures upon the feature vector (such as random feature selection) to produce decorrelated-correlated trees — a requirement to guarantee its effectiveness [Breiman, 2001].

1.2 Objectives

In this work, we developed a general framework for L2R, named Generalized BROOF-L2R that explores the advantages of boosting and Random Forests, by combining them in a non-trivial fashion. More specifically, at each iteration of the boosting algorithm, a Random Forest model is learned by training examples sampled according to a probability distribution. Such probability distribution is updated at the end of each iteration in order to force the subsequent learners to focus on hard to classify regions of the input space. In particular, the use of RFs as weak learners has its own advantages, since they are capable of providing robust estimates of expected error

through out-of-bag error estimates [Breiman, 1996b]. Moreover, by means of a selective updating of the the weights of the out-of-bag samples, one can effectively slow down the tendency of boosting strategies to overfit (a well-known phenomenon that becomes critical as the noise level of the dataset being analyzed increases) [Salles et al., 2015].

As we shall detail in this master dissertation, the key aspects of the proposed Generalized BROOF-L2R have to do with how to update the probability distribution and how such update should be performed, as well as the underlying loss function used to produce the final set of results. In this work, we discuss a set of possible instantiations of the proposed general framework, in order to highlight the behavior and potential of the proposed L2R solution.

In summary, the main research questions that we address are: *(i)* Can the combination of these two machine learning approaches based on Boosting and Bagged Trees help each other in order to enhance rank effectiveness in the context of L2R? *(ii)* How should the samples distribution be updated at each iteration of the boosting meta-algorithm? *(iii)* How should the loss functions be implemented in order to better capture the main features of Boosting and Bagging in the context of L2R? *(iv)* Are the instantiations computationally efficient? *(v)* Is it statistically and computationally feasible to build and apply ensemble models in large real-world datasets?

The answers to those questions are scattered throughout the dissertation, and in the next section, we highlight the main findings of this work.

1.3 Achievements

We develop a L2R framework named BROOF-L2R that allows the use of out-of-bag samples as validation technique and at each boosting iteration we apply one of four distinguished loss functions. Amongst all of our instances, the one that optimizes the residue by minimizing the gradient descent loss function achieves the strongest results in terms of Mean Average Precision (MAP) and Normalized Discounted Cumulative Gain (NDCG), with significant improvements over the explored adversary algorithms in 5 traditional benchmark datasets. Our alternative instances were also able to achieve competitive (or superior) results when compared to the baselines in individual collections.

As our experimental evaluation shows, our general framework is able to produce top-notch results with substantially less training samples and less iterations compared to the evaluated baselines. Such data efficiency and high generalization capabilities are key to guarantee practical feasibility since obtaining labeled data and machinery-

power are very costly. We also provide extensive statistical analysis of our findings using well-known statistical designs and hypothesis tests to demonstrate the benefits of the BROOF-L2R framework.

To summarize, the contributions of this work are three-fold: *(i)* we provide a general framework for L2R that is able to combine two strong methods (boosting and Random Forests) in an original way, which can be specialized in several ways and produce highly effective L2R solutions; *(ii)* we propose and discuss a set of alternative instantiations of such a framework, in order to highlight the behavior and effectiveness of each possible choice; and *(iii)* we advance the state of the art in L2R by means of some instantiations of our proposed framework that are able to outperform top-notch solutions, according to an extensive benchmark evaluation considering five datasets and seven L2R baseline algorithms.

The potential of our approach is demonstrated by two published papers, one in a national level [de Sá et al., 2015] (KDMile) and another in an international level [de Sá et al., 2016], in which this last one is the major Information Retrieval conference (SIGIR). In the first paper, is shown an initial study of this two machine learning algorithms applied in the L2R context with a general idea of how they could be merged into a single elegant algorithm. The second published paper deepens into the possible ways of making this two algorithms work together by defining an extensible and general framework for L2R based in the combination of this two ensemble machines.

The following section contains a Roadmap with a brief description of the organization of each chapter of this dissertation.

1.4 Outline

The remainder of this work is described as follows:

- In Chapter 2, we formalize what is the task of L2R and the main differences from other classification and regression problems. We also introduce the notations and conventions that are necessary to better understand the techniques and algorithms used in the proposed framework.

- In Chapter 3, we provide a brief description of related work using Boosting, committee of additive trees such as Bagging and RF or even the combination or enhancement of one or another approach in the context of L2R.

- In Chapter 4, we discuss the BROOF-L2R framework and how to instantiate it

by modifying individual steps that generate stronger models with higher generalization capabilities.

- In Chapter 5, we describe the experimental statistical methods used to summarize the obtained results.
- In Chapter 6, we detail our results considering the experiments performed as described in Chapter 5.
- Finally, in Chapter 7, we conclude the dissertation, summarizing our main findings and proposing some directions for further investigation.

Chapter 2

Problem Statement and Algorithmic Background

In this chapter, we briefly describe what is L2R and give an overview of the algorithms used in the presented framework.

2.1 Learning to Rank Framework

As described by [Baeza-Yates and Ribeiro-Neto, 1999], the task of ranking is at the core of information retrieval by directly retrieving to individual users an ordered list of documents containing the most relevant documents at the top while pushing away the less relevant ones. This is usually done by using a set of ranking functions that are combined in order to increase ranking effectiveness. To achieve this effectiveness in a feasible way, ML approaches are used to figure out the relevance of a document regarding pairs of query and documents [He et al., 2008].

Although it is known that there exists research in L2R that considers semi-supervised learning, such as inductive approaches that propagate the ground-truth known labels to the unknown documents, or even completely unsupervised ones, such as on-line L2R by using implicit feedback, in this work we only consider it as a supervised technique which exploits the query dimension. Therefore, we can use any ML algorithm for classification or regression to estimate the relevance of a document. To better exemplify, Figure 2.1 shows a chart that aids to visualize how ML is applied in the L2R context. As any supervised classification approach, to build a ML model to rank documents, it is necessary to have a training dataset that is composed of a set of queries $Q = \{q_1, q_2, q_3, \ldots, q_m\}$. Each individual query q is accompanied by a set of

documents $X = \{x_1, x_2, x_3, \ldots, x_n\}$ that are represented as feature vectors, in which each feature is a ranking function by itself or a combination of them.

As we can also see in Figure 2.1, each document in the training set has its own annotated relevance judgment y_n that identifies the "importance" of a document x_n to answer a given query q_m. Such importance of a document x_n may vary for different queries. The representativeness of a document is usually defined as a binary or multi-graded relevance judgment. The first one implies that a document can either be 0) non-relevant or 1) relevant for a given search. The second one considers that the importance of a document can range in a graded scale, for instance, from 0 to 4, being 0 the least relevant and 4 the most relevant one [Liu, 2011].

Given the training set, a machine learning system is applied to the discriminative data to figure out a hypothesis h that will evaluate each sample document in the input space X and then assign a prediction $\hat{y}$ for each document based on its features $h(\overline{x}_n)$. By means of this prediction, it is possible to compute its distance from the ground truth relevance y, which allows us to identify by means of an evaluation metric the generalization capabilities of an algorithm by using some loss function l.

After the construction of the model, it is possible to refine its predictions by evaluating different parameters using cross-validation techniques. When the final model is ready, it is possible to apply the resulting mechanism in a test set by passing a list of documents for individual queries and, as a result, to obtain the prediction for each document in the form of a class, in case of classification, or regression scores values. Although some papers mention that, for L2R the use of classification or regression algorithms are statistically equivalent and that the best approach is dataset dependent [Geurts and Louppe, 2011], in this work we consider only the regression approach, since it provides a way of differentiating how much the prediction of a document is more important than another one. After the computation of the importance of the documents, the last step is to sort the documents according to its predicted score $\hat{y}$ [Liu, 2009, Liu, 2011].

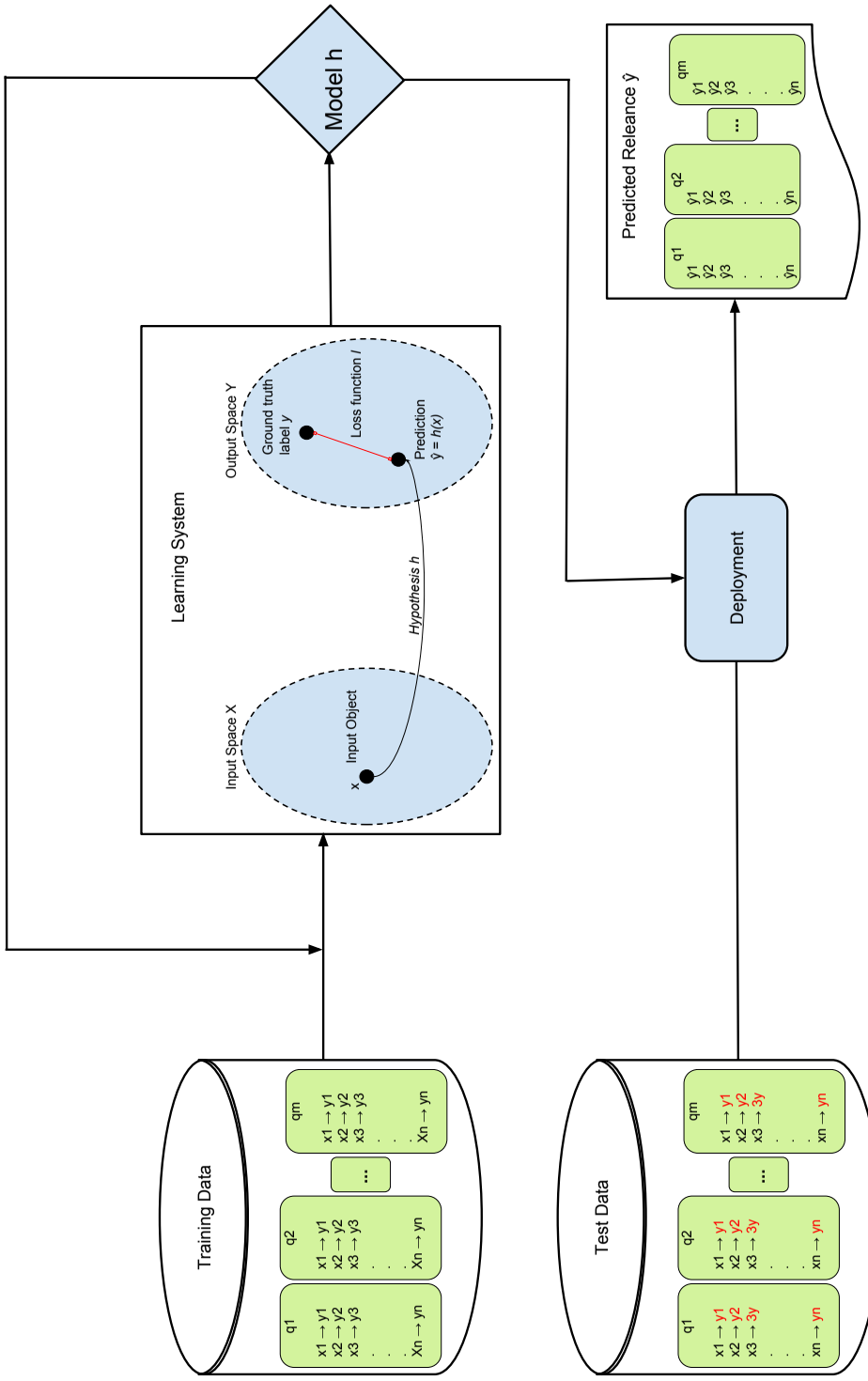


Figure 2.1: Learning to Rank Model

2.2 Decision Trees

Decision trees are known to be one of the most popular ML algorithms amongst researchers. Its popularity is mainly due to: (i) their high generalization capabilities; (ii) their generality, allowing their application in many fields of study such as statistics, machine learning, data mining, pattern recognition and many others; (iii) their interpretability, since it is possible to trace the pieces of evidence by descending through the nodes of the tree and verifying the many criteria of impurity chosen in order to split the data through the nodes [Maimon and Rokach, 2010].

There are many ways of instantiating a model based on decision trees: CART [Breiman et al., 1984], ID3 [Quinlan, 1986], C4.5 [Quinlan, 1993] are some of the most popular algorithms. In this work, we only highlight the use of CART as our primary algorithm of study, since there are many freely available implementations of it such as the highly known python library by [Pedregosa et al., 2011]. The CART acronym stands for classification and regression trees, and it works by recursively dividing the input space by making orthogonal splits considering an univariate splitting criteria of impurity [Breiman et al., 1984].

For classification problems usually Gini Index, Entropy or Classification Error are used as measure of impurity. These three measures are described in Equations 2.1, 2.2 and 2.3:

$$\text{Classification Error} = 1 - \max[p(i|t)] \tag{2.1}$$

$$\text{Gini} = 1 - \sum_{i=0}^{c-1}[p(i|t)]^2 \tag{2.2}$$

$$\text{Entropy} = -\sum_{i=0}^{c-1} p(i|t) log_2 p(i|t), \tag{2.3}$$

in which c is the total amount of individual annotated relevance judgments of documents in a given node, p is the probability of documents with class i regarding the total number of documents t. For the regression case, the most known equivalent splitting criteria is known as Mean Squared Error (MSE) shown in Equation 2.4:

$$\text{MSE} = \min_{j,s}\left[\min_{c_1}\sum_{x_i \in R_1(j,s)}(y_i - c_1)^2 + \min_{c_2}\sum_{x_i \in R_2(j,s)}(y_i - c_2)^2\right], \tag{2.4}$$

In here R_1 and R_2 are pairs of half-planes of a node t that are chosen by a

greedy algorithm that considers a splitting variable j and a split point s. The inner minimization considers the average of documents in each individual region given by c_1 and c_2. The greedy algorithm is necessary in order to maintain the feasibility of the solution (required in order to process large amounts of data) since to find the best tree structure is considered NP-hard [Hancock et al., 1996]. This splitting criterion is recursively processed until one of the stopping rules are achieved (total number of nodes, the total number of leaves, the tree depth, the number of attributes used), or until all tree nodes are pure, which achieves the tree's maximum length. The problem of letting the tree grow to its maximum extent is that, as it grows, it starts to loose its generalization capabilities and probably overfitting on training or validation set, which requires a set of pruning steps in order to reduce the complexity of the model. To further understanding decision trees, we refer the reader to [Breiman et al., 1984, Quinlan, 1986, Tan et al., 2005, Maimon and Rokach, 2010].

2.3 Ensemble Methods

Although there is no formal definition of what is an ensemble method, theoretical and empirical studies have shown the importance of committee of aggregated classifiers. The general classifier which assembles the individual ones using a combiner is usually better than the single counterparts [Kuncheva, 2014]. The two most known ensembles of additive trees are Random Forests and Boosting, and in the two following subsections we provide a brief overview of each one of this two ML models.

2.3.1 Random Forests

As a variant of bagging (**b**ootstrap **agg**regatio**n**) approach, RF is one of the most powerful ML ensemble techniques, being extremely efficient and effective in several tasks such as genome data analysis [Chen and Ishwaran, 2012], image detection [Antonio Criminisi, 2009], tag recommendation [Canuto et al., 2013] and name disambiguation [Treeratpituk and Giles, 2009] to name a few. Its high generalization power is mainly due to its efficiency in minimizing the variance while not increasing too much the bias. Thus, when building the individual trees of the ensemble, a set of randomization techniques are applied upon the training data and feature vector of documents. Since the randomization of training samples are performed with resampling, a Poisson distribution estimates that roughly 63% of the original set of documents should be used. The remaining 37% of the samples, named as out-of-bag (oob) samples, may be used as validation technique of the fitted model. The randomization of the features

is usually the proportion of $\sqrt{p}$ in which p refers to the dimensionality of predictors and the intuition of this randomization is to decrease even further the variance of the model [Breiman, 2001].

2.3.2 Boosting

Boosting is a meta-algorithm that exploits the weak learner assumption, improving the efficiency of any classifier in which the accuracy is better than random guessing [Solomatine and Shrestha, 2004]. To increase the likelihood of getting a better classifier in each round of the iterative procedure it modifies the importance of samples in the input space by resampling the documents according to a given probability distribution function [Quinlan, 1996] or by associating weights to each training sample and iteratively modifying this weight distribution [Solomatine and Shrestha, 2004].

The associative weights' distribution has the same uniform probability distribution at the initial step, and as the number of iterations grows the weights are modified in order to represent the samples that are more difficult to predict. This updating scheme of the distribution has the intention of iteratively identifying the "hard to predict" regions of the input space and heuristically building new weak classifiers on specific hard to predict regions. As new specialized classifiers are built upon these hard to predict regions the bias tends to minimize. A problem with this technique is that boosting is very susceptible to noise data, which can cause overfitting as the number of iterations grow [Schapire, 1999].

As a final remark, in contrast to the RF approach, the variation required in boosting to identify the hard to predict samples is by fitting decision stumps or small trees, whilst RF tends to keep variation through bagging while fitting fully grown trees.

Chapter 3

Related Work

Due to the effectiveness of boosting and RF, there are plenty of research aiming at improving and/or assembling one of these two ML mechanisms. Some of them can be found in [Fernández-Delgado et al., 2014] and [Tax et al., 2015]. The first one shows a comparison of 179 algorithms and the second one is a selective cross-benchmark with specifically tailored solutions to improve document retrieval containing 87 L2R approaches. The most interesting aspect of these two works is that independent of the search domain, the top performers are always ensembles of additive trees. In the sections that follow, we provide a brief description of related work that attempts at improving ensemble of additive trees approaches.

3.1 Major L2R Approaches

Learning to Rank solutions are divided into three major approaches: pointwise, pairwise and listwise. Pointwise L2R algorithms are probably the simplest (yet successful) approaches, directly translating the ranking problem to a classification/regression one. In this case, the training set for the supervised learning algorithm consists of pairs $\{q_m, (x_n^m, y_n^m)\}$ of queries q_m and a list of associated documents x_n^m (n^{th} document of query m), each one with its relevance judgment y_n^m (relevance judgment of document x_n of query q_m). In this case, each triple (q_m, x_n^m, y_n^m) is considered to be a single training example. The goal is to learn a classifier/regressor model capable of accurately predicting the relevance score of a document x, with relation to a query q_m, thus producing a partial ordering over documents. Pairwise algorithms, on the other hand, transform the ranking problem into a pairwise classification problem. In this case, learning algorithms are used to predict orders of document pairs, thus exploring more ground-truth information than the pointwise approaches. Unlike both mentioned

strategies, the listwise approaches essentially treat the pair $\{q_m, (x_n^m, y_n^m)\}$ as a single training instance (that is, considering a ranked list of documents for a query q_m as a single training example), capturing more information from the training set (namely, group structure) than the previous alternatives.

Although there are ranker methods in all three L2R approaches in the literature, ensembles of Random Forests (RFs) and boosting demonstrate to be strong solutions according to published benchmarks [Mohan et al., 2011, Geurts et al., 2006, Canuto et al., 2013]. More specifically, RFs (and the variations thereof [Geurts and Louppe, 2011]) as well as boosting algorithms such as Gradient Boosted Regression Trees (GBRT) [Friedman, 2000] and LambdaMART [Xu et al., 2012], are considered by many researchers [Lucchese et al., 2015] to be the state of the art in L2R tasks. This success is due to the fact that these ensembles rely on a divide and conquer approach by maintaining the strength of the individual learners of the committee in several parts of the predictive task. Thus, when mixing the individual predictive abilities of the classifiers, it is possible to maintain a set of specialists in smaller portions of the general problem [Kuncheva, 2014].

This advantage in using a mixture of experts is observed by the authors of [Busa-Fekete et al., 2013], which build an ensemble of standard pointwise multiclass Adaboost.MH. The novelty of their strategy is to individually calibrate this ML algorithm by estimating the probability distribution of the class labels given a feature vector representing the query document pair $\{q_m, (x_n^m, y_n^m)\}$. The estimates are computed using a set of different techniques and then combined by aggregating each estimate with exponential weight, which seems to be better than the usual uniformly weighted aggregation. As a conclusion, the authors argue that in general, their pointwise approach is more competitive than their counterparts pairwise and listwise, since it scales better and is able to surpass the baselines in terms of NDCG as the size of training data grows in multi-relevance judgment collections. This can be explained by the fact that being able to better capture training data information when learning a ranking function comes with a price: usually, pairwise and mainly listwise approaches are harder to train since they require more sophisticated (e.g. query-level) loss functions [Liu, 2011].

Another problem that arises with sophisticated solutions such as pairwise or listwise ones, discussed by [Niu et al., 2012], is the high-level of disagreement in real world data as the number of factors that define the importance of a document increases, making it unfeasible for wide use on the web due to the increase in complexity. One possible solution for this complexity issue relies on better choosing the pairs of documents to be judged, and the way of choosing the correct pairs of documents. The authors suggest to consider a transitivity rule of preference using heap sort. Their ranking approach

basically builds an ensemble using a listwise loss function to model the order of top k elements and a pairwise loss function to model the preference of top items to each of the k items. The final model is the ensemble of listwise approaches SVM^{MAP}, AdaRank and ListNet combined with the pairwise models RankSVM, RankBoost and RankNet. This ensemble technique minimizes the complexity of the main pairwise problem by only evaluating a few combination of documents, instead of judging all possible pairs of documents during the creation of the model.

Although we devise a series of loss functions that work upon the queries dimension to improve the ranking performance towards minimizing the residues, we do not use any information retrieval metric that directly computes the current relevance of the documents being ranked at a given iteration to improve the ranking effectiveness. Therefore, we see our approaches as pointwise methods. In the following section, we highlight some related work that attempts at improving the tree structure of ensemble models in order to improve its efficiency, which is a requirement to be competitive nowadays.

3.2 Ensemble Design: Improving Efficiency

Although ensemble machines generate very effective models, they are not without drawbacks. The general ensembles of additive trees are usually known to require large amounts of memory due to the large number of trees in the final committee. This becomes a real problem when considering general purposes hand-held systems such as wearables, smartphones, embedded systems and Web applications.

To overcome this issue, the authors of the Boosted Random Forest [Mishina et al., 2014] algorithm build an ensemble method by introducing boosting into a RF. This introduction of boosting is intended to reduce the amount of memory allocated for the RF by effectively applying the boosting algorithm to each individual tree of the ensemble and then heuristically selecting only the trees that increase the overall effectiveness of the ensemble in the training stage process. According to their findings, this process reduces the number of trees on the ensemble while increasing the effectiveness of the final model. Therefore, they are applying boosting to individual trees and then assembling them into a RF model containing only the best learners. As shown in their experimental results, this process is able to effectively reduce the number of individual trees in the final ensemble with better ranking performance and low memory cost.

Another enhancement on an ensemble of additive trees towards the performance

of the models is the QuickScorer algorithm, which modifies the tree structure in order to boost up the tree efficiency of the final model. The novelty of the QuickScorer is the use of bitwise operations to traverse the tree in a feature-wise order, thus making the tree traversal cache-aware. According to the authors [Lucchese et al., 2015], the trees in the ensemble are simultaneously traversed by interleaving the features of each tree, which enables efficiency up to 6.5 times faster than the original tree. Another attempt of improving the tree ensemble by the authors [Lucchese et al., 2016b] is through vectorization of the tree in the QuickScorer algorithm, which enables them to parallelize the tree traversal in the algorithm using SIMD extensions.

Another enhancement in an ensemble of an additive tree is proposed in [Lucchese et al., 2016a], which suggests a series of modifications in the structure of the ensemble by making a set of pruning strategies in each tree of the ensemble and then removing trees that are too much correlated in their structure. This cleaning up of trees have the same purpose of the aforementioned work by [Mishina et al., 2014], but instead of minimizing the complexity of the final ensemble using boosting, they re-weight the trees that were left on the ensemble using a greedy line search algorithm that optimizes the weights of the trees by minimizing a given loss function. According to their findings, this strategy, named CLEaVER, is up to 2.6 times faster than the original ensemble without losing its generalization effectiveness.

3.3 Deriving Ensembles of Decision Trees

This section highlights a series of works that attempt to derive improved versions of an ensemble of decision trees in order to optimize its effectiveness. We first highlight the improvements over RF derivations, then we describe a few works that make some derivations over the traditional boosting meta-algorithm. For last, we cite a few works that elegantly improve ensemble models by combining these two strategies into a single committee.

3.3.1 Random Forests

As mentioned so far, it is natural to expect several extensions of RF and Boosting not only towards optimizing its efficiency but improving its effectiveness as well. One such extension in the classification realm for ranking is proposed by [Jiang, 2011], which derives a RF model by modifying the tree node measure of impurity with the replacement of the traditional Information Gain (when using entropy as measure of impurity) for the Average Gain. According to the authors, this minimizes the tendency of Infor-

mation Gain towards selecting predictors with a large number of distinct values while decreasing the correlation of trees in the ensemble. This procedure of decorrelating the trees is also envisioned by the authors [Amaratunga et al., 2008], which modifies the random procedure of select the features in each node of the tree with a weighted approach, which reduces the overfitting of the model in domains with high dimensionality such as text classification or gene sequence.

The alternative approach to derive ensembles of randomized trees proposed by [Breiman, 2001] that modifies the node splitting criteria of impurity, as suggested by the authors [Menze et al., 2011] is the use of regularization techniques such as Lasso and Ridge Regression [Hastie et al., 2015]. This variation enables multivariate splitting rules in the boundaries of the input space of each node in the decision tree, and as such, more than a single predictor is used to decide how the samples should be divided into the nodes of each tree, allowing instantiations of oblique RF. As pinpointed by the authors [Menze et al., 2011], the variance of oblique RF is lower than the traditional univariate scheme of RF, thus, in their findings the oblique version performs better than the original RF in most cases.

Another extension of randomized trees is the ensemble algorithm named Extremely Randomized Trees (ERT) proposed by [Geurts et al., 2006] and its application for L2R [Geurts and Louppe, 2011]. The ultimate goal of ERTs is to reduce the correlation between the trees composing the ensemble, a requirement to guarantee the high effectiveness of RF models. This is achieved by modifying the RF algorithm in, essentially, two aspects: (i) each tree is learned considering the entire training set, instead of bootstrapped samples; and (ii) in order to determine the decision splits after the random attribute selection, instead of selecting a cut-point that optimizes node purity, ERTs simply select a random cut-point threshold that is combined in each tree node with the best possible combination of the random set of attributes. This ultimately reduces tree correlation, potentially improving the generalization capability of the learned model. According to the authors [Geurts and Louppe, 2011], this approach was competitive with the major approaches in the YAHOO! L2R competition.

3.3.2 Boosting

Ensembles of boosted trees have been shown to be remarkable models by introducing perturbations in the input space. The most well-known boosting framework is AdaBoost, which iteratively modifies the input space by associating weights with each sample. At each iteration AdaBoost re-weights the sample distribution considering the samples that were erroneously predicted at each iteration. In the classification

task, this is quite easy, since only a comparison of labels is used in order to determine the wrongness of a sample in the training set. However, this strategy does not work for regression problems. One derivation of AdaBoost is proposed by [Drucker, 1997], which applies loss functions that capture the residue of a sample and then update the weights' distribution proportionally to the residues. Another derivation of AdaBoost is proposed by [Solomatine and Shrestha, 2004] that uses a constant threshold value to determine the correctness or wrongness of a prediction. In other words, they translate the regression problem into a classification one. The benchmark comparison of [Shrestha and Solomatine, 2006] shows that this translation of regression to the classification is quite effective, surpassing most of the evaluated baselines.

A pairwise boosting approach derived from AdaBoost is the algorithm RankBoost, which, just like the original approach, requires a set of iterative steps in order to define the hard to predict regions of the input space. The key aspect of RankBoost [Freund et al., 2003] when compared to the traditional algorithm is the fact that it does not rely on the predictions of decision trees as weak learners to devise regression scores for the samples. Instead, it translates the ranking approach to a binary classification of instance pairs. This pairwise comparison of samples is computed by comparing feature values to a threshold constant, which allows to increase the weights of pairs of documents that are correctly predicted while decreasing the weights of incorrectly predicted pairs during the update phase of the weights' distribution.

Another Boosting approach that does not rely on the use of decision trees as weak learners is the AdaRank algorithm proposed by [Xu and Li, 2007]. The main idea of AdaRank is to optimize ranking measures while updating the "samples" distribution that represents their importance by a weak learner. This corresponds to a listwise approach that employs exponential loss functions based on IR performance measures. Differently from the aforementioned approaches, AdaRank maintains the weights' distribution over queries and, at each iteration, this weights distribution is updated in order to leverage the performance of weak learners on hard queries. Moreover, the authors consider a single feature as weak ranker that is linearly combined with the set of features used as weak rankers in previous iterations. The chosen feature as weak-ranker is the one that has the optimally weighted performance amongst the features. As a result, the authors were able to surpass the baselines RankBoost and Rank SVM.

Another class of boosting algorithms that are derived from decision trees is GBRT [Friedman, 2000] (a.k.a, MART[1] – Multiple Additive Regression Trees). GBRT successfully builds an ensemble of additive trees by learning a ranking function that ap-

[1]From now on, we will use MART and GBRT as synonyms.

proximates the root mean squared error (RMSE) on the training set through gradient descent. As with typical boosting algorithms, the goal of GBRT is to focus on regions of the input space where predicting the correct relevance score is a hard task. Since this algorithm aims at approximating the RMSE on the training data, it can be regarded as a pointwise approach. A variation of GBRT that also attempts at minimizing the gradient descent is Lambda-MART [Burges, 2010], a listwise approach that directly optimizes the ranked list of documents according to some retrieval measure, such as NDCG (instead of simply approximating the RMSE of the training documents' relevance scores in isolation). To this end, Lambda-MART learns a ranking function that generates a list of relevant documents to a query that is as close as possible to the correct rank.

3.3.3 Combining Bagged and Boosted Trees

Beyond focusing on the improvement of each individual ensemble strategy, some authors also propose to combine them in order to come up with better-learned models by capturing the benefits of each individual approach. For example, in [Mohan et al., 2011] GBRTs and RFs are independently explored in order to learn better ranking functions. More specifically, the GBRT model is initialized with the residues of the RF algorithm, followed by the traditional iterations of a GBRT algorithm. The main motivation behind this approach in using RF predictions as start point gradients is that RFs are less prone to overfitting, being ideal to initialize the GBRT algorithm instead of the usual uniform initialization. Therefore, the main advantage in using this initialization provided by the residues of the RF prediction is that it allows the GBRT to start very close to the global minimum and merely refine the RF predictions. According to the reported benchmark, such strategy was shown to be superior to the original GBRT algorithm.

Another attempt at improving the generalization capabilities by assembling individual learners into ensemble models is the work proposed by [Bernard et al., 2012], in which the main idea is to perform a reweight of the training data to each individual tree in the RF algorithm. The key aspect of this strategy known as Dynamic Random Forests is to maintain the randomization process of bagging and feature selection with the advantages of the boosting. The difference of their approach to the original boosting procedure is that each new induced tree is evaluated accordingly with the already trees composing the ensemble instead of relying only in the last tree as the original boosting procedure. The combination of randomized approaches with boosting strategies is also envisioned by [Kotsiantis, 2011]. In their work, bagging, boosting, rotation

forests and random subspace models are combined with a simple sum voting strategy that counts the majority votes for each class of the individual algorithms. According to the authors, the combination relying on the sum strategy showed satisfying results when contrasted with the individual algorithms, which allowed them to conclude that Boosting and Rotation Forests assist in regions with smaller noise, while bagging and random subspace methods are more robust in noisy regions of the input space.

Differently from the aforementioned related works, we base ourselves in a recent development for text classification, namely, the BROOF algorithm [Salles et al., 2015]. In their approach, a similar approach to the one of [Zhang and Xie, 2010] is used, in which a RF machine is applied as the weak learner algorithm of the boosting meta-algorithm. The advantages of BROOF is that the RF and boosting strategies are tightly coupled in order to exploit their unique advantages: by exploiting out-of-bag error estimates as well as selectively updating training weights according to out-of-bag samples, the BROOF model is able to focus on hard-to-classify regions of the input space, without being compromised by the boosting tendency to overfit. This ultimately leads to competitive results when compared to the state-of-the-art algorithms. In here, we generalize such approach specifically for L2R tasks in order to come up with better ranking functions: we called the Generalized BROOF-L2R. As we shall see, this general framework is flexible enough so that it can be instantiated in several ways, exploiting distinct characteristics of the ranking tasks being addressed. In special, with this general framework, we are able to achieve state-of-the-art results, with rankers superior to the top-notch algorithms proposed so far in all evaluated cases.

Chapter 4

Generalized BROOF-L2R

In this chapter, we detail our proposed Generalized BROOF-L2R framework. Briefly speaking, this framework allows the definition of learners based on the combination of Random Forests and the Boosting meta-algorithm, in a non-trivial fashion. In doing so, we capture the advantages of each individual algorithm to build a stronger model, capable of maintaining the minimization of the variance by disturbing the input space through randomization techniques such as Bagging [Breiman, 1996a]. And, with the disturbance in the input space through manipulation of the hard regions acquired by the boosting procedure, our instantiations might help to reduce the bias just like the original AdaBoost proposal described in [Schapire and Freund, 2012]. Therefore, our proposed combination of this two ML approaches can effectively help each other in order to enhance the effectiveness of the final model and provide a better control of the bias/variance trade-off.

As we shall see, this framework establishes a set of operations to be performed during the boosting iterations in a well-defined order of application. The goal is to drive the weak learners towards hard to predict regions of the underlying data representation, in order to come up with an optimized additive combination of weak learners to form the final predictor. The extension points that we describe in this proposed framework can produce a heterogeneous set of instantiations that typically produce very competitive results for L2R. In the following, we present the generalized framework for L2R, as well as some pointwise instantiations. Although we only describe the most descriptive derivations in this work, it is important to stress out that the set of derived combinations discussed here is far from exhaustive, being possible to elaborate even better possibilities, which we will let open as future work. We first start by giving a description of how we combine these two ML algorithms and how to make instantiations by following a set of procedures. We then describe each of the instantiations that

were able to achieve statistical gains when compared to the baselines.

4.1 Framework Description

Based on the ideas of the algorithm BROOF, which was proposed by [Salles et al., 2015] to solve text classification tasks, we here extend it in order to exploit the combination of Random Forests and Boosting for the specific task of L2R. However, instead of directly adapting the original algorithm to a single L2R method, we here generalize it into an extensible framework that is flexible enough to permit a series of possible instantiations. The proposed framework named Generalized BROOF-L2R is an additive model composed of several Random Forest models, which act as weak learners. Each fitted model influences the final decision proportionally to its accuracy, focusing – as the boosting iterations go by – on more complex regions of the input space, in order to drive down the expected error. As usual in a boosting strategy, three aspects play a key role: (i) the influence β_t of each weak learner in the fitted additive model; (ii) the strategy to update the samples distribution w_n^m for a document x_n in query q_m in each iteration t of the boosting meta-algorithm and (iii) how to combine the individual weak learners created in each iteration of the boosting procedure in order to enhance the performance in terms of effectiveness of the model.

The basic structure of the framework is outlined in Algorithm 1, together with a brief explanation of what we call its extension points – the general functions exploited by the framework to determine how the optimization process works. There is a set of 5 general functions whose purpose is to specify the weight distribution update process, the error estimation, and the underlying input data representation that the algorithm should focus on minimizing. Particularly, the use of the Random Forest classifier as a weak learner extends the range of possible instantiations of the framework, since it enables us to come up with better error rate estimates and a more selective approach to update the examples' weights, through the use of the so-called out-of-bag samples.

Following the pseudo code described in this same Algorithm, we can verify that the function Fit accepts as parameter a set of queries $Q_{trn} = \{q_m, (x_n^m, y_n^m)\}$, each one with its set of documents x_n^m with its associated graded relevance judgment y_n^m that are used to build the final ensemble. The parameter $max\_iter = T$ is a requirement to identify the maximum number of rounds of boosting that must be performed in case the heuristic used as stopping criteria is not achieved during the iterations. Finally, the shrinkage factor η is a measure that controls the learning rate of the algorithm. This

Algorithm 1 Generalized BROOF-L2R: Pseudocode

function Fit($Q_{trn} = \{q_m | \{x_n^m, y_n^m\}\}$, max_iter=$T$, num_trees=$N$, shrinkage=$\eta$)
  w_n^m = InitializeWeights(Q_{trn})
  $dy_n^m \leftarrow y_n^m$
  for $t = 1$ **to** T **do**
    $dy_n^m \leftarrow$UpdateExamples(Q_{trn}, dy_n^m)
    $RF_t \leftarrow RF_{Regressor}$.Fit($Q_{trn}, dy_n^m, N$)
    $\{(\hat{y}_{n,t}^m, y_{n,t}^m)\} \leftarrow$ValidationSet($RF_t, Q_{trn}$)
    $\langle e_{n,t}^m, \beta_t \rangle \leftarrow$ComputeLearnerWeights($RF_t, \{(\hat{y}_{n,t}^m, y_{n,t}^m)\}$)
    if $\sum_1^m e_{n,t}^m \times w_n^m \geq 0.5$ **then**
      T = t; **break**
    end if
    $w_n^m \leftarrow$UpdateExampleWeights($e_{n,t}^m, \beta_t, \{(\hat{y}_{n,t}^m, y_{n,t}^m)\}$)
  end for
  return $\{(RF_t, \beta_t)\}|_{t=1}^T$
end function

Function	Description
InitializeWeights	Initial weights associated to each example, resembling boosting by re-weighting. **Uniform:** Equal weights for each example, $w_n^m = \frac{1}{\sum_1^m n_m}$. **Random:** Randomly initialized weights, $w_n^m =$Random(), $0 \leq w_n^m \leq 1$.
UpdateExamples	Determines the underlying representation of the input data, directly defining what the algorithm should optimize for. **Identity:** Maintains the original representation of input data, $dy_n^m = y_n^m$. **Residue:** Optimizes for the residues: $dy_n^m = \begin{cases} dy_n^m - \eta \hat{y}_{n,t-1}^m & \text{if } t > 1 \\ y_{i,j} & \text{otherwise} \end{cases}$, where η is a shrinkage factor.
ValidationSet	Determines which training data will be considered during weight update and error rate estimation, with direct influence on the algorithm robustness to overfitting. **OOB:** The set of out-of-bag examples OOB_t related to RF_t. **Train:** The entire training set Q_{trn}.
CompLearnerWeights	Determines how to compute the influence of the current weak learner on the final predictor. **Absolute:** $\beta_t = \eta \frac{\epsilon}{1-\epsilon}$, where $\epsilon = \sum_{i=0}^m \bar{e}_n^m \times \bar{w}_n^m$, $\bar{e}_n^m = \lvert y_{i,j} - \hat{y}_{i,j} \rvert$ and η is a shrinkage factor. **Median:** Similarly to the above variant, $\beta_t = \eta \frac{\epsilon}{1-\epsilon}$ and $\epsilon = \sum_{i=0}^m \bar{e}_n^m \times \bar{w}_n^m$. However, the errors are given by $\bar{e}_n^m = \lvert$Median$(R_{\hat{y}_n^m}) - \hat{y}_{i,j} \rvert$, where $R_{\hat{y}_n^m}$ denotes the region of correctness. **Height:** Similarly to the variants above, both $\beta_t = \eta \frac{\epsilon}{1-\epsilon}$ and $\epsilon = \sum_{i=0}^m \bar{e}_n^m \times \bar{w}_n^m$. The main difference of them is: $\bar{e}_n^m = \begin{cases} \#\text{ irrelevant documents above} x_n^m & \text{if } x_n^m \text{is relevant} \\ \#\text{relevant documents below } x_n^m & \text{otherwise} \end{cases}$, in the ordered list of results. **Constant:** Produces constant coefficients, $\beta_t = \eta$.
UpdExampleWeights	Specifies how to update the training examples weights to be used in the next iteration. **OOB:** Updates the weights associated with the out of bag samples according to β_t and the difficulty involved in predicting the samples' outcomes. **Train:** Updates the weights associated the entire training set. Similarly to the above variant, the update strategy considers both the coefficient β_t and $\bar{e}_n^m$. **Constant:** Keeps the same weights during the boosting iterations, $w_{i,j} = w_{i,j}$.

learning rate is highly correlated with the number of iterations, since a small value for η might achieve maximum effectiveness in minimizing a given loss function with a cost of a large number of iterations, which might cause overfitting on training data. On the other hand, choosing a large value for the learning rate η will require less iterations to achieve the minimum local, but it might as well overpass it, which may cause the model to lose its generalization capabilities. As seen in most boosting algorithms, the largest variations in effectiveness by modifying this parameter occurs when minimizing the gradient with the least square loss function.

Given the set of aforementioned parameters, the first procedure of Algorithm 1 is the *InitializeWeights* function, which is responsible for the initialization of the samples distribution that defines the importance of a document x_n during the construction of weak learners in each iteration t of the boosting procedure. There are a few ways of initializing theses weights when starting the boosting procedure, such as Dirichlet Randomization to allow a more uniform distribution by applying random values amongst the samples, or simply using the uniform initialization, which considers that all samples are equally important at the beginning of the boosting.

At each boosting iteration, the input data representation may be updated, through the general function UPDATEEXAMPLES. This second step defines the underlying data representation that the algorithm should optimize for. The two possibilities are to optimize for the original ground truth y_n^m of the input space and the second one is to optimize for the minimization of the residues, by updating at each step the ground truth of the samples using gradient descent. Therefore this function considerably extends the range of possible implementations of the framework by allowing to instantiate derived versions of the Gradient Boosting Machine [Mason et al., 2000, Hastie et al., 2009]. After defining the underlying data representation that the algorithm should optimize, a RF regressor is built upon the set of queries Q_{trn} considering the current configuration.

In order to evaluate the generalization capabilities of a RF_t at a given iteration t, a validation technique is applied during the creation of the model by predicting the relevance scores $\hat{y}$ for a set of training documents given by VALIDATIONSET. The general function VALIDATIONSET serves the purpose of specifying which training examples should be used during error estimation and weights update. The samples that are used for the validation technique can be the original set of samples in the input space or the left apart out-of-bag samples of each individual tree in the committee. The output of this step is paramount to guide the optimization process towards hard to classify regions of the input space. Although being of great importance to boosting effectiveness, this focuses on hard to classify regions of the input space may also be

harmful to the optimization process, especially when dealing with noisy data. As noted by [Freund and Schapire, 1996, Jin et al., 2003], boosting tends to increase the weights of a few hard-to-classify examples (e.g., noisy ones). Thus, the decision boundaries may only be suitable for those noisy regions of the input space while not necessarily general enough for the most common examples. In order to improve robustness against such a problem, our framework exploits an intermediary step related to how the examples weights get updated as the boosting iterations go by. The main goal here is to provide some mechanism to slow down overfitting as well as to provide more robust estimates of error in order to increase the generalization power of each weak learner and to determine how they should influence the final predictor.

The selected training examples are then used to compute both the error rate of the model and the influence β_t of the weak learner on the final model, by means of the ComputeLearnerWeights function. This fourth (and most important) step allows to devise the loss functions that are used to compute the influence of the current weak learner at a given iteration t by capturing the residues of the samples selected by the ValidationSet function. In this work, we devised 4 loss functions for the L2R context: *(i)* The first one, which we named Absolute loss computes the difference in prediction of its predicted regression value $\hat{y}_n^m$ to its ground truth y_n^m relevance judgment. *(ii)* The second loss function which we call Median Region computes the median distance of related relevant judgments samples. *(iii)* The third one named Height computes the height of a document, by pushing non-relevant documents to the bottom of the ranked list while pushing relevant ones to the top. *(iv)* The fourth loss function which we name GBROOF considers constant coefficients, and therefore it relies on the minimization of residues by using the gradient descent minimization.

Finally, the training examples' weight distribution is updated by the function UpdateExampleWeights. This updating process should, ideally, take into account the generalization capability of the current weak learner RF_t, as well as how hard is to correctly predict the ranked lists of the validation examples. Validation examples whose outcome is hard to predict by an accurate learner should influence more in the following boosting iterations, so the updates should indicate which samples will have a better preference in the foreseeable iterations of the boosting procedure for a given iteration t. So far, we considered 3 approaches for updating the weights distribution. The first one is to consider the entire training set, such that all training samples are updated. The second updating scheme considers only the left apart samples in the out-of-bag, which produces predictions for all samples in the training if the number of trees is large enough, since the trees are built with bootstrapped samples with replacement. The third variation does not update the samples in order to induce the

future weak learners in the ensemble since the minimization of the residues is done by the gradient descent. It is also worth mentioning that depending on the possible choices of combinations, an early stopping strategy is adopted, which terminates the boosting iterations if the current learner has an estimated error rate greater than 0.5. With this heuristic, although not ideal, the intention is to stop the boosting iterations in case the model starts to overfit during its creation.

Considering the set of possible combinations for the given set of 5 procedures, the final prediction of the algorithm is given by combining the weak learners RF_t of each iteration t weighted by its weight β_t and the learning rate η. For derived gradient instantiations of the framework, this combination is the additive combination of predictions shown in Equation 4.1. For the remaining derivations that rely on the minimization through disturbance of the inputs space by modifying the associative weights, the final prediction is the additive combination of predictions normalized by the summation of weights in each iteration as shown in Equation 4.2.

$$prediction = \sum_{t=1}^{T} RF_t(Q_{test}) \times \eta \tag{4.1}$$

$$prediction = \frac{\sum_{t=1}^{T} \left(log\frac{1}{\beta_t} \times RF_t(Q_{test}) \times \eta \right)}{\sum_{t=1}^{T} \left(log\frac{1}{\beta_t} \right)} \tag{4.2}$$

The next session describes the possible combinations and specific details of implementation.

4.2 Possible Instantiations

In this section, we describe a set of possible instantiations of the proposed framework, stressing out the four most effective instantiations (regarding the loss functions) that highlight the flexibility of the proposed framework to produce L2R solutions that typically produce very competitive results. In order to derive instantiations that are effective in inducing L2R models based on the Generalized BROOF-L2R framework, one needs to specify and tune the choices for the five generic functions discussed earlier. The set of instantiations are displayed in the Table 4.1. In that table, we specify which alternatives were chosen for each generic function, providing details on how they are implemented.

As it can be observed, $\text{BROOF}_{\text{absolute}}$, $\text{BROOF}_{\text{median}}$ and $\text{BROOF}_{\text{height}}$ rely on

Instantiation	Description	
	Extension Point	Variation
$\text{BROOF}_{\text{absolute}}$	InitializeWeights	**Uniform, Random**
	UpdateExamples	**Identity**
	ValidationSet	**OOB, Train**
	ComputeLearnerWeights	**Absolute**
	UpdateExampleWeights	**OOB, Train**
$\text{BROOF}_{\text{median}}$	InitializeWeights	**Uniform, Random**
	UpdateExamples	**Identity**
	ValidationSet	**OOB, Train**
	ComputeLearnerWeights	**Median**
	UpdateExampleWeights	**OOB, Train**
$\text{BROOF}_{\text{height}}$	InitializeWeights	**Uniform & Random**
	UpdateExamples	**Identity**
	ValidationSet	**OOB, Train**
	ComputeLearnerWeights	**Height**
	UpdateExampleWeights	**OOB, Train**
$\text{BROOF}_{\text{gradient}}$	InitializeWeights	**Uniform & Random**
	UpdateExamples	**Residue**
	ValidationSet	**OOB, Train**
	ComputeLearnerWeights	**Constant**
	UpdateExampleWeights	**Constant, OOB**

Table 4.1: Generalized BROOF-L2R: Possible instantiations.

the use of out-of-bag samples or the whole set of training samples in order to drive the weak learners of the boosting meta-algorithm further on hard to predict regions of the input space. Such samples can be explored when estimating the weak learners' error rate through out-of-bag or as usual in the original boosting procedure assessing the errors to measure the residues through a loss function using the training set. It is worth to mention that, as the size of the data grows, using the training data is too optimistic, since the same data that was used to train the model is used as a measure of error. By using the out-of-bag samples we are able to produce better error estimates in large collections, being more effective and efficient, since the out-of-bag samples constitute an independent set of samples that was left apart during the construction of the model. By doing so, we are able to better approximate the expected error rate of the learner with a more reliable measure than the usual training error rate [Breiman, 1996b, Salles et al., 2015, de Sá et al., 2016].

In addition, the validation samples estimates are used to identify the weights' distribution that should be applied on following iterations of the procedure, which allows the model to focus on hard to predict regions of the input space. We hypothesize that such selective update strategy can slow down the algorithm's tendency to overfit in real large-scale collections. The major difference amongst our instantiations is the restriction on how each weak-learner influences the final predictor. To better clarify the instantiations, we outline the specifics of each instantiation in the pseudocode of

Algorithms 2 to 5 along with a set of figures that represent how the loss functions work upon the samples.

As we see in Table 4.1, for all instantiations, we derived models considering random initialization of the samples distribution weights using Dirichlet Randomization, which allows uniform random values between [0, 1], and the uniform initialization, which considers that all samples are equivalent and equally weighted in the first iteration. The three first instances $\text{BROOF}_{absolute}$, BROOF_{median} and BROOF_{height} set the configuration for the procedure UpdateExamples to optimize for the original ground truth of samples, therefore, the instances use boosting by re-weighting. This is different for $\text{BROOF}_{gradient}$ that minimizes the residue in each boosting iteration through gradient descent. All derivations were validated with training and out-of-bag samples.

The specific details of the first instantiation are shown in Algorithm 2 with a visual representation of the loss function in Figure 4.1. In that figure, it is considered that the maximum relevance judgment is 4 for completely relevant documents while the representation for non-relevant documents is 0. Let us also consider that each point is the prediction of an RF model for a given document chosen during the validation procedure (e.g.: out-of-bag document), where the red ones stand for non-relevant documents (ground truth equals 0) and the blue ones are relevant documents (ground truth equals 4). The absolute regression loss computes the absolute value of the prediction $|\hat{y}_n^m - y_n^m|$ for those samples, and then proportionally updates the weights' distribution according to this residue. As we can observe in this figure, all samples weights are updated regardless of the position that they occupy in the ranking for a given query

Algorithm 2 $\text{BROOF}_{\text{absolute}}$: Pseudocode

function FIT($\{(q_i, \{x_{i,j}, y_{i,j}\}|_{j=1}^{m_i}\}$, M, N, η)
  $w_{i,j} = \frac{1}{\sum_{i,j} m_{i,j}}$
  $x'_{i,j} \leftarrow y_{i,j}$
  for each $t = 1$ **to** M **do**
    $x'_{i,j} \leftarrow x_{i,j}$
    $RF_t \leftarrow RF_{Regressor}$.FIT($\{(x'_{i,j}, y_{i,j})\}, N$)
    $\{(\hat{y}^t_{i,j}, y^t_{i,j})\} \leftarrow RF_t$.OOB
    $e^t_{i,j} \leftarrow |y_{i,j} - \hat{y}_{i,j}|$
    $\epsilon \leftarrow \sum_{i,j} e^t_{i,j} w_{i,j}$
    $\beta_t \leftarrow \eta \frac{\epsilon}{1-\epsilon}$
    if $\epsilon \geq 0.5$ t = T; **break**
    $w_{i,j} \leftarrow w_{i,j} \beta_t^{1-e^t_{i,j}}$
  end for
  return $\{(RF_t, \beta_t)\}|_{t=1}^{M}$
end function

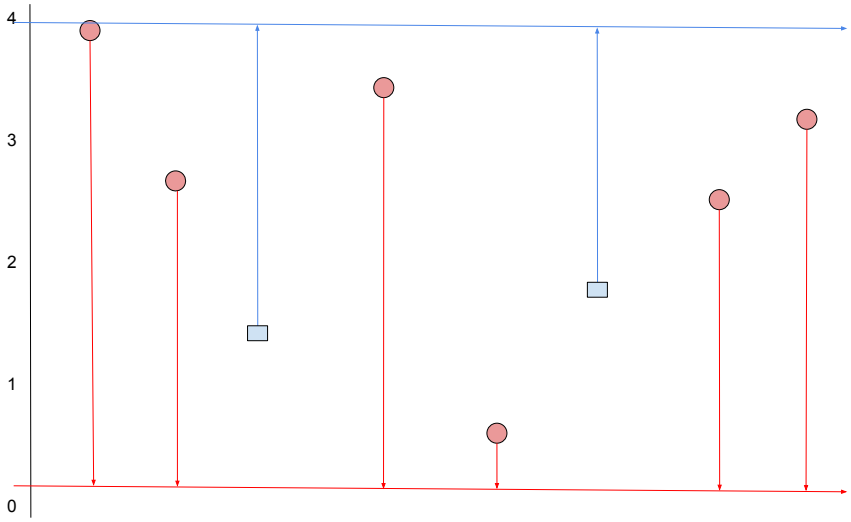
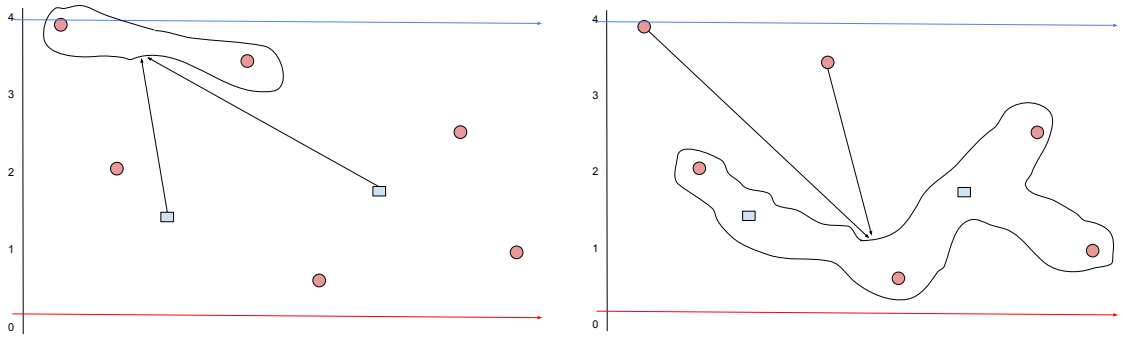


Figure 4.1: Residues when minimizing the absolute loss-function

m.

To address the ranking position of a document in a query, the derived instances BROOF$_{median}$ and BROOF$_{height}$ use loss functions that are able to capture the correctness of a document prediction. If the prediction for a document is considered correct, its weight remains the same. The ones that were wrongly predicted have the weights updated in order to reflect the wrongness of the prediction and induce specialized models that are better at predicting these hard documents. The pseudo code for the BROOF$_{median}$ is shown in Algorithm 3 with the loss function in Figure 4.2.



(a) (b)

Figure 4.2: Residues when minimizing the median of a region.

In order to explain the loss function exemplified in Figure 4.2 for the BROOF$_{median}$ instantiation, it is assumed once more that the red points stand for non-relevant documents and the blue ones for the relevant documents. This instance

of the framework considers regions of the input space that define the "importance" of a document. Each region is defined as the amount of samples of each individual annotated relevance judgment. Therefore, for a multi-relevance judgment scenario with 5 relevance judgments, the loss function would divide the input space into 5 levels, in which in the perfect ranking, each level would contain only documents that are really alike in terms of importance (i.e: the same annotated relevance judgment).

For the sake of our argument, let us suppose that a given query, as shown in Figure 4.2, only contains samples with relevance judgments 4 (relevant) and 0 (non-relevant). Thus, the input space is divided into two levels. In the perfect ranking, the topmost level would contain two documents that are relevant, and the second level would contain the other six, non-relevant documents. However, as we can see in Figure 4.2a, the two topmost documents are irrelevant, with two relevant documents hanging in the middle of the non-relevant ones. Taking this into consideration, the two relevant documents and the two top most, non-relevant documents should be swapped in order to get the perfect ranking. This is done by re-weighting the weights' distribution for these samples in the wrong region of the input space. These samples are updated with the absolute difference of the ground truth of those samples with the median of the samples in its correct region $|\text{MEDIAN}(R_{\hat{y}_n^m}) - \hat{y}_n^m|$. For example, in Figure 4.2a, the two relevant documents have their weights updated with the difference of their regression value score to the median of the circled region containing the topmost, non-relevant documents. In Figure 4.2b the two topmost non-relevant documents are updated with the difference of its regression value with the median of its correct region, which is

Algorithm 3 $\text{BROOF}_{\text{median}}$: Pseudocode

function FIT($\{(q_i, \{x_{i,j}, y_{i,j}\}|_{j=1}^{m_i}\}$, M, N, η)
  $w_{i,j} = \frac{1}{\sum_{i,j} m_{i,j}}$
  $x'_{i,j} \leftarrow y_{i,j}$
  for each $t = 1$ **to** M **do**
    $x'_{i,j} \leftarrow x_{i,j}$
    $RF_t \leftarrow RF_{Regressor}$.FIT($\{(x'_{i,j}, y_{i,j})\}, N$)
    $\{(\hat{y}^t_{i,j}, y^t_{i,j})\} \leftarrow RF_t$.OOB
    $e^t_{i,j} \leftarrow \text{MEDIAN}(pos(y_{i,j}) - pos(\hat{y}_{i,j}))$
    $\epsilon \leftarrow \sum_{i,j} e^t_{i,j} w_{i,j}$
    $\beta_t \leftarrow \eta \frac{\epsilon}{1-\epsilon}$
    if $\epsilon \geq 0.5$ **break**
    $w_{i,j} \leftarrow w_{i,j} \beta_t^{1-e^t_{i,j}}$
  end for
  return $\{(RF_t, \beta_t)\}|_{t=1}^{M}$
end function

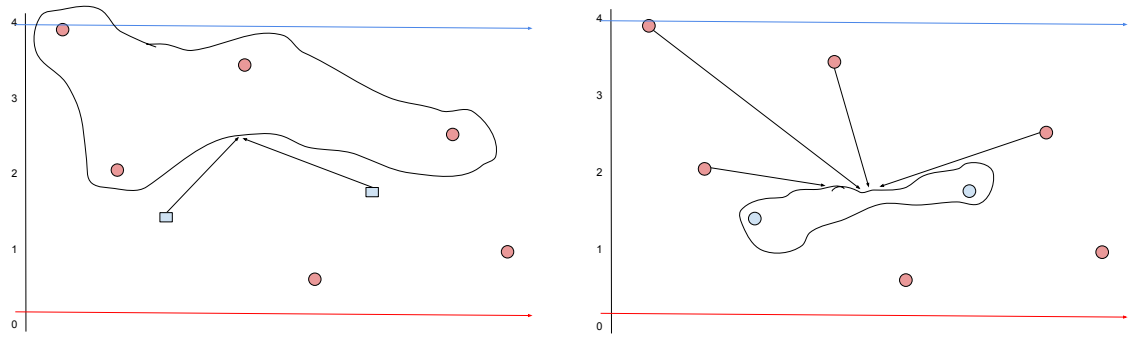
composed of the circled area containing the 6 samples.

As observed in the two previous derived instantiations of the BROOF-L2R framework, the main difference between is in how they identify the samples that should be updated. The first one updates all samples while the second one only updates the samples that were wrongly predicted. In BROOF$_{height}$, the same scheme of updating the wrongly predicted samples is used, but instead of comparing regions that define the correctness of a sample, it analysis the height of the documents in the ranked list. The height of a document x_n^m is dependent on its position in the ranked list and on its annotated relevance judgment. In this case, the height of a relevant document is defined as the amount of non-relevant documents that were ranked higher than it, while the height of a non-relevant document is defined as the amount of documents that were ranked below it. The pseudo code for the derived instantiation is in Algorithm 4 with the visualization for the loss function in Figure 4.3.

To better understand the concept of the height of a document, let us consider that in Figure 4.3 the red points are irrelevant documents with ground truth equivalent to 0 whereas the blue ones are relevant documents with relevance judgment equals to 4. Thus, in Figure 4.3a, the height for the relevant documents is the summation of non-relevant documents ranked above it, i.e., the height for the relevant documents is the four documents in the circled area. The same interpretation is applied for Figure 4.3b, which shows that the height for the irrelevant documents is the number of relevant documents ranked below them, which, in this example, corresponds to the two relevant

Algorithm 4 BROOF-L2R$_{\text{height}}$: Pseudocode

function FIT($\{(q_i, \{x_{i,j}, y_{i,j}\}|_{j=1}^{m_i}\}$, M, N, η)
  $w_{i,j} = \frac{1}{\sum_{i,j} m_{i,j}}$
  $x'_{i,j} \leftarrow y_{i,j}$
  for each $t = 1$ **to** M **do**
    $x'_{i,j} \leftarrow x_{i,j}$
    $RF_t \leftarrow RF_{Regressor}$.FIT($\{(x'_{i,j}, y_{i,j})\}, N$)
    $\{(\hat{y}^t_{i,j}, y^t_{i,j})\} \leftarrow RF_t$.OOB
    $e^t_{i,j} \leftarrow \begin{cases} \#\text{ irrelevant documents above } x_{i,j} & \text{if } x_{i,j}\text{is relevant} \\ \#\text{ relevant documents below } x_{i,j} & \textit{otherwise} \end{cases}$
    $\epsilon \leftarrow \sum_{i,j} e^t_{i,j} w_{i,j}$
    $\beta_t \leftarrow \eta \frac{\epsilon}{1-\epsilon}$
    if $\epsilon \geq 0.5$ **break**
    $w_{i,j} \leftarrow w_{i,j} \beta_t^{1-e^t_{i,j}}$
  end for
  return $\{(RF_t, \beta_t)\}|_{t=1}^{M}$
end function



(a) (b)

Figure 4.3: Residues when minimizing the height of a regions.

samples in the circled area. The main idea of this approach is to push the hard to predict relevant document to the top while pushing down the hard to predict non-relevant documents proportionally to its current position in the ranked list at a given iteration t of the boosting procedure.

Finally, in order to illustrate the generality of our proposed framework, we provide a fourth instantiation, $\text{BROOF}_{\text{gradient}}$, that resembles the gradient boosting machines (GBM) that optimize the gradient descent [Hastie et al., 2009] over the residues that are iteratively modified in order to find the minimum local in each iteration of the boosting procedure. More specifically, by a suitable combination of alternative implementations for each general function outlined in Algorithm 5, one can come up with an algorithm that could be named Gradient Boosted Random Forests (GBRF).

This derivation of the framework considers an alternative representation of the input data, that optimizes for the residues, such as $y_n^m - \hat{y}_n^m$, instead of the original input ground truth representation, updating them according to the negative gradient of the cost function (in this case, Root Mean Squared Error – RMSE). Such alternative is outlined in Algorithm 5 with an illustration of the loss function in Figure 4.4.

In order to simplify the explanation of how the minimization of the residues work in the derived version of the loss function illustrated in Figure 4.4, we will assume the minimization for a single relevant document with relevance judgment of four (the blue point in the first slot of the Figure). At each iteration of the boosting procedure, a weak learner (RF) makes a prediction of this sample generated by means of the internal validation procedure. For the first slot in the example, the prediction was 0.5, while the ground truth was of 4. On the second iteration, the ground truth is updated with the difference of its original value and the predicted regression value of the document. At the beginning of the second iteration the new ground truth for this sample will be 3.5. Then a new RF model is built, which will attempt at optimizing for the newly

updated ground truth of 3.5 with a prediction of 0.4, and then the ground truth is updated again. This process is recursively repeated until the minimum local for the sample is achieved.

As we shall see in our experimental evaluation, our proposed instantiations achieve very strong results compared to seven state-of-the-art baseline algorithms in five representative datasets. In particular, $\text{BROOF}_{\text{absolute}}$ and $\text{BROOF}_{\text{gradient}}$ were shown to be the strongest instantiations, obtaining significant improvements over the best baselines.

