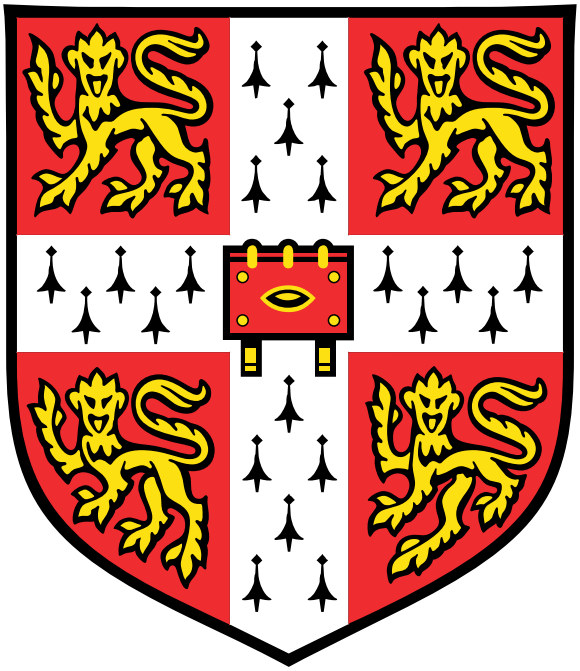
Parameter Optimization using high-dimensional Bayesian Optimization

Bachelor Thesis



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This dissertation is submitted for the degree of

March 2018

0.1 Project Proposal for Bachelor Thesis

0.1.1 Motivation

Tuning hyperparameters is considered a computationally intensive and tedious task, be it for neural networks, or complex physical instruments such as free electron lasers. Users for such applications could benefit from a 'one-click-search' feature, which would find optimal parameters in as few function evaluations as possible. This project aims to find such an algorithm which is both efficient and holds certain convergence guarantees. We focus our efforts on Bayesian Optimization (BO) and revise techniques for high-dimensional BO.

0.1.2 Background

In Bayesian Optimization, we want to use a Gaussian Process to find an optimal parameter setting $\mathbf{x}^*$ that maximizes a given utility function f. We assume the response surface to be Lipschitz-continuous.

Assume we have observations $\mathscr{Y} = \{y^{(1)}, \ldots, y^{(N)}\}$, each evaluated at a point $\mathscr{X} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\}$. The relationship between the observations y and individual parameter settings $\mathbf{x}$ is $y = f(\mathbf{x}) + \varepsilon$ where $\varepsilon \sim \mathscr{N}\left(0, \sigma_n^2\right)$. Any quantity to be predicted has a subscript-star (e.g. y_* is the function evaluation we want to predict).

In it's simplest form, a Gaussian Process is described by the following equation:

$$\begin{pmatrix} y \\ y_* \end{pmatrix} \sim N\left(\mu, \begin{pmatrix} K & K_*^T \\ K_* & K_{**} \end{pmatrix}\right), \tag{1}$$

Where μ is a mean function, $K = \text{kernel}(\mathbf{X}, \mathbf{X})$, $K_* = \text{kernel}(\mathbf{x}_*, \mathbf{X})$ and $K_{**} = \text{kernel}(\mathbf{x}_*, \mathbf{x}_*)$. We predict any new point y_*, (given all previously sampled points y) by estimating the probability $p(y_*|y) \sim N(K_* K^{-1} y, K_{**} - K_* K^{-1} K_*')$

This, in turn, can be used to build an acquisition function. This acquisition function describes where to best sample points next. Some popular acquisition functions include GP-UCB, Most probable improvement (MPI) and Expected Improvement (EI). The choice of the acquisition function has great influence on the performance of the optimization procedure.

We will talk about the problems and possible solutions for the task at hand in the next section.

0.1.3 Scope of the Project

Bayesian optimization suffers from the curse of dimensionality. The goal of this project is to arrive at a solution that resolves the curse of dimensionality for the specific task with regards to Bayesian optimization. This project includes, but is not limited to the following methods.

1. [7] Assume $f(x) \approx g(\mathbf{W}^T x)$ where $\mathbf{W} \in \mathbb{R}^{D \times d}$ and $D >> d$. We assume that $\mathbf{W}$ is orthogonal.

   This algorithm does not require gradient-information (thus, easier to implement, and robust to noise). The standard-deviation, kernel parameters and $\mathbf{W}$ can be found iteratively. First we fix $\mathbf{W}$, and optimize over the standard-deviation, kernel parameters. Then we fix the standard-deviation, kernel parameters. and optimize over $\mathbf{W}$. We repeat this procedure until the change of the log-likelihood between iterations is below some ε_l.

2. [6] Assume $f(x) = f^{(1)}(x^{(1)}) + f^{(2)}(x^{(2)}) + \ldots + f^{(M)}(x^{(M)})$ where $x^{(i)} \in \mathscr{X}^{(i)} \subseteq \mathscr{X}$, i.e. each function component $f^{(i)}$ takes some lower-dimensional subspace as the input. The lower-dimensional subspaces may overlap. The mean and covariance of $f(x)$ is then the sum of the individual component's means and covariances.

   An additive decomposition (as described above) can be represented by a dependency graph. The dependency graph is built by joining variables i and j with an edge whenever they appear together within some set $x(k)$.

   The goal is to maximize an acquisition function $\phi_t(x) = \sum_{i=1}^{M} \phi_t^{(i)}(x^{(i)})$. This maximization is achieved by maximizing the probability of Markov Random Fields within the graph. A junction tree is created from the graph, which is then used to find the global maximum of the acquisition function.

   The dependencies between the variable-subsets are represented through a graph, which can be learned through Gibbs sampling. This, in turn, is used to create a kernel for the GP.

3. [**?**] A function $f : \mathbf{R}^D \to \mathbf{R}$ is said to have effective dimensionality d_e (where $d_e < D$), if there exists a linear subspace $\mathscr{T}$ of dimension d_e such that for all $x_\top \in \mathscr{T} \subset \mathbf{R}^D$ and $x_\perp \in \mathscr{T}_\perp \subset \mathbf{R}^D$, we have $f(x) = f(x_\top + x_\perp) = f(x_\top)$. $\mathscr{T}^\perp$ is the orthogonal complement of $\mathscr{T}$.

   Assume $f : \mathbf{R}^D \to \mathbf{R}$ has effective dimensionality d_e. Given a random matrix $\mathbf{A} \in \mathbf{R}^{D \times d}$ (where $d \geq d_e$) with independent entries sampled fom $\mathscr{N}(0,1)$. For any $x \in \mathbf{R}^D$, there

exists a $y \in \mathbf{R}^d$ such that $f(x) = f(\mathbf{A}y)$. We now only need to optimize over all possible $y \in \mathbf{R}^d$, instead of all possible $x \in \mathbf{R}^D$.

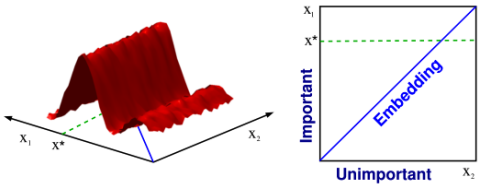

Fig. 1 This function in D=2 dimesions only has d=1 effective dimension. Hence, the 1-dimensional embedding includes the 2-dimensional function's optimizer. It is more efficient to search for the optimum along the 1-dimensional random embedding than in the original 2-dimensional space

If, for some reason, finding an active subspace or an effective lower dimension is not possible, we are open to adapt the procedure of optimization.

Abstract

This is where you write your abstract ...

Table of contents

0.1 Project Proposal for Bachelor Thesis ii
0.1.1 Motivation ii
0.1.2 Background ii
0.1.3 Scope of the Project iii

List of figures **ix**

List of tables **xi**

1 Background **1**
1.1 1

2 Existing Approaches **3**
2.1 Using a projection matrix 3
2.1.1 Active learning of linear subspace 3
2.1.2 High dimensional Gaussian bandits 3
2.1.3 Random embeddings (REMBO) 4
2.1.4 Applications to high-dimensional uncertainