Bayesian Optimization for Optimizing Retrieval Systems

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ABSTRACT
The effectiveness of information retrieval systems heavily depends on a large number of hyperparameters that need to be tuned. Hyperparameters range from the choice of different system components, e.g., stopword lists, stemming methods, or retrieval models, to model parameters, such as $k_1$ and $b$ in BM25, or the number of query expansion terms. Grid and random search, the dominant methods to search for the optimal system configuration, lack a search strategy that can guide them in the hyperparameter space. This makes them inefficient and ineffective. In this paper, we propose to use Bayesian Optimization to jointly search and optimize over the hyperparameter space. Bayesian Optimization, a sequential decision making method, suggests the next most promising configuration to be tested on the basis of the retrieval effectiveness of configurations that have been examined so far. To demonstrate the efficiency and effectiveness of Bayesian Optimization we conduct experiments on TREC collections, and show that Bayesian Optimization outperforms manual tuning, grid search and random search, both in terms of retrieval effectiveness of the configuration found, and in terms of efficiency in finding this configuration.

CCS CONCEPTS
- Information systems → Retrieval models and ranking:

KEYWORDS
Retrieval system; Hyperparameter optimisation; Bayesian Optimization; Covariance function

ACM Reference Format:

1 INTRODUCTION
The effectiveness of information retrieval (IR) systems heavily depends on a large number of hyperparameters that need to be tuned. Hyperparameters range from the choice of different system components, e.g., stopword lists, stemming methods, retrieval models, to model parameters, such as $k_1$ and $b$ in BM25, number of top-ranked documents to consider in pseudo-relevance feedback, and number of query expansion terms.

Retrieval performance is rather sensitive to parameter (or hyperparameter) tuning. Zhai and Lafferty [37] demonstrated this sensitivity for the smoothing parameters in language models, and Trotman et al. [31] for parameters in BM25. Automatic techniques for optimizing model parameters have attracted the attention of the research community in recent years [12–15, 20, 23, 24]. However, parameters are usually optimized in isolation, while their mutual dependencies are, to a great extent, unexplored [1, 19]. Ferro and Silvello [11] recently examined this mutual dependency between choices of stopword lists, stemmers and retrieval models, and concluded that parameter interactions have a strong effect on system performance.

Grid search has been the most widely used strategy for automatic joint optimization of hyperparameters in information retrieval [33]. Grid search is easy to implement, parallelization is trivial, and it is reliable in low dimensional spaces [3]. However, grid search suffers from the curse of dimensionality because the number of configurations grows exponentially with the number of hyperparameters [2]. To reduce the number of candidate configurations to be explored researchers often apply grid search on one dimension/hyperparameter at a time, while fixing the values of the rest hyperparameters until all of them have been traversed. However, this approach is not guaranteed to find a global optimum. Bergstra and Bengio [3] instead propose random search as a more efficient search algorithm. Random search generates candidate configurations drawn uniformly from the same configuration space as would be spanned by a regular grid. Bergstra and Bengio [3] show that random search is more efficient than grid search in high-dimensional spaces because objective functions of interest often have a low effective dimensionality, i.e., they are more sensitive to changes in some dimensions than others [7]. Nevertheless, random search remains agnostic to the effect that a $\delta$-step in the hyperparameter space that would have to the effectiveness of an IR system. Quantifying this effect could lead to more efficient search strategies.

Bayesian Optimization has risen as a promising framework for efficient and effective search in the candidate configuration space [4, 5, 17, 25, 26, 29, 36]. Under the Bayesian Optimization framework, one does not need to explicitly specify the objective function; what is only necessary is the ability to query this function and get an observation. In the case of information retrieval, one does not need to analytically express system effectiveness as a function of the hyperparameters, but only observe the effectiveness of a system configuration in terms of an evaluation measure, e.g., average precision. Bayesian Optimization uses a surrogate model to approximate system effectiveness. Taking a prior belief over this surrogate model allows Bayesian Optimization to sequentially refine it. Further, the
surrogate model, which indicates a probability distribution over
the possible system effectiveness functions, allows designing dif-
ferent strategies for selecting the next configuration to be tested,
exploiting hyperparameter subspaces that have shown to contain
high performance configurations, or exploring hyperparameter
subspaces with high potential [25].

In this paper, we use Bayesian Optimization to automatically op-
timize the retrieval system hyperparameters. Information retrieval
effectiveness, however, as a function of the hyperparameter space
exhibits high irregularity. Furthermore, hyperparameters can be
continuous, or categorical [10], with the latter contributing most of
the irregularity of the objective function. To tackle this we model
the effect of a δ-step in the hyperparameter space to the effectiveness
of the IR system, by suggesting to use different similarity functions
(covariance functions) for continuous and categorical hyperparam-
eters, and examine their ability to effectively and efficiently guide
the search in the hyperparameter space. We compare Bayesian Op-
timization to manual tuning, grid search, and random search using
TREC collections, and demonstrate that Bayesian Optimization is
able to find better configurations in terms of retrieval effectiveness
when all methods are granted the same computational budget. To
the best of our knowledge, this is the first work that uses Bayesian
Optimization to find optimal configurations of retrieval systems.

Therefore, the main contributions of this work are the following:
(1) We propose the use of Bayesian Optimization for retrieval
system configuration;
(2) We decompose the components of Bayesian Optimization
that affect the effectiveness of the method and suggest an
instantiation of it that fits the IR hyperparameter space; and
(3) We demonstrate the effectiveness of the method in building
IR systems and explain the reason in terms of optimization
behaviour.

2 RELATED WORK

We first discuss prior work on hyperparameter optimization in IR.
Next, we give an overview of Bayesian Optimization methods and
the domains they have been applied to.

2.1 Hyperparameter optimization in IR

Optimizing the hyperparameters of a retrieval system is inevitable
in order to achieve optimal performance [33]. Different methods
have been proposed in the literature for automatically optimizing in-
dividual components of a retrieval system [12–15, 20, 23, 24, 30, 38].
Taylor et al. [30] use gradient descent method to optimize the pa-
rameters of ranking functions like BM25F. Their approach however
makes the assumption that the cost functions must be differentiable.
Bigot et al. [6] propose a method for hyperparameter optimization
on a per-query basis. However, this method is hard to generalise as
it only works on queries already seen in the training set. Deveaud
et al. [8] cast the problem of system configuration optimization as a
ranking problem and use learning to rank approaches to select the
best combination of hyperparameters for IR systems. The drawback
is that all the configurations to be ranked must be run in advance
for training and the element number of configurations (e.g. about
10,000 in the paper) grows exponentially with the number of space
dimension. The work of [6] and [8] is orthogonal to the work in this
paper. In both aforementioned works all candidate configurations
need to be considered and the focus lies in finding the best one of
them for each query. Instead, in this paper we propose a search
strategy that avoids considering all candidate configurations and
focuses search in the most promising sub-spaces of hyperparameter
space.

2.2 Bayesian Optimization

The problem of hyperparameter optimization appears in many
machine learning applications, and lately it has attracted a wide in-
terest in that community [4, 5, 17, 25, 26, 29, 36]. Bayesian Optimiza-
tion has emerged rapidly as a promising framework for efficiently
identifying effective configurations. Popular Bayesian Optimization
approaches include sequential model-based optimization (SMBO)
[26], sequential model-based algorithm configuration (SMAC) [17],
tree-based Parzen estimator (TPE) [5] and multi-task Bayesian Op-
timization [29] etc. Bayesian Optimization methods have been ap-
plied successfully in many tasks [28, 34, 36]. For example, Bayesian
Optimization can find better hyperparameters for deep neural net-
works in MNIST digit recognition and CIFAR-10 object recognition
[28]. Also, by applying TPE in feature selection, basic machine
learning algorithms like logistic regression and SVM are proven to
outperform state-of-art neural network models in topic classifi-
cation and sentiment analysis task in NLP [36]. As an important
surrogate model, Gaussian process as well as its covariance func-
tions have been also studied extensively [18, 28]. These successful
applications have inspired us to use Bayesian Optimization to opti-
mize retrieval systems.

3 PRELIMINARIES

3.1 Bayesian Optimization

The Bayesian Optimization framework provides a mechanism to
sequentially search for the global optimum x of an objective func-
tion f(x) : X → R. There are two key components in Bayesian
Optimization [25]. The first is a probabilistic surrogate model used
to predict the objective function value y given a point x. For every
x, there is a random variable y, whose distribution p(y|x) is given
by the surrogate model. One example of the predictive distribution
p(y|x) can be observed in the top panels of Figure 1. In this example
the surrogate model is a Gaussian Process (described in Section 3.2).
The black curve depicts the original objective function (for instance
mean average precision), while the x-axis in the figure represents
an 1-dimensional hyperparameter space, e.g. the parameter μ of a
Language Model with Dirichlet smoothing. The predictive distribu-
tion of y can then be used to construct an acquisition function.
An acquisition function is a policy for selecting the sequence of
points {x1, x2, ..., xn, ...}, i.e. a mechanism to select the next con-
figuration x_{n+1} to test given D_{n} := {(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)}. As
the acquisition function x is usually a closed-form expression of
hyperparameters it is easier to be optimized than the original
objective function. The bottom panel of Figure 1 demonstrates an
acquisition function. The acquisition function values for different
configurations (i.e. along the x-axis) dictate the potential of a certain
configuration to yield a high objective function value.

The second component is the objective function itself, a func-
tion of the target model requiring hyperparameter optimization. In
our case the objective function can be any retrieval effectiveness measure, such as average precision, normalized discount cumulative gain and so on. Computing the objective function for different system configurations is the most time-consuming step [5].

Algorithm 1

Require: surrogate model $M$, acquisition function $\alpha_M$, objective function $f$, input space $X$
1: Initially sample $k$ points $\{x_1, x_2, \ldots, x_k\}$ from $X$, query $f$ to get $(y_1, y_2, \ldots, y_k)$
2: Update $M$
3: for $n = 1, 2, \ldots$ do
4: Select $x_{n+1} \leftarrow \text{argmax } \alpha_M(x; D_n)$
5: Calculate $y_{n+1} \leftarrow f(x_{n+1})$
6: Augment $D_{n+1} = \{D_n, (x_{n+1}, y_{n+1})\}$
7: Update $M$
8: end for
9: Select the best $y$ from $D$

3.2 Gaussian Process

The Gaussian Process (GP) is the most commonly-used surrogate model in Bayesian Optimization [21]. The key hypothesis underlying GP is that any finite set of $\{y_i\}$ follows a Multivariate Gaussian Distribution. There is an analytic expression for the joint distribution $p(y_1:n|x_1:n) \sim N(0, K)$, with $K$ being the covariance matrix,

$$K = \begin{bmatrix}
    k(x_1, x_1) & \cdots & k(x_1, x_n) \\
    \vdots & \ddots & \vdots \\
    k(x_n, x_1) & \cdots & k(x_n, x_n)
\end{bmatrix}$$

and $k(x_i, x_j)$ being a covariance function. The conditional distribution of the objective function value given the sequence of past observations and a new point $x_{n+1}$ is $p(y_{n+1}|x_{n+1}, D_{1:n}) \sim N(\mu_n(x_{n+1}), \sigma^2_n(x_{n+1}))$, where $\mu_n(x_{n+1})$ and $\sigma^2_n(x_{n+1})$ are the mean and the variance of the posterior distribution, respectively. They are defined as

$$\mu_n(x_{n+1}) = k^T K^{-1} y_{1:n}$$

$$\sigma^2_n(x_{n+1}) = k(x_{n+1}, x_{n+1}) - k^T K^{-1} k$$

The covariance function models the effect of taking a $\delta$-step in the hyperparameter space to the objective function. In Section 4.2 we suggest covariance functions we believe to be appropriate for the continuous, and categorical hyperparameters of a retrieval system.

3.3 Acquisition Function

A good acquisition function is the one that finds an optimal trade-off between exploration and exploitation in the hyperparameter space. In practice, an acquisition function balances between configurations for which the predicted function value $f(x)$ is high (exploitation) and configurations for which the predicted variance $\sigma(x)$ is high (exploration) [25].

In this work, we consider three acquisition functions: probability of improvement (PI), expected improvement (EI) [9] and upper confidence bound (UCB), defined as follows:

$$\alpha_{PI}(x|D_n) := P(y > y^*) = \Phi(\frac{\mu_n(x) - y^*}{\sigma_n(x)})$$

$$\alpha_{EI}(x|D_n) := \mathbb{E}(\max(y - y^*, 0))$$

$$= (\mu_n(x) - y^*)\Phi(\frac{\mu_n(x) - y^*}{\sigma_n(x)}) + \sigma(x)\phi(\frac{\mu_n(x) - y^*}{\sigma_n(x)})$$

$$\alpha_{UCB}(x|D_n) := \mu_n(x) + \beta\sigma_n(x)$$

where $\alpha(\cdot)$ is the acquisition function, $y^*$ is a target value which is often set to $\max(\{y_i\})$ [35], and $\Phi$ and $\phi$ are the Cumulative Distribution Function and Probability Density Function of the standard normal distribution, respectively. $\beta$ is a hyperparameter that can be set according to some theoretically motivated guidelines.

A drawback of PI, intuitively, is that it is pure exploitive. Configurations that have a high probability their effectiveness being infinitesimally greater than $y^*$ will be drawn over configurations that offer larger gains but with less certainty. EI on the other hand considers the magnitude of the improvement a configuration can potentially yield, instead of PI. In UCB it is the parameter $\beta$ that controls the trade-off between exploration and exploitation. These three acquisition functions are point-wise, that is they only care about the improvement over $y^*$ on each single point. There are also entropy-based acquisition functions that make use of what
has been observed about the objective function to pick up the most informative point, which will be left for the future study.

3.4 Initialization

The first posterior distribution of the surrogate model can be obtained by using the predefined prior distribution to draw the first hyperparameter point, i.e. the first configuration. This strategy runs the risk of getting stuck in a local optimum, since it heavily depends on the first point that will be used. A more general strategy, which we follow in this work is to sample a set of configurations randomly in the search space so that the surrogate model can observe the overall ‘landscape’ of configurations. In this work we test three sampling methods: Latin hypercube sampling, random sampling, and sampling from Sobol sequences [16].

3.5 Selecting the Optimal Configuration

At the end of the optimization process one needs to decide which configuration is the optimal one. The natural choice is to select the configuration with the best observed effectiveness. However, this strategy runs the risk of overfitting the observed objective function values. A different strategy is to select the configuration with the highest predicted value, instead of the actual observed value, which can accommodate noisy outputs. The two strategies are called incumbent and latent, respectively [16], and we test both in this work.

4 METHODOLOGY

In this section we first elaborate the hyperparameter optimization process, then we focus on the particular characteristics of the retrieval systems hyperparameter space and discuss the covariance functions we consider appropriate for this space.

4.1 Hyperparameter Optimization Process

Following the Bayesian Optimization framework, we have two major modules in our algorithmic pipeline, the IR module and the BO module (see Figure 2). The IR module tackles the conditional hyperparameters, and computes the objective function value \( y_n \), given a hyperparameter configuration \( x_n \). The BO module adds \((x_n, y_n)\) into the sample set, updates the posterior distribution of the surrogate models, selects the next hyperparameter configuration \( x_{n+1} \), and passes it back to IR module.

4.2 Hyperparameter Structure and Covariance functions

Snoek et al. [26] suggest that it is the choice of the covariance functions that has the strongest effect on the performance of Bayesian Optimization. In this paper we only consider a simple case, stationery covariance function, which is defined as a function of \(|x - x'| = r\). The mean square differentiability of a stationary covariance function around 0 determine the smoothness properties of the samples drawn from the corresponding Gaussian process [22], which essentially dictates the expected response in the objective function if a \(\delta\)-step is taken in the hyperparameter space.

The squared exponential covariance function (SE) is a widely made choice for smooth objective functions; it is mean square differentiable at any order and thus very smooth. It is defined as:

\[
K_{\text{SE}}(x, x') = \exp\left(-\frac{r^2}{2}\right)
\]

where \(x\) and \(x'\) are two points in the hyperparameter space, and \(r\) is the distance between \(x\) and \(x'\).

The Matérn1 covariance function (Matérn1) is appropriate to model rough objective functions, as it is only first-order mean square differentiable. Matérn1 is defined as follows:

\[
K_{\text{Matérn1}}(x, x') = \exp(-r).
\]

Selecting a covariance function requires examining the hyperparameter space of an IR system. Retrieval model parameters, e.g. the smoothness parameter \(\lambda\) in Jelinek-Mercer Smoothing of Language Models, or the parameter \(b\) in BM25, are typically continuous. On the other hand, the choice of the retrieval model itself can be expressed with a categorical hyperparameter; the use or not of relevance feedback algorithms is also categorical, as is the choice of a stopword list, or a stemmer. The default distance used in either SE covariance function or Matérn1 covariance function is Euclidean distance, defined as

\[
r_E := \sqrt{\sum_{d=1}^{N} (x_d - x'_d)^2}.
\]

It would treat categorical hyperparameters as ordinal, whereas this should not be the case. Therefore, considering the heterogeneity of the hyperparameters of IR systems, Euclidean distance is not a good fit. Instead, inspired by [17], we use Hamming distance for categorical dimensions, while Euclidean distance for continuous or discrete dimensions. The Hamming distance is defined as

\[
r_H := \sum_{d=1}^{N} (1 - \delta(x_d, x'_d))
\]

where \(\delta\) is the Kronecker delta function (equalling one if its two arguments are identical and zero otherwise).

In order to accommodate both continuous and categorical hyperparameters, we combine the Euclidean distance and the Hamming

![Figure 2: Hyperparameter optimization architecture.](image-url)
distance into a mixture distance, the Hamming Euclidean mixture distance (HE distance). HE treats continuous and categorical hyper-parameters differently; it is defined as
\[
    r_{HE} := \sqrt{\sum_{d \in \text{con}} (x_d - x'_d)^2 + \sum_{d \in \text{cat}} (1 - \delta(x_d, x'_d))}
\]
where \(\text{con}\) is the set of continuous dimensions and \(\text{cat}\) the set of categorical dimensions. It is easy to prove that HE is a distance (or metric). By replace the original distance function \(r_{SE}\) with \(r_{HE}\), we get two new covariance functions,
\[
    K_{HSE}(x, x') = \exp(-\frac{r_{HE}^2}{2})
\]
\[
    K_{HMatérn1}(x, x') = \exp(-r_{HE}).
\]

Compared with SE and Matérn1, HSE and HMatérn1 are designed to handle heterogeneous space where the continuity property of different dimensions are not the same. To sum up, in this work, we test the performance of SE, HSE, Matérn1 and HMatérn1 as four representative covariance functions for continuous and categorical hyperparameters.

5 EXPERIMENT SETUP

5.1 Research questions
In the remainder of the paper we aim to answer the following three research questions:

RQ1 What is the most critical component of the Bayesian Optimization framework for identifying the best retrieval system configuration?

RQ2 How effective is Bayesian Optimization in searching the configuration space, and in finding configurations that generalize across queries and collections?

RQ3 How to explain the optimization behaviour of Bayesian Optimization in terms of exploration and exploitation?

5.2 Implementation of Retrieval System and Bayesian Optimization
We use Pyndri [32], a Python Interface to the Indri Search Engine [27], as the IR module in our pipeline, which is mainly decomposed to indexing, retrieval, and pseudo-relevance feedback. All the three modules are considered in our optimization experiments.

The objective function can be any retrieval effectiveness measure. In this work we optimize for the Mean Average Precision (MAP), Normalized Discounted Cumulative Gain (NDCG) and Mean Reciprocal Rank (MRR) and use \texttt{trec_eval} \(^1\) for the computations.

We use Pybo [16] in our experiments, a Python package for Bayesian Optimization. Pybo supports the default version of the SE covariance function and the Matérn1 covariance function which use Euclidean distance to measure the distance of two points; we implemented the HSE covariance function and the HMatérn1 covariance function within Pybo ourselves.

5.3 Candidate Configurations
There are two major choices to make when indexing documents: the stopword list and the stemmer. Ferro and Silvello [11] has shown that the choice of different stopword lists, like that of indri, Lucene, Smart and Terrier, has limited effect to the performance of a IR system; however, having stopword list or not makes a big difference. On the other hand, indexing document collections takes a long time. Therefore for efficiency and convenience we only set two values for the categorical hyperparameter \textit{stopper}: TRUE means using Indri stopword list and FALSE means not using any stopword list. The situation is similar for \textit{stemmer}: TRUE means using Krovetz stemmer and FALSE means not using any stemmer.

There are three retrieval models implemented in Indri: TF-IDF with BM25 term weighting, Okapi BM25, and Language Models. Language Models supports three different smoothing methods, Jelinek-Mercer (JM), Dirichlet (DIR), and two-stage smoothing (TS). Let \(\text{rm}\) denote a categorical hyperparameter that represents the retrieval model type and takes values in \{TF-IDF, BM25, LM-JM, LM-DIR, LM-TS\}, that is the TF-IDF model with BM25 term weighting, the Okapi BM25 model, the Language Model with JM smoothing, the Language Model with Dirichlet smoothing, and the Language Model with two-stage smoothing respectively. There is a number of hyperparameters per model: \(k\) and \(b\) for TF-IDF, \(k\), \(k\), and \(b\) for Okapi BM25, \(\lambda_{col}\) and \(\lambda_{doc}\) for the JM smoothing, \(\mu\) for the Dirichlet smoothing, and \(\lambda\) and \(\mu\) for the two stage smoothing. The parameters of these models lay in a continuous space.

Indri also supports pseudo-relevance feedback models. We consider a binary hyperparameter \(\text{prf}\) that takes the value TRUE if pseudo-relevance feedback is used, and FALSE otherwise. There are four hyperparameters that need to be set for the pseudo-relevance feedback models, the number of feedback documents to be considered, \(\text{fbDocs}\), the number of feedback terms, \(\text{fbTerms}\), the Dirichlet smoothing parameter used for the feedback document language model, \(\text{fbMu}\), and the weight of the original query, \(\text{fbOrigWeight}\), in the mixture model between the original query and the feedback documents. In total, we have a conditional hyperparameter space of 18 dimensions (see Figure 3).

5.4 Test collections
We conduct our experiments on the ad-hoc test collections of TREC 5-8 and TREC Robust 2004, as well as the web test collections of TREC 2010-2012 in order to thoroughly evaluate the proposed method in diversified datasets. The details can be found in Table 1. As we can see, ad-hoc tracks and web tracks are quite different methods in diversified datasets. The details can be found in Table 1. As we can see, ad-hoc tracks and web tracks are quite different test collections. Web tracks have much more documents and the average length of documents is also longer, indicating they are more challenging compared with ad-hoc tracks.

5.5 Baselines

Manual Search. The first baseline is obtained by running Indri with its default hyperparameters. Then we manually select the best performing model among TF-IDF/BM25/Language Models, with/without pseudo-relevance feedback.

Grid Search. The second baseline is grid search. Grid search is the most widely used method for hyperparameter tuning. For each of the five retrieval model (TF-IDF, BM25, LM-JM, LM-DIR, LM-TS)
6 RESULTS AND ANALYSIS

6.1 Decompose component effect of Bayesian Optimization

This experiment is designed to answer RQ1. In order to study which components of Bayesian Optimization has the strongest effect on the performance of Bayesian Optimization in finding optimal system configurations we run a full factorial experiment, using 54 joint strategies of Bayesian Optimization: the 3 initialization strategies \( \times \) the 3 covariance functions \( \times \) the 3 acquisition functions \( \times \) the 2 selection strategies. The experiment was run on the Robust 2004 dataset. We measure performance on the basis of MAP and we run an analysis of variance (ANOVA) considering only the main effects of the Bayesian Optimization components (that is we ignore any interactions between them, since we do not have enough data points for a detailed analysis).

The results of the ANOVA can be seen in Table 2. The important observation lays in the last column of the table; this is the \( \rho \)-value that designates whether a factor has a significant effect when \( \rho > 0.05 \), or there is not enough evidence to reach that conclusions otherwise. As we can observe, and in accordance to previous work [26] ANOVA suggests that the choice of the covariance function is the most important decision one needs to make when instantiating Bayesian Optimization, at least among the components we considered in this work. Therefore, we vary covariance functions and fix the rest strategies by selecting the respective best ones, that is Sobol + EI + Incumbent in the following sections.

6.2 Optimizing IR systems using Bayesian Optimization

This experiment is designed to answer RQ2. We first run the four methods on Robust 2004 or Web 2012 as the training set, then we tested the corresponding optimal configurations on TREC 5-8 or Web 2011-2012. In order to have a thorough study of Bayesian Optimization, we further experimented on the 2-dimensional space which is is \( \lambda \) and \( \mu \) for the two stage smoothing, and the 18-dimensional space which includes the complete hyperparameters introduced in Section 5.3 respectively.

Table 3 shows the performance of the best configurations found by each method. As expected, there is no big difference among...
the four search methods in 2-dimensional space. It is because both grid search and random search are able to cover the space in low dimensional space. However, grid search needs more budget compared with Bayesian Optimization and random search. Therefore, Bayesian Optimization, grid search and random search can achieve comparable performance, but Bayesian Optimization and random search are more efficient in 2-dimensional spaces than grid search. The situation changes with the number of dimension increasing. We can see Bayesian Optimization performs slightly better than random search, grid search and manual method in 18-dimensional space. Random search is comparable with Bayesian Optimization in low (2) dimensional space, but it fails in high (18) dimensional space. However, there seems no significant difference among the four methods according to the results in Table 3.

6.3 Optimization behaviour of Bayesian Optimization

This experiment is designed to answer RQ3. We study how Bayesian Optimization searches points in the search space and how different covariance functions affect this behaviour. For visualisation convenience we take 1-dimensional and 2-dimensional hyperparameter space as examples.

The hyperparameter considered in 1-dimensional space is \( \mu \) in language model with Dirichlet smoothing. We initialised the posterior of the surrogate model with 2 points, and iteratively searched 32 points. We also recorded the predictive function predicted by the surrogate model in round 1 and 32. The result is show in Figure 4. We can see that the intensive red lines tend to appear near the global optimum for most datasets and measures, indicating that Bayesian Optimization spends more efforts and exploits much near the global optimum. It is more obvious when the objective function is highly irregular like MRR. By “irregular” we mean there are many local optimums. On the right panel of Figure 4a, we find that Bayesian Optimization prefers exploitation near these local optimums and allows exploration in other areas, and finally it spends most efforts near the global optimum. Figure 4b shows the zoomed-in result on TREC 6 + MRR. The posterior of the surrogate model in round 1 does not know much about the objective function and predicts the same value for most points except the area near the two initial points. Whereas in round 32, the predictive function can model the rough trend quite well, where several local maximums and minimums are quite consistent with the real objective function. Overall speaking, Bayesian Optimization’s performance in 1-dimensional space is as good as we expect in terms of exploration and exploitation. Its preference of exploitation near global optimum makes it a reliable optimization approach.

The hyperparameters considered in 2-dimensional space are \( \mu \) and \( \lambda \) in language model with two-stage smoothing. We initialised the posterior of the surrogate model with 4 points, and iteratively searched 32 points. Same as 1-dimensional case, we also recorded the predictive function in round 1 and 32. In Figure 5 we plotted the results of the SE covariance function and the Matérn1 covariance function respectively. The first two panels of Figure 5a shows the effect of Matérn1 on the predictive function. In round the surrogate model predicts that the lower left corner has the potential of getting high values. In round 32 the predictive function is quite rugged because multiple local optimums are observed. It predicts the area around \((2800, 0.7)\) having a global optimum, which is quite consistent with the real objective function. The right panel compares the point traces of Bayesian Optimization, random search and manual search. At the beginning, Bayesian Optimization prefers exploration and tries to cover a large area of the search space. Later it prefers exploitation as we can see it spends more efforts near the global optimum. It is also interesting to compare the way how the two covariance functions model the real objective function. We know that the smoothness of the samples generated by the two covariance functions conforms to the order: SE > Matérn1. This is consistent with Figure 5. The real objective function in this case is quite smooth and seems to have one optimum, therefore SE is enough to model its irregularity. As an evidence we can see that more points are searched within green contour line on the most right side in Figure 5b compared with Figure 5a.

Figure 4: Optimization behaviour of Bayesian Optimization in 1-dimensional space \( X = [0, 3000] \).
To sum up, Bayesian Optimization balances exploitation and exploration by spending more search budget near the global optimum or local optima, which makes it a reliable optimization approach. This optimization behaviour is affected by the covariance function. If the objective function is very irregular like MRR, Matérn1 is recommended; while SE is recommended if relative objective functions like MAP and NDCG.

7 CONCLUSIONS AND FUTURE WORK
In this paper we study the problem of retrieval system optimization. We propose the use of Bayesian Optimization to jointly search and optimize over the hyperparameter space. Given the heterogeneous hyperparameters in retrieval systems we suggest the use of four covariance functions that can handle both continuous and categorical hyperparameters, the SE, HSE, Matérn1 and HMatérn1 covariance function. We analyze the effect of the different components of Bayesian Optimization and reach at the same conclusion as prior research on the topic [26] that it is the choice of the covariance functions that have the strongest effect on the performance of Bayesian Optimization. To demonstrate the effectiveness and efficiency of Bayesian Optimization to identify a good system configuration, we performed manual tuning, grid search and random search, both in terms of exploitation and exploration. We found it spends more search budget near the global optimum or local optima, and this optimization behaviour is affected by covariance functions of different smoothness.

One should note that for the Gaussian Process the bounds for all dimensions of the search space are axis-aligned, i.e. the search space is a hyper-rectangle [25]. This is contradictory with the conditional structure of IR hyperparameters, which means that our instantiation of Bayesian Optimization wastes time in searching in invarient dimensions. We leave the study of surrogate model that can solve conditional hyperparameters as a future work.

REFERENCES

Figure 5: Optimization behaviour of Bayesian Optimization in 2-dimensional space $X = \{ (\mu, \lambda) | \mu \in [0, 3000], \lambda \in [0, 1] \}$. Objective function: MAP. Data set: TREC-WEB12. The contour lines depict the predictive functions in round 1 and 32 on the first two panels, and the real objective function on last panel. The red numbers denote Bayesian Optimization searches which point and in which round; the black dots denote the point trace of random search; and the star denotes the point of manual search.