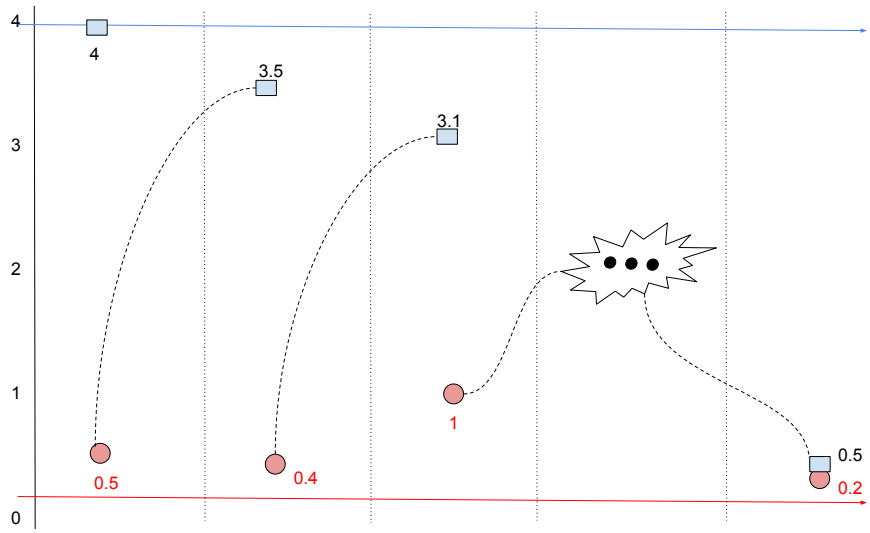


Figure 4.4: Residues when minimizing the gradient descent with least square.

Algorithm 5 $\text{BROOF}_{\text{gradient}}$: Pseudocode

function FIT($\{(q_i, \{x_{i,j}, y_{i,j}\}|_{j=1}^{m_i}\}$, M, N, η)
  $w_{i,j} = \frac{1}{\sum_{i,j} m_{i,j}}$
  $x'_{i,j} \leftarrow y_{i,j}$
  for each $t = 1$ **to** M **do**
    $x'_{i,j} \leftarrow \begin{cases} x'_{i,j} - \eta \hat{y}_{i,j}^{t-1} & \text{if } t > 1 \\ y_{i,j} & \text{otherwise} \end{cases}$
    $RF_t \leftarrow RF_{Regressor}$.FIT($\{(x'_{i,j}, y_{i,j})\}, N$)
    $\{(\hat{y}_{i,j}^t, y_{i,j}^t)\} \leftarrow RF_t$.OOB
    $e_{i,j}^t \leftarrow |y_{i,j} - \eta \hat{y}_{i,j}|$
    $\epsilon \leftarrow \sum_{i,j} e_{i,j}^t w_{i,j}$
    $\beta_t \leftarrow \eta$
    if $\epsilon \geq 0.5$ **break**
    $w_{i,j} \leftarrow w_{i,j}$
  end for
  return $\{(RF_t, \beta_t)\}|_{t=1}^{M}$
end function

Chapter 5

Experimental Protocol and Evaluation

This chapter describes an extensive set of experiments in well-known L2R benchmarks. In the following, we describe the characteristics of the datasets, baseline algorithms and the experimental protocol and setup.

5.1 Datasets

The corpora we use to evaluate the effectiveness of the studied algorithms are freely available online for scientific purposes. Such datasets can be divided into two groups considering the relevance judgments and their sizes. The two largest datasets contains {query, document} pairs with five relevance judgment levels, ranging from 0 (completely irrelevant) to 4 (highly relevant). In this group we have the WEB10K[1] dataset that consists of a subset of 10,000 random queries extracted from the web search engine Microsoft Bing. The second largest collection, YAHOO! Webscope Learning to Rank Challenge[2], contains 6,330 queries. In contrast to the Microsoft collection, which is partitioned into 5 folds for cross-validation purposes (3 partitions used for training, 1 for validation and 1 for the test in each one of the 5 folds), the YAHOO! Webscope contains a single fold that splits the data into three subsets: training and validation containing 1,266 queries each and test containing 3,798 queries.

The second group of datasets corresponds to the well-known LETOR 3.0 Topic Distillation tasks (TD) (a.k.a., informational queries), of the Web track in the Text Retrieval Conference 2003 (TD2003) and 2004 (TD2004)[3]. These datasets contain

[1] `https://www.microsoft.com/en-us/research/project/mslr/`
[2] `https://webscope.sandbox.yahoo.com/`
[3] `http://research.microsoft.com/en-us/um/beijing/projects/letor/`

	Train	Validation	Test
Fold1	s1, s2, s3	s4	s5
Fold2	s2, s3, s4	s5	s1
Fold3	s3, s4, s5	s1	s2
Fold4	s4, s5, s1	s2	s3
Fold5	s5, s1, s2	s3	s4

Table 5.1: Splitting strategy amongst the Folds

binary relevance judgments. Similarly to the WEB10K benchmark, these datasets are partitioned into 5 folds to be used in a folded cross-validation procedure.

For comparative purposes, considering that the Microsoft and the TD datasets were designed for a folded cross-validation procedure, we applied the same splitting criteria upon the YAHOO! dataset. This procedure consisted in merging the three original partitions into a single set, and then splitting the sorted queries into 5 subsets that were equally distributed into 5 folds as shown in Table 5.1. As we can observe in this Table, the distribution of the sets {s1, s2, s3, s4, s5} was kept in order to maintain the proportion of 3 partitions for training, 1 for validation and 1 for the test in each one of the five folds. In the reported results we address both YAHOO! partitions by naming the original single fold version as YAHOOV1S2 and the new 5-fold strategy as YAHOOV1S2-F5.

The statistics that summarize the distribution of documents in each annotated relevance judgment amongst the folds for each collection are shown in Table 5.2. As it is possible to observe, the folds for the TD2003 contain 30 queries for each training data, while the validation and test set contain 10 queries per fold. In the same table, it is also possible to identify the amount of samples of each annotated relevance judgment in each subset of training, validation and test for each fold of a given collection. For instance, we have 169 relevant documents (relevance equals 1) and 28,889 non-relevant documents (relevance equals 0) in the training set for the Fold1 in the smallest collection TD2003. The interpretation for the remaining folds and collections are the same. For instance, 3,798 queries for the training data containing 26,069 non-relevant documents (relevance equals 0) and 1,921 relevant ones (relevance equals 4) in Fold1 of the YAHOOV1S2 dataset.

5.2 Baselines

In our experiments, we consider as baselines freely available implementations of state-of-the-art L2R methods, including AdaRank (with MAP and NDCG as loss func-

Collection	Part.	Rel. Judg.	Fold1	Fold2	Fold3	Fold4	Fold5	Queries
TD2003	Train	1	169	254	283	309	206	30
		0	28889	28804	29717	29691	28852	
	Test	1	82	71	53	45	156	10
		0	9918	9929	9005	9955	9844	
	Vali	1	156	82	71	53	45	10
		0	9844	9918	9929	9005	9955	
TD2004	Train	1	576	729	723	737	583	45
		0	43570	43417	43423	44263	44417	
	Test	1	190	197	196	183	350	15
		0	14810	14803	14804	13963	14650	
	Vali	1	350	190	197	196	183	15
		0	14650	14810	14803	14804	13963	
WEB10K	Train	0	377957	373029	371725	372756	377322	6000
		1	232569	230368	232302	231727	231874	
		2	95082	95117	96663	96244	95247	
		3	12658	12814	12903	12712	12864	
		4	5146	5355	5518	5329	5295	
	Test	0	124784	126450	126088	125419	121522	2000
		1	77896	78016	75962	78591	75815	
		2	32459	31875	30913	32294	31910	
		3	4450	4053	4361	4244	4209	
		4	1932	1594	1769	1783	1803	
	Vali	0	121522	124784	126450	126088	125419	2000
		1	75815	77896	78016	75962	78591	
		2	31910	32459	31875	30913	32294	
		3	4209	4450	4053	4361	4244	
		4	1803	1932	1594	1769	1783	
YAHOOV1S2-F5	Train	0	26069	25450	22461	19569	20142	3798
		1	58823	57112	51598	45400	47500	
		2	27099	25763	23167	19229	20437	
		3	4258	4375	4234	3702	3528	
		4	1921	1894	1714	1615	1550	
	Test	0	4706	7741	7695	10633	7122	1266
		1	12287	17412	17801	23610	15701	
		2	5039	7763	7635	11701	6427	
		3	1063	1261	1204	1793	1378	
		4	366	638	546	737	611	
	Vali	0	7122	4706	7741	7695	10633	1266
		1	15701	12287	17412	17801	23610	
		2	6427	5039	7763	7635	11701	
		3	1378	1063	1261	1204	1793	
		4	611	366	638	546	737	

Table 5.2: Statistics of the evaluated collections in the main experiments.

tions), Random Forests, SVM^{rank}, MART, LambdaMART and RankBoost. We used the RankLib[4] (under the Lemur project) implementations of RankBoost, MART and LambdaMART. For AdaRank we used the implementation available by Microsoft Research[5]. For SVM^{rank}, we used the original implementation of [Joachims, 2006][6]. Finally, for Random Forests, we used the implementation available in Scikit-Learn[Pedregosa et al., 2011] library, which is also the basis of our implementations.

5.3 Experimental Protocol and Setup

To validate the performance of our approaches, we use two statistical tests to assess the statistical significance of our main results, namely, the Wilcoxon signed-rank test and the paired Student's t-test. We consider the Wilcoxon signed-rank test since it is a non-parametric statistical hypothesis testing procedure that requires no previous knowledge of the samples distribution. In fact, some authors believe that it is one of the best choices for the analysis of two independent samples [Demšar, 2006]. However, there is also some discussion in the literature favoring the Student's t-test when comparing L2R methods [Park, 2010]. Due to the lack of consensus, we perform our analysis with both tests, considering a two-sided hypothesis with the significance level of 0.95% in both tests. These statistical analyses were performed with the package "stats" available in the R language for statistics and graphic computing.

The statistical tests are computed over the values for Mean Average Precision (MAP) and the Normalized Discounted Cumulative Gain at the top 10 retrieved documents (hereafter, NDCG@10), the two most frequently used performance metrics to evaluate a given permutation of a ranked list using binary and multi-relevance order [Tax et al., 2015]. To compute these metrics we used the standard evaluation tool available for the LETOR 3.0 benchmark (for binary datasets), as well as the tool available for the Microsoft dataset for all multi-graded relevance judgment datasets[7]. These tools simply compute MAP as the mean of Average precision over all test queries considering the precision at position of each document in the ranked list. The Equation 5.1 and 5.2 shows the procedure for computing this metric:

[4] `http://sourceforge.net/p/lemur/wiki/RankLib/`

[5] `http://research.microsoft.com/en-us/downloads/0eae7224-8c9b-4f1e-b515-515c71675d5c/`

[6] `https://www.cs.cornell.edu/people/tj/svm_light/svm_rank.html`

[7] Reminding that, at the time of the writing of this paper, the evaluation tool used in the YAHOO! competition was not available online.

$$\text{AveragePrecision(q)} = \frac{\sum_{i=1}^{k} Precision \times Relevance\ judgment@i}{relevant\ documents\ until\ position\ k} \tag{5.1}$$

$$MAP = \sum_{q \in Q} \frac{\text{AveragePrecision}(q)}{|Q|}, \tag{5.2}$$

in which Average Precision (AP) is the average of precision for the query q in the set of queries Q. Thus, MAP is the mean of AP for all queries.

Regarding NDCG, we assume that NDCG@k is 0 (zero) for empty queries, i.e., queries with no relevant documents. Some of the available evaluations tools (e.g., the one from YAHOO!) assume the value of 1 for these cases, which may lead to higher values of NDCG [Busa-Fekete et al., 2013]. We chose to standardize this issue, using the same criterion used by most evaluation tools, e.g., those available for the Letor (3.0 and 4.0) and Microsoft datasets, in order to allow fairer comparisons. Accordingly, let IDCG_p be the maximum possible discounted cumulative gain for a given query. These tools implement DCG@k as shown in Equation 5.3 and NDCG@k as in Equation 5.4:

$$DCG_p = \sum_{i=1}^{p} \frac{2^{rel_i} - 1}{log_2(i+1)} \tag{5.3}$$

$$NDCG@p = \frac{DCG_p}{IDCG_p}. \tag{5.4}$$

In terms of algorithm tuning, we follow the usual procedure of tuning the hyper-parameters using training and validation sets. Considering the Random Forest based approaches we vary the number of trees from 10 to 100 in ranges of 10 and then scaling up to 1000 in ranges of 100. We achieved convergence around 300 trees. We also optimized the percentage of features to be considered as candidates during node splitting, as well as the maximum allowed number of leaf nodes. The optimal values were 0.3 and 100, respectively.

For $\text{BROOF}_{\text{absolute}}$, $\text{BROOF}_{\text{median}}$ and $\text{BROOF}_{\text{height}}$, we limited the number of iterations to 500, reminding that the algorithms have an early stopping criterion that prevents further boosting iterations when the error rate exceeds 0.5. On average, our strategies converge at about 15 iterations on the LETOR datasets, and around 5 to 10 iterations on the multi-relevance judgment datasets. An exception was $\text{BROOF}_{\text{gradient}}$ which converged at about 100 iterations for the largest datasets.

Concerning the SVM^{rank} baseline, we favored the use of a linear kernel considering the fact that we verified in our analysis that a polynomial kernel is infeasible on large

scale benchmarks such as WEB10K. The cost parameter C was calibrated using the training and validation sets with the explored values: 0.001, 0.01, 0.1, 1, 10, 100 and 1000. For the boosting methods Mart and LambdaMART, we tuned, always considering the validation set, the number of iterations ranging from one to a hundred, with a step of 1, and then scaling it up to 1000 iterations, with steps of 100. For the shrinkage factor of the predictive models, we tested the values of 0.025, 0.05, 0.075 and 0.1. The best found values for the MART and LambdaMART were ensembles of 1000 trees with shrinkage factor η of 0.1. For the AdaRank$_{MAP}$, AdaRank$_{NDCG@5}$ and for the RankBoost algorithm, similar procedures were performed in the validation set to configure the number of iterations.

Finally, we performed 5, 10 and 30 runs of the 5-fold cross validation procedure for WEB10K, YAHOO! and LETOR datasets, respectively. The differences in the number of repetitions are due to the size of the datasets and the need to properly address the variance of the results. The reported results on Tables 6.1 and 6.2 are the average of all these runs, being the statistical tests applied to these results.

Chapter 6

Experimental Results

In this chapter, we report the results of our approaches over state-of-the-art baselines in 5 known L2R datasets. We first present the benchmark comparisons that demonstrate the benefits of our instantiations over the evaluated baselines, then we present a convergence analysis of the strongest instantiations in the most representative collections. We also address the issue of the generalization capabilities of our approaches under a constrained number of training samples, which shows that our approaches are capable of achieving the strongest results with smaller percentages of training data. In the sequence, we investigate the advantages of wisely choosing the correct way of setting the ValidationSet function of Algorithm 1. Finally, we conclude the chapter with a discussion of the main factors that influence the proposed instantiations with an analysis design that shows the advances of our induced loss functions for L2R.

6.1 Benchmark Comparisons

In this section we analyze our proposals in terms of effectiveness, comparing the derived instances of the framework to 7 baseline algorithms in 5 datasets. The main results containing the statistical significance of 0.95% of confidence using the T-student and the Wilcoxon Signed Rank Sum hypothesis test are reported on Table 6.1 considering the Mean Average Precision (MAP). Table 6.2 shows the outcomes for the Normalized Discounted Cumulative Gain (NDCG@10). To make the interpretation of the results easier to understand, the values in red boxes are the stronger baselines, while the ones with an underline are the strongest baselines that tied with at least one of our instantiations (which is also underlined in the case of a tie) in both statistical hypothesis tests. The values in the green box represent our strongest instantiation. The starred values ($\star$) means that the derived instantiation of the framework was able to achieve

statistical significance with the Wilcoxon test, while the signed plus values (+) represent statistical gains with the statistical analysis of the T-student test.

6.1.1 Mean Average Precision – MAP

We start by considering the MAP metric on Table 6.1. As it is possible to observe, the MAP results show that in general our proposed framework outperforms or ties with the strongest baselines in all collections. More specifically, the BROOF$_{absolute}$ instantiation obtained the highest value in MAP with gain regarding the statistical hypothesis test Wilcoxon with of 0.288 of effectiveness against 0.278 for the strongest baseline – RF – in the collection TD2003. We can also note for this collection that the remaining derived instantiations of the framework were able to achieve similar gains, with BROOF$_{median}$ outperforming the strongest baseline with the T-student test and BROOF$_{height}$ successfully bypassing the RF baseline in both statistical tests. As it is possible to observe, BROOF$_{gradient}$ ties with the strongest baseline.

Considering the collection TD2004, the ensemble model BROOF$_{\text{absolute}}$ was considered the top performer amongst the proposed solutions, being tied with the strongest baseline RankBoost. Although not explicitly shown in this table, it is worth to mention that all four of our instantiations achieve statistical gains by overcoming all other baselines in both Wilcoxon and T-Student test. Regarding the WEB10K dataset, we observe the same patterns, which shows that our approaches BROOF$_{absolute}$, BROOF$_{median}$ and BROOF$_{height}$ were also able to achieve statistical gains over distinct baselines with strong evidence for the BROOF$_{gradient}$ as the leading winner model, since

Algorithm	Datasets				
	TD2003	TD2004	WEB10K	YAHOOV1S2	YAHOOV1S2-5F
Mart	0.192633	0.193744	0.352491	0.559721	0.568821
LambdaMart	0.165181	0.169605	0.350263	0.5545	0.563694
RF	0.278644	0.2522	0.337702	0.563355	0.559019
RankBoost	0.235189	0.255467	0.316201	0.544887	0.547524
AdaRank-MAP	0.2003	0.196801	0.294792	0.413846	0.480190
Adarank-NDCG	0.121672	0.132435	0.304359	0.540243	0.538514
SVM-Rank	0.257490	0.220392	0.324552	0.544887	0.551333
BROOF$_{\text{absolute}}$	0.288039$_{+}$	0.263288	0.342437	0.565486$^{*}_{+}$	0.563729
BROOF$_{\text{median}}$	0.282427*	0.259941	0.347665	0.567696$^{*}_{+}$	0.567284
BROOF$_{\text{height}}$	0.285937$^{*}_{+}$	0.259058	0.340340	0.564774$^{*}_{+}$	0.557727
BROOF$_{\text{gradient}}$	0.280634	0.252342	0.36251$^{*}_{+}$	0.572918$^{*}_{+}$	0.57656$^{*}_{+}$

'$*$': statistical significance according to Wilcoxon Test
'+': statistical significance according to Student's t-test
'n': statistically tied results considering both tests

Table 6.1: Mean Average Precision (MAP): Obtained results.

it was able to overcome the results of the strongest baseline MART in both statistical hypothesis tests.

Finally, in the YAHOOV1S2 dataset, the strongest baseline was the algorithm RF, which showed to be inferior to all four of our proposed algorithms in both statistical hypothesis tests. As noted on the Table, it is clear that BROOF$_{gradient}$ is the winner derivation of our framework in both YAHOO! collections with gains in both statistical hypothesis tests. In sum, according to the MAP metric, our results clearly show that the proposed instantiations of the Generalized BROOF-L2R framework produce very competitive results as the best algorithm is superior in the majority of cases, tying in a few others – a very significant result.

6.1.2 Normalized Discounted Cumulative Gain – NDCG

Turning our attention to the NDCG results reported on Table 6.2, a similar behavior can be observed: our proposed instantiations are no worse than the strongest baselines in all cases, being superior in the majority of cases. Considering the TD2003 and TD2004 datasets, our solutions were no worse than any baseline, being statistically tied with the strongest one (RF, in both cases). For the respective collections, our instantiations BROOF$_{\text{gradient}}$ and BROOF$_{absolute}$ were favored in the respective dataset obtaining the highest average value of NDCG.

The results for WEB10K show that BROOF$_{gradient}$ is able to surpass the strongest baseline LambdaMart in both statistical hypothesis tests, and the same observation of the MAP in this collection is applied in the remaining derivations of the framework,

Algorithm	Datasets				
	TD2003	TD2004	WEB10K	YAHOOV1S2	YAHOOV1S2-5F
Mart	0.271274	0.263926	0.4404	0.703757	0.714763
LambdaMart	0.224536	0.237338	0.445437	0.69619	0.706287
RF	0.36346	0.350582	0.424498	0.703139	0.702384
RankBoost	0.31613	0.33399	0.397071	0.682478	0.681796
AdaRank-MAP	0.271921	0.281035	0.35732	0.51767	0.607867
AdaRank-NDCG	0.166241	0.182031	0.385761	0.66309	0.664115
SVM-Rank	0.344177	0.303471	0.399902	0.682478	0.691064
BROOF$_{\text{absolute}}$	0.360802	0.358146	0.434964	0.70633	0.706954
BROOF$_{\text{median}}$	0.36798	0.350466	0.436284	0.708538_{+}	0.709148
BROOF$_{\text{height}}$	0.368195	0.355356	0.42882	0.70383	0.701985
BROOF$_{\text{gradient}}$	0.368695	0.348532	0.456081^{*}_{+}	0.717271^{*}_{+}	0.725129^{*}_{+}

'$*$': statistical significance according to Wilcoxon Test
'$+$': statistical significance according to Student's t-test
'n': statistically tied results considering both tests

Table 6.2: Normalized Discounted Cumulative Gain (NDCG@10): Obtained results.

noting that they were able to achieve statistically significant gains over the remaining individual baselines.

Furthermore, $\text{BROOF}_{\text{median}}$ was also superior to the best baseline ensemble MART in the YAHOOV1S2 dataset according to the Student's t-test. For the same collection, $\text{BROOF}_{gradient}$ surpassed the strongest baseline in both Wilcoxon and T-Student hypothesis tests. The remaining derivations $\text{BROOF}_{\text{absolute}}$ and $\text{BROOF}_{\text{height}}$ tied with the MART algorithm, which highlights once more the effectiveness of the proposed approaches, since we always surpass or tie with all baselines. Finally for the multi-folded version YAHOOV1S2-F5 dataset, the instantiation $\text{BROOF}_{gradient}$ show its potential by surpassing the strongest baseline in both employed statistical tests.

6.2 Behavioral Analysis

We now turn our attention to some behavioral aspects of our algorithms namely convergence rate, learning effectiveness towards optimizing training data and validation analysis. We start by contrasting the convergence rate of the boosting baseline approaches with our best derivation in the largest collections. Then we discuss the effectiveness of the algorithms in generalizing its predictive abilities under constrained training data. Finally, we address the use of training or out-of-bag samples in order to update the samples distribution towards hard to predict regions of the input space.

6.2.1 Convergence Rate

In order to better understand the convergence rate of our proposals, we provide an empirical evaluation of our most effective solution $\text{BROOF}_{\text{gradient}}$, by analyzing the obtained NDCG@10 as we vary the number of rounds of boosting. We here focus on contrasting the results on the three largest datasets: WEB10K, YAHOOV1S2, and its multi-fold version YAHOOV1S2-F5. The findings for this experiment can be found in Figure 6.1.

As can be observed, $\text{BROOF}_{\text{gradient}}$ share a similar behavior with three explored boosting algorithms, namely, MART, RankBoost and AdaRank-NDCG for all collections. The four algorithms show fast convergence rates, and differ in two key aspects: (i) our approach is able to achieve significantly better results at the initial boosting iterations, which leads to the second aspect (ii) that our $\text{BROOF}_{\text{gradient}}$ converges to a higher asymptote than the other algorithms. Therefore it was able to surpass the strongest baseline MART with only a few rounds of boosting. On the other hand, the convergence rate of LambdaMART was significantly slower than the convergence rate

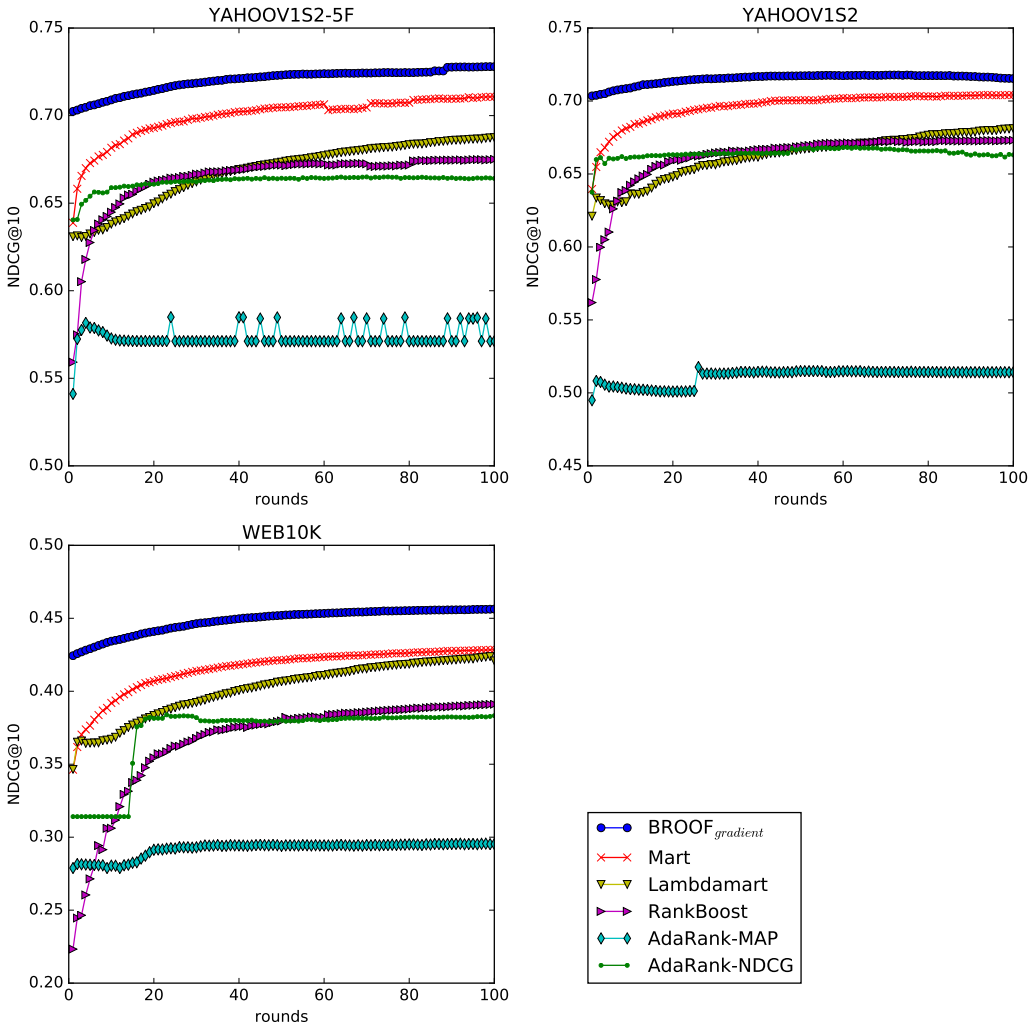


Figure 6.1: Convergence analysis: NDCG as the number of boosting iterations increases.

of the mentioned algorithms. In sum, BROOF$_{\text{gradient}}$ enjoys faster convergence rates, with higher NDCG values at the initial boosting iterations and higher asymptote. This efficiency in being able to effectively generalize better results is paramount to guarantee practical feasibility of our solutions. Although high effectiveness is a requirement, achieving such high effectiveness with just a few boosting iterations is key to minimize running time. We can also parallelize the trees in each round of the boosting mechanism achieving the effectiveness with less rounds of boosting and less running time.

6.2.2 Data Analysis

Another behavioral aspect of direct impact on the practical feasibility of our derived solutions is to what extent our approaches are considered "data effective". That is, to what extent each algorithm is capable of delivering highly effective rankings with reduced training sets. We evaluate the solutions under this dimension by analyzing each algorithm's learning curve obtained with the measure of its effectiveness as we vary the training set size. To explore this result, we randomly sample portions of queries from the original training set in ranges of size 10 from 10% to a 100% of the collection. The obtained results for this experiment can be found in Figure 6.2.

Considering the WEB10K dataset, we can observe the surprising result that $\text{BROOF}_{\text{gradient}}$ is able to outperform all baseline algorithms with only 20% of the original training set. As a comparison, the strongest baseline MART achieved only ≈ 0.44 of NDCG using the entire training set, while our approach surpassed it with ≈ 0.45 using only 20% of the original training set. It can also be noted that $\text{BROOF}_{\text{absolute}}$ is no worse than the baseline algorithms RF and SVM^{rank}, since it is able to surpass these baselines with the smaller fractions of 20% and 10% respectively of the original training set. In fact, with about 40% of the training set $\text{BROOF}_{\text{gradient}}$ starts to achieve its maximum effectiveness, and starts to smooth the learning curve as the training set size increases; whereas the $\text{BROOF}_{\text{absolute}}$ starts to smooth the learning curve with 10% of the data.

For both YAHOO datasets our instantiations show to be more susceptible to the increases of training data. However a similar pattern found in WEB10K was observed: with 30% to 40% of the training set our approach $\text{BROOF}_{gradient}$ was able to outperform the strongest baseline MART using the entire training set in both collections. The $\text{BROOF}_{absolute}$ instantiation was also able to surpass the strongest baseline MART with 40% of training in the YAHOOV1S2 collection. For the multi-fold version, YAHOOV1S2-F5 the $\text{BROOF}_{absolute}$ surpassed the baselines RF and SVM^{rank} with 10% of training. In these datasets, our algorithms were also able to achieve maximum effectiveness and smooth out the gains around 50% to 80% of the original training set.

Considering the TD2003 and TD2004 datasets, the RF baseline was a bit more competitive and exhibit a similar behavior in effectiveness as the training set size varies. For TD2003, 50% of the training allowed $\text{BROOF}_{gradient}$ to surpass all baselines. As can be observed, there is a small decrease of effectiveness around the 60% of training data, which can be explained by the increase of noise within the additional partition of the data. After 60%, the learning curve starts to increase and surpasses all baselines

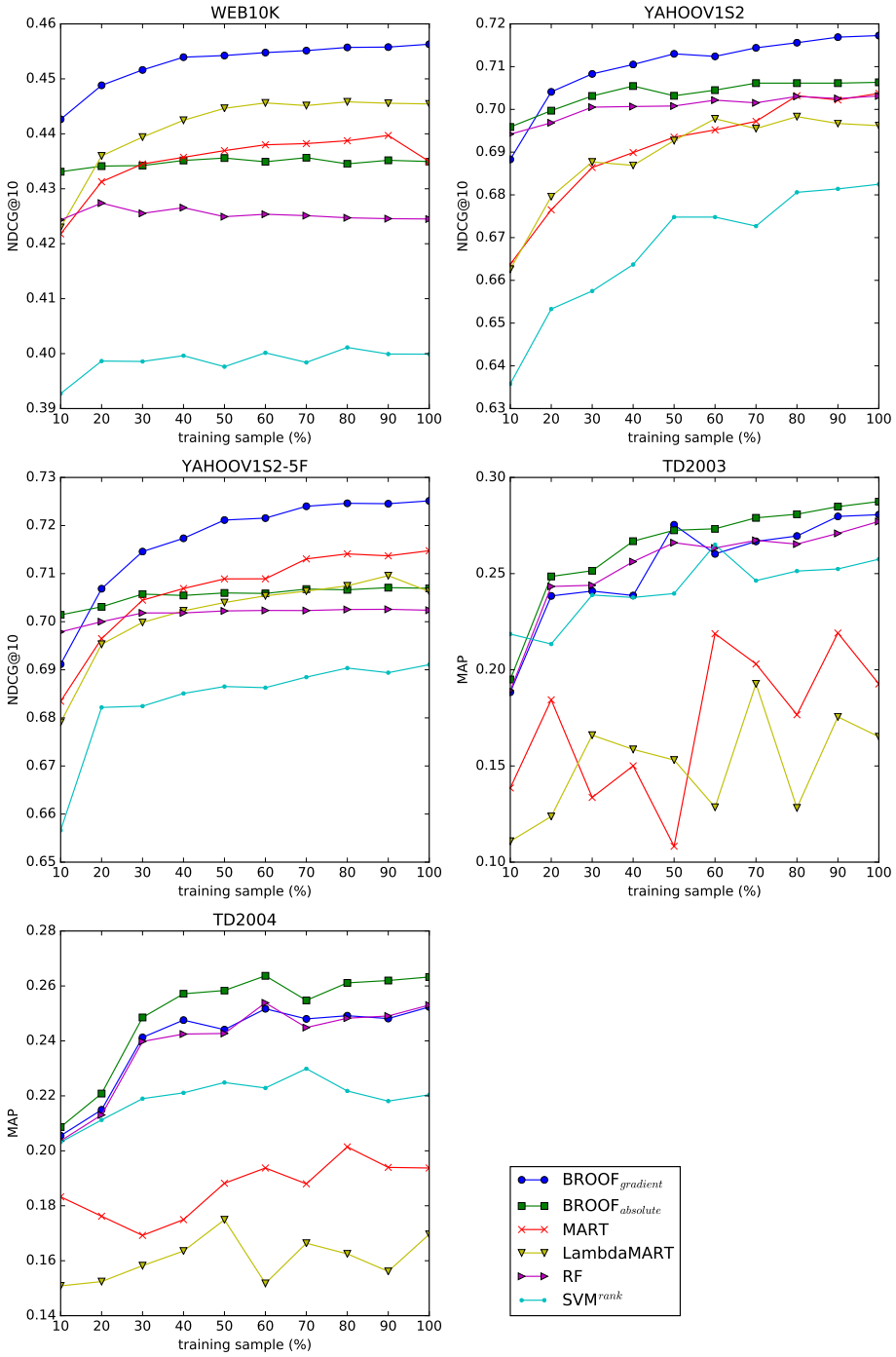


Figure 6.2: Learning curve analysis for the boosting algorithms.

once again, achieving its maximum effectiveness with 90% of training data. The gains with BROOF$_{absolute}$ are clearer since there is almost a smooth linear learning curve by overcoming all baselines around 50% of the training data. The analysis for the collection TD2004 shows that our best instantiation has a higher advantage over all baselines, with clear evidence of the effectiveness of the algorithm BROOF$_{absolute}$ around 40% of

training against the entire training data for the strongest baseline RF. BROOF$_{gradient}$ is also quite competitive since it is tied with the RF surpassing all remaining baselines.

These findings have also a direct influence on the practical feasibility of our solutions. First, smaller training set translates to smaller running times. Second, obtaining labeled data is critical but also costly, thus it is clear that being able to produce highly effective models from smaller training set is an important characteristic of a successful approach.

6.2.3 Validation Analysis

As mentioned in the description of the extension points for Algorithm 1, the validation set function in our boosting approaches enables to determine which training data samples will be considered during the weight update step. As described in the extension points, there are basically two ways of selectively update the samples distribution. The default procedure in most of the boosting strategies is to use the entire set of training samples. As we argued during the description of the extension points, this update strategy is in theory too optimistic, because it uses samples that were already used during the construction of the model, which might cause overfitting as the number of iterations increases. A better solution would be to use a cross-validation procedure of the training samples, and apply these samples to assess the performance of the model at each round of the boosting mechanism. Since we are using a RF model as the inner procedure of the boosting, we recommend the use of out-of-bag samples as an option of the validation procedure of our instances. Therefore, it is worth to assess the effect of the use of the validation procedure with both training and out-of-bag samples to be updated at each round of boosting. The results of this experiment are shown in Figure 6.3 for the three largest collections depicting the effectiveness of the BROOF$_{gradient}$ approach (the best algorithm in these collections) as the number of rounds of boosting increases. In these charts, the circled blue points represent the configuration for the training samples while the red cross points represent the out-of-bag samples.

As we can observe in the charts for the depicted experiment, the results for the YAHOOV1S2 collection show no difference in effectiveness in both validation techniques until the round ≈ 50 of the boosting procedure. After this round, the learning curve shows to overfit for the configuration of the validation procedure set to the out-of-bag samples, while the configuration set to the training samples seems to grow as the number of rounds increase. This is an interesting finding when contrasted with the results for the folded version of the same collection using the 5-fold cross validation procedure. As we can observe, the chart for the YAHOOV1S2-5F shows that there is

no difference in the effectiveness of the two evaluated procedures in almost the entirety of the learning curve, with a tenuous difference around round 90. This difference shows that the use of out-of-bag samples allows the algorithm to converge faster, with the penalty of obtaining smaller gains while the approach that makes use of the training samples still increases with a thin advantage as the number of iterations grows. In contrast to the two previous analysis, the findings for the collection WEB10K in the same Figure 6.3 reports that the out-of-bag error estimation produces more effective results than the simple training error estimate. Moreover, the use of out-of-bag as validation technique not only produces more realistic predictions with higher values for the NDCG as it also shows that the differences between the two validation techniques increase in favor of the use of out-of-bag as the number of boosting iterations grow.

To discuss these results a bit further, we consider the number of queries in each one of the three collections. As noted in the description of Section 5.1 and mainly in Table 5.2, the training set for the collection YAHOOV1S2 contains only $1,266$ queries. The modified cross-validated collection YAHOOV1S2-F5 is three times larger than the original representation of the data in terms of training queries, while the total amount of queries for the training dataset in the folds in the WEB10K is almost five times larger than the YAHOOV1S2. Therefore, a possible explanation for the reported differences in the behavior of the algorithms' generalization capabilities in using the train/out-of-bag samples in the two versions of the collection YAHOOV1S2 and WEB10K is that the effectiveness of the boosting mechanism is proportional to the amount of queries in the training data. Consequently, the recommendation for the two approaches for smaller collections is to use the training samples as the validation technique while larger collections containing larger amounts of queries will benefit in using the out-of-bag samples as the inner validation technique of the boosting mechanism. Although

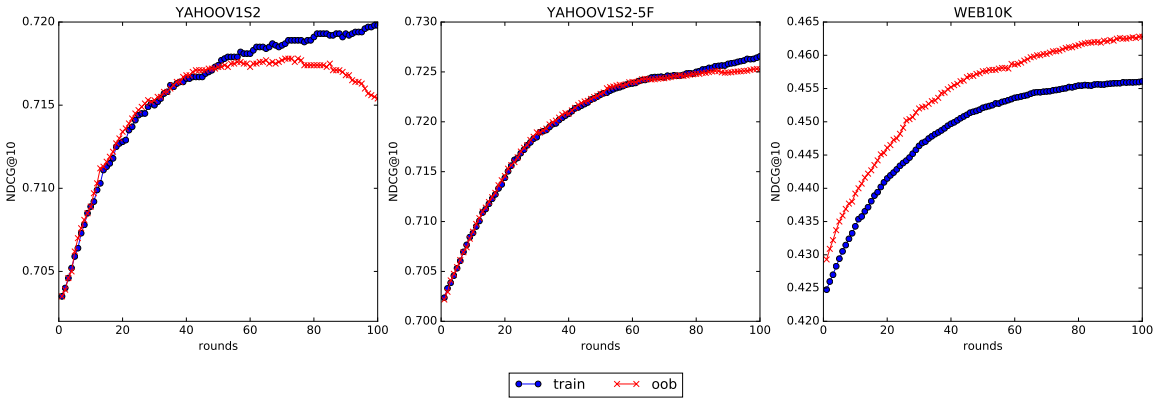


Figure 6.3: $\text{BROOF}_{\text{gradient}}$: Effect of out-of-bag samples versus entire training set.

this is not a general rule of thumb, it is a good start point to take into consideration before building boosted ensemble models based in bagged decision trees such as RF.

This highlights the importance of exploiting the validation set function as described in Algorithm 1 in our proposed framework instantiations. As a final remark, as it can be observed in the results of Figure 6.3, the variants that use the training error rate are also able to outperform the baselines. This is also an important aspect that highlights the quality of the proposed framework.

6.3 Quantitative Analysis

In this section, we report the full factorial experimental design with replication used to explain the importance of the factors of the proposed framework and how they interact among themselves. The importance of each factor and its interaction is given by the computation of the allocation of variation and the statistical analysis of variance as described by [Jain, 1991].

6.3.1 Full Factorial Design

As discussed in the previous analysis of this chapter, two factors are the most important ones in the derived instantiations of our framework. They are: *(i)* the validation set function and *(ii)* the loss functions used to minimize the residues at each boosting iteration. The analysis for each individual L2R collection was managed considering a full factorial design with the two aforementioned factors at two and four levels respectively. The first factor considers whether the inner validation technique makes use of training or out-of-bag samples in the updating strategy of the samples weights' distribution while the second factor takes into consideration each one the loss functions that generates the derived instances of the framework named BROOF$_{absolute}$, BROOF$_{region}$, BROOF$_{height}$ and BROOF$_{gradient}$.

The sample representation of the factorial design is shown in Table 6.3 for the collection WEB10K. The columns out-of-bag and training represent the two levels of the factor validation set function while the column containing the conglomeration of algorithms in the rows of the table represents the second discrete factor: loss functions. In order to discriminate the interactions and influence of the factors isolating the experimental errors, each experiment was repeated under each configuration 10 times for each one of the evaluated collections.

The model of the full two-factor design with repetition is given by: $y_{ijk} = \mu + \alpha_j + \beta_i + \gamma_{ij} + e_{ij}$ and the explanation of the fragmented parts of the equation are:

Algorithm	Exp. Number	Out-of-Bag	Training
$\text{BROOF}_{absolute}$	1	0.43498	0.43384
	2	0.43506	0.43396
	3	0.43498	0.43388
	⋮	⋮	⋮
	10	0.43476	0.43498
BROOF_{median}	1	0.43566	0.43634
	2	0.43604	0.43584
	3	0.43568	0.43626
	⋮	⋮	⋮
	10	0.4355	0.43514
BROOF_{height}	1	0.4288	0.4281
	2	0.42902	0.42842
	3	0.42904	0.42858
	⋮	⋮	⋮
	10	0.4288	0.4277
$\text{BROOF}_{gradient}$	1	0.45614	0.45608
	2	0.45614	0.45584
	3	0.4564	0.45614
	⋮	⋮	⋮
	10	0.45628	0.45576

Table 6.3: NDCG@10 for the 4 instantiations of the proposed framework applied upon the WEB10K in order to represent the full factor factorial design.

y_{ijk} is the k^{nth} observation of the factor A (validation set) at level j and factor B (loss function) at level i

μ is the mean response for the k repetitions

α_j is the effect of factor A at level j

β_i is the effect of factor B at level i

γ_{ij} is the interaction for the factors A at level i and B at level j.

e_{ijk} is the experimental error

6.3.2 Computation of effects

To compute the factors' effects, it is necessary to arrange the observations in a two-dimensional matrix such as the one shown in Table 6.3 consisting of b rows and a columns such that the $(i, j)^{th}$ entry y_{ij} corresponds to the response in the experiment in which factor A is at level j and factor B is at level i, which produces $\bar{y}_{ij} = \mu+\alpha_j+\beta_i+\gamma_{ij}$. After the arrangement of the collected data, it is necessary to average the k repetitions

under each cell configuration in a new matrix as shown in Table 6.4 for each collection (the measure metric is MAP for binary collections and NDCG@10 for multi-relevance judgment collections averaged over the 10 replications under each configuration), and then compute the means and sums of the observation for the new rows and columns of the newly created table. As we can observe in this new table, by averaging over all means observations we obtain the overall mean or mean response μ. The difference of the row mean at level j minus the overall mean is the β_i effect for the factor B at level j which leads to the equation $\beta_i = \bar{y}_{i..} - \mu$ that computes the column effects. The same procedure applied on columns of this new table produces the effects α_j for the factor A, leading to the equation $\alpha_i = \bar{y}_{.j.} - \mu$ to compute the row effects.

The interpretation of the effects in Table 6.4 is as follows: the overall mean μ explains that an average algorithm, using both the training and training and out-of-bag samples, would obtain the values 0.2779 for TD2003, 0.2531 for TD2004, 0.7102 for YAHOOV1S2, 0.7111 for YAHOOV1S2-F5 and 0.43875 for WEB10K, considering MAP and NDCG@10. It is also possible to observe in the column effect that the use of out-of-bag samples provides a better ranking model than using the training samples for the collections TD2003, TD2004 and WEB10K. Regarding the row effect that shows the representativeness of the loss functions when compared to the average algorithm, it is possible to observe that $BROOF_{gradient}$ and $BROOF_{absolute}$ are better predictors in TD2003. The collection TD2004 shows that three of the derived instantiations are better than an average algorithm. For the three largest collections, $\text{BROOF}_{gradient}$ is the only instance that showed to have an increase in NDCG@10.

The interactions of the two factors shown in Table 6.5 are computed by subtracting the $\mu + \alpha_j + \beta_i$ from the cell mean $y_{ij.}$ in Table 6.4. Each produced cell corresponds to the interaction of the two evaluated factors and its related levels. In this table is possible to summarize that $BROOF_{gradient}$ and $BROOF_{absolute}$ are 0.0049 and 0.0082 bellow the average derivations of the framework, while BROOF_{median} and BROOF_{height} show an increase in the performance for collection TD2003. When observing the findings for TD2004 we can observe the same behavior for the algorithms $BROOF_{gradient}$, $BROOF_{absolute}$ and $BROOF_{height}$ with the instantiation $BROOF_{median}$ above the average instantiations of the framework. The findings for YAHOOV1S2 shows that 3 out of 4 derived instantiations are able to surpass the average case, with BROOF_{height} being the only one which does not achieve the average algorithm. The interactions for YAHOOV1S2 show that $\text{BROOF}_{gradient}$ and BROOF_{median} are the only derivations capable of surpassing an average algorithm, while YAHOOV1S2-5F only the instantiations BROOF_{median} and BROOF_{height} have some advantage over the average derived instantiations of the framework in both alternatives of the validation set function.

Collection	Algorithm	Using OOB	Using Training Samples	Row Sum	Row Mean	Row Effect
TD2003	$BROOF_{gradient}$	0.2817651363	0.280847105	0.5626122413	0.2813061206	0.0034003269
	$BROOF_{median}$	0.2800920993	0.2684889027	0.548581002	0.274290501	-0.0036152927
	$BROOF_{absolute}$	0.2866742102	0.2923861856	0.5790603958	0.2895301979	0.0116244041
	$BROOF_{height}$	0.2848318632	0.2481608478	0.532992711	0.2664963555	-0.0114094383
	Column Sum	1.1333633089	1.0898830412			
	Column Mean	0.2833408272	0.2724707603		μ 0.277905793754	
	Column Effect	0.0054350335	-0.0054350335			
TD2004	$BROOF_{gradient}$	0.2530611972	0.2546295395	0.5076907367	0.2538453684	0.0006924604
	$BROOF_{median}$	0.2603905641	0.218422483	0.478813047	0.2394065235	-0.0137463844
	$BROOF_{absolute}$	0.2638140393	0.2647743971	0.5285884364	0.2642942182	0.0111413102
	$BROOF_{height}$	0.2596135105	0.250517533	0.5101310435	0.2550655218	0.0019126138
	Column Sum	1.036879311	0.9883439526			
	Column Mean	0.2592198278	0.2470859881		μ 0.25315290795	
	Column Effect	0.0060669198	-0.0060669198			
YAHOOV1S2	$BROOF_{gradient}$	0.71727	0.71935	1.43662	0.71831	0.00805375
	$BROOF_{median}$	0.70854	0.70941	1.41795	0.708975	-0.00128125
	$BROOF_{absolute}$	0.70632	0.70734	1.41366	0.70683	-0.00342625
	$BROOF_{height}$	0.70377	0.71005	1.41382	0.70691	-0.00334625
	Column Sum	2.8359	2.84615			
	Column Mean	0.708975	0.7115375		μ 0.71025625	
	Column Effect	-0.00128125	0.00128125			
YAHOOV1S2F5	$BROOF_{gradient}$	0.725176	0.726496	1.451672	0.725836	0.014723
	$BROOF_{median}$	0.709148	0.709148	1.418296	0.709148	-0.001965
	$BROOF_{absolute}$	0.705106	0.707538	1.412644	0.706322	-0.004791
	$BROOF_{height}$	0.703196	0.703096	1.406292	0.703146	-0.007967
	Column Sum	2.842626	2.846278			
	Column Mean	0.7106565	0.7115695		μ 0.711113	
	Column Effect	-0.0004565	0.0004565			
WEB10K	$BROOF_{gradient}$	0.45614	0.455926	0.912066	0.456033	0.017283
	$BROOF_{median}$	0.435554	0.435702	0.871256	0.435628	-0.003122
	$BROOF_{absolute}$	0.434942	0.434696	0.869638	0.434819	-0.003931
	$BROOF_{height}$	0.428812	0.42822	0.85704	0.42852	-0.01023
	Column Sum	1.755448	1.754552			
	Column Mean	0.438862	0.438638		μ 0.43875	
	Column Effect	0.000112	-0.000112			

Table 6.4: Computation of effects with uniform initialization of weights

Algorithm	$BROOF_{gradient}$	$BROOF_{median}$	$BROOF_{height}$	$BROOF_{absolute}$
TD2003	-0.004976	0.000366	0.012900	-0.008291
TD2004	-0.006851	0.014917	-0.00151	-0.006547
YAHOOV1S2	0.000241	0.000846	-0.001858	0.000771
YAHOOV1S2-5F	-0.000203	0.000456	0.000506	-0.000759
WEB10K	-0.000004	-0.000186	0.00018	0.000011

Table 6.5: Computation of interactions – Using OOB

6.3.3 Allocation of variation

The allocation of variation determines the importance of a factor in the final model and the total allocation is composed by the two factors, its interactions and the experimental

errors. The computation of the variation is done by squaring both sides of the model equation across all observations, which leads to the following equation:

$$\sum_{ijk} y_{ijk}^2 = abr\mu^2 + br\sum_{j}\alpha_j^2 + ar\sum_{i}\beta_i^2 + r\sum_{ij}\gamma_{ij}^2 + \sum_{ijk} e_{ijk}^2 \tag{6.1}$$

The independent parts of Equation 6.1 represent the independent fractions of the total sum-of-squares. The sum of squares of the observed response SSY is given by the summation $\sum_{ijk} y_{ijk}^2$, while the sum of squares of the overall mean SS0 is given by the multiplication of the number of levels a in A by the number of levels b in B times the number of replications r in each configuration of the project, thus SS0 is equals to $abr\mu^2$. The sum of squares for the factor A named SSA represents the variation of the model for factor A, and it is equal to $br\sum_{j}\alpha_j^2$. This same summation can be used to compute the sum of squares for the factor B by replacing the levels of the correspondent factor in the multiplication, thus SSB is equal to $ar\sum_{i}\beta_i^2$. The explanation of the interactions is given by the sum of squares $SSAB$ which is computed by $r\sum_{ij}\gamma_{ij}^2$. The unexplained portion of the total variation is given by the sum-of-square of the errors SSE and it is computed by $\sum_{ijk} e_{ijk}^2$. The total explanation of the variation of the model is given by the SST which can be derived from either $SSY - SS0$ or $SSA + SSB + SSAB + SSE$. The explained variation of the model is given by dividing each individual sum-of-squares in Equation 6.1 by the total sum of squares SST and the results for each collection is shown Table 6.6.

By analyzing the table, we can verify that the possibilities allowed by the function Validation Set represent an amount of 13.45% and 17.46% for TD2003 and TD2004. In both collections, the factor Algorithm has the higher percentage of variation, which consists of 33.01% and 37.62% for the respective collections. The interactions of the factors are quite descriptive, considering that they represent 23.91% and 37.31% in both TD2003 and TD2004 collections. The unexplained portion of variation in all evaluated datasets can be assigned to the differences in each individual algorithm, such as other

%	TD2003	TD2004	YAHOOV1S2	YAHOOV1S25F	WEB10K
Explained by OOB	13.45	17.46	4.99	0.26	0.01
Explained by Algorithm	33.01	37.62	68.05	99.32	99.89
Explained by Interactions	29.61	37.31	3.67	0.35	0.01
Unexplained	23.91	7.59	23.27	0.05	0.07
Total Explanation	76.08	92.40	76.72	99.94	99.92

Table 6.6: Allocation of variation explained by factors in all evaluated L2R sets.

individual minor factors not studied in this analysis (g.e.: number of trees or depth of trees). For the three largest datasets WEB10K, YAHOOV1S2, and YAHOOV1S2-5F the model showed to be more representative with smaller unexplained variations. In these collections, the higher percentage of explanation is attributed to the different loss functions that allow the derived instantiations of the framework with 68.05%, 99.32% and 99.89% of the total variation.

As a summary we can consider that the model for the factorial design is representative, since the smaller total explanation consists of 76.08% and 76.72% for the collections TD2003 and YAHOOV1S2, while for the remaining collections the variation is explained almost in its entirety with 92.40%, 99.94% and 99.92% for the collections TD2004, YAHOOV1S2-5F and WEB10K respectively. Therefore, when building a boosting machine model derived from our framework, the recommendation would be to focus on the definition of the loss functions that derive the instantiations, paying attention in which loss function to use, since as previously argued the best choice for the loss function is dataset dependent.

6.3.4 Analysis of variance

Although the allocation of variation is a great tool to define the most important factors of a model, it only provides the percentage of variation that explains the importance of a factor, which puts in evidence whether the level of importance is or not significant under the view of a statistical analysis. If the unexplained variation of a model attributed to the errors is high, a factor explaining a large fraction of the variation might turn out to be statistically insignificant. To address the issue of whether the explained percentage of variation of the studied factors are really significant, an analysis of variance (ANOVA) test is normally applied in order to investigate the significance of the factors. In this work, we applied the ANOVA test by considering 95% of confidence using the F-distribution table for each collection. The results for this computations are shown in Table 6.7.

In this Table, the statistical significance is computed for the two evaluated factors that define the samples used to fit the model at each iteration of the boosting provided by the function ValidationSet and the 4 loss functions that generate the algorithms provided by the function ComputeLearnerWeights according with the Algorithm 1. In the ANOVA analysis, the factors and its interactions are said to have a significant effect only if the computed ratio of its sum of squares and the mean square of errors are greater than the value read from the F-distribution table. In the results shown in Table 6.7, the ratios are in the column F-computed while the quantiles from the

Collection	Component	Sum of Squares	% of Variation	Deg. of Fr.	Mean Square	F-computed	F-Table
TD2003	y	6.196094		80			
	$\hat{y}\ldots$	6.178530		1			
	$y-\hat{y}\ldots$	0.017563	100.0	79			
	Use Of OOB	0.002363	13.454867	1	0.002363	0.031254	3.973896
	Algorithm	0.005798	33.015286	3	0.001932	0.025563	2.731807
	Interactions	0.005201	29.613235	3	0.001733	0.022929	2.731807
	Errors	0.004200	23.916609	72	0.075611		
				$s_e = 0.027497$			
TD2004	y	5.143774		80			
	$\hat{y}\ldots$	5.126911		1			
	$y-\hat{y}\ldots$	0.016862	100.0	79			
	Use Of OOB	0.002944	17.461974	1	0.002944	0.127688	3.973896
	Algorithm	0.006344	37.624468	3	0.002114	0.091708	2.731807
	Interactions	0.006292	37.316113	3	0.002097	0.090956	2.731807
	Errors	0.001281	7.597443	72	0.023060		
				$s_e = 0.015185$			
YAHOOV1S2	y	40.359743		80			
	$\hat{y}\ldots$	40.357115		1			
	y-$\hat{y}\ldots$	0.002628	100	79			
	Use Of OOB	0.000131	4.996548	1	0.000131	0.011926	3.973896
	Algorithm	0.001788	68.058024	3	0.000596	0.054150	2.731807
	Interactions	9.6482375e-05	3.670796	3	3.21607916667e-05	0.002920	2.731807
	Errors	0.000611	23.274630	72	0.011011		
				$s_e = 0.010493$			
YAHOOV1S2F5	y	40.460718		80			
	$\hat{y}\ldots$	40.454535		1			
	y-$\hat{y}\ldots$	0.006182	100	79			
	Use Of OOB	1.667138e-05	0.269644	1	1.667138e-05	0.281338	3.973896
	Algorithm	0.006141	99.326717	3	0.002047	34.544717	2.731807
	Interactions	2.166374e-05	0.350391	3	7.22124666667e-06	0.121862	2.731807
	Errors	3.29207998409e-06	0.053246	72	5.92574397136e-05		
				$s_e = 0.000769$			
WEB10K	y	15.408704		80			
	$\hat{y}\ldots$	15.400125		1			
	y-$\hat{y}\ldots$	0.008579	100	79			
	Use Of OOB	1.00352e-06	0.011696	1	1.00352e-06	0.008508	3.973896
	Algorithm	0.008571	99.896287	3	0.002857	24.224673	2.731807
	Interactions	1.34284e-06	0.015650	3	4.47613333333e-07	0.003795	2.731807
	Errors	6.55216000306e-06	0.076365	72	0.000117		
				$s_e = 0.001085$			

Table 6.7: ANOVA using 95% of confidence level

F-distribution are shown in the column F-Table.

By analyzing the ratio of all three components of the allocation of variation shown in these two columns for the collection TD2003, we can conclude that there is no statistical evidence that one factor alone or even its interactions provides significant difference amongst the obtained results of the derived instantiations and that the observed difference in the obtained metric measures are mostly due to the unexplained variation, which is congruent to the obtained results shown in the allocation of variation analysis for the collection TD2003. The same behavior is observed for the collections TD2004 and YAHOOV1S2 in all three evaluated components allowing us to conclude that the obtained results are merely due to the experimental errors and not to any

significant difference between the loss functions or the different out-of-bag or training samples used during the boosting iterations. For both collections, YAHOOV1S2-F5 and WEB10K are possible to observe a different behavior from the three previously one, which allow us to conclude that the choice of the loss functions is congruent to the higher percentage of variation of over 99% in both collections. In summary, we can conclude that regarding the instantiations of the framework the most significant factor is the use of the right loss function since it is more prone to give advantages with statistical evidence using an ANOVA test than using the training or out-of-bag samples.

Chapter 7

Conclusions and Future Work

In this chapter, we summarize the research contributions of this master degree thesis and point out some lines of research for further investigation.

7.1 The Framework

In this work, we proposed an extensible framework for L2R, called Generalized BROOF-L2R, which smoothly combines two successful strategies for Learning to Rank, namely, Random Forests and Boosting. Such combination, that uses Random Forests models as weak learners for the boosting algorithm, relies on a set of functions that must be set in order to derive instantiations of the framework. The main characteristics of the framework are: (i) to make use of the training or out-of-bag samples produced by bagging procedures such as Random Forests to determine the influence of each weak learner in the final additive model and (ii) to update the sample distribution weights by means of a more reliable error rate estimate through the applied loss functions. In fact, the framework is general enough to provide a rather heterogeneous set of instantiations that, according to our empirical evaluation, are able to achieve competitive results compared to state-of-the-art algorithms for L2R.

Amongst the set of possible combinations, we only evaluated a total of eight possible instantiations by setting the validation set to training an out-of-bag with 4 distinct loss functions. Regarding the loss functions used in the derived instantiations, three of them relate to boosting by re-weighting. They sequentially minimize the residues at each iteration by building Random Forests as weak learners that are specialists in hard to predict regions by means of perturbation of the input space in the samples weights' distributions. The fourth loss function is based on gradient descent optimization, which

sequentially minimizes the residues by updating the original underlying ground truth for the training samples, thus making boosted gradient random forests models.

Despite the fact that all derived instances of the framework provide very competitive results when compared to the evaluated baselines, BROOF$_{gradient}$ seems to be consistently the top performer in the larger collections, followed by the remaining derivations that are also superior to most baselines. For the smaller collections, BROOF$_{absolute}$ seems to be the best performer, with all other derivations being very competitive, surpassing or tying with most baselines. According to our experimental analysis, all our instantiations are prone to achieve superior results when contrasted to the baseline algorithms under a scenario of a constrained amount of training samples with faster convergence rate. Another observed trend when contrasting the use of the validations set techniques is that using training samples seems to be a better choice for smaller collections, while the use of out-of-bag samples increases the algorithms generalization capabilities as the size of the data increases. We also investigated the effects and the allocation of variation for the two main factors of the proposed framework, which lead led us to conclude that amongst the eight derived instantiations by varying the 4 loss functions and the two inner validation techniques, the most representative factor is the set of the loss function, explaining the largest evidence in the allocation of variation and in the ANOVA test.

7.2 Future Work

We believe that there is a lot of ground to cover regarding our ML approaches. For instance, based on our initial analysis, besides the envisioned loss functions, there are other important factors that can be generalized in our previous solution, including: (i) the initialization strategy to define the importance of samples in each query on the training set; (ii) how to update the samples. Moreover, although we quantify the use of the four loss functions and the use of samples in the inner validation technique of the boosting procedure in a factorial design, we still need to really quantify the impact of the remaining components of our solution in the final results in order to analyze the most promising ways of improving instantiations of the framework. The allocation of variation that was possible to identify with statistical significance were only observed in WEB10K and YAHOOV1S2-F5, with unexplained variation for the remaining collections, which can be attributed to the remaining not studied factors. In fact, based on the aspects we can vary in our procedures we have envisioned a minimum of 16 possible instantiations of our general L2R framework by combining

the possibilities shown in Algorithm 1, from which we tested only 8, which are already superior to the state-of-the-art. This demonstrates the potential of continuing to pursue this line of research. One possibility, for instance, is to modify the initial distribution to a more uniform model, such as the Dirichlet randomization factor, and assess the performance of the variations over the training set (original boosting procedures) and out-of-bag procedures. It is also possible to modify the validation procedure, such that the inner validation technique of the boosting procedure induces leave-one-out queries in the training, instead of relying only on the out-of-bag or training samples to lead the weak learners to the hard regions of the input space.

Other possible extension regards our fourth loss function. This relates to its resemblance to the Mart algorithm (one of the most effective ones in L2R). We conjecture that, by considering that *(i)* Mart is an additive tree procedure that minimizes the least-square regression loss using gradient descent and *(ii)* our approach is an additive tree procedure based on an ensemble of averaged trees generated by the RF model, we believe that we can use the same technique used by LambdaMart to enhance our results by specifying appropriate gradients generated by the LambdaRank function in each iteration of our weak-learners. Hitherto we were able to verify that LambdaMart was able to surpass its base model Mart in some of the datasets by using the multi-relevance judgment ranking metric NDCG, which if correctly applied upon our base weak-learner will allow us to instantiate a new listwise approach using the same properties of LambdaMart, but in our case with a larger potential.

Another hard to tackle issue regarding our boosting procedures refers to the number of iterations to stop the boosting. In all our approaches we stop the boosting iterations by setting a number of rounds that the algorithm must have. However, if the chosen number is too large, a heuristic is applied that considers at each iteration if the current model has an error higher than 1/2, and if so, the training is stopped and no further weak learner is built to compose the ensemble. Although this approach yields satisfying (statistically significant) results, we verified that it is far from perfect and that by choosing a better strategy to stop the number of iterations would allow us to leverage the performance of our rankers even further.

7.2.1 A few Guidelines for Future Investigation

To summarize, we intend to answer the following research questions in future work, that we were not able to be investigate so far:

1. Is it worth to extend our current approach to a listwise one by exploring different loss functions in the learning phase? Before our current approach (a

pointwise one), the state-of-the-art in several datasets was a listwise approach – LambdaMART. We are confident that we can extend BROOF-L2R in a listwise manner by exploiting the LambdaRank gradients used by LambdaMart. In this algorithm, there is a large gap when we vary the underlying metric from ERR to NDCG in different datasets. We propose to investigate these differences in our framework and arrive in a feasible solution that does not require too much parameterization on the training phase.

2. What is the best way to choose the stopping criteria in a boosting procedure? We will investigate the possibility of assessing the best strategy to stop the boosting iteration of our current approaches. One possibility is to use the correlation of the number of rounds.

3. Is it worth to identify the statistical query dependencies based on a "leave-one-out" strategy? We observed that by validating the training phase using leave-one-out of the queries increases the performance of our approaches. We are investigating the possibility of using this procedure as the underlying mechanism to induce the weak learners into the hard to predict regions of the input space.

4. What are the main factors and their interactions in our current approaches? We have considered only eight instantiations of our framework, and by simply modifying some key concepts in each of them we are able to extend it to a whole new family of algorithms.

5. What are the *theoretical properties* of our solutions? We have not delved deeper into such questions in order to understand why our solutions work so well. For instance, are we achieving a better trade-off between the bias and the variance of the learned models with our solution? We intend to perform such investigations and investigate how we can improve our framework with the use of regularization techniques such as the ones proposed by [Hastie et al., 2015] and [Saha et al., 2013].

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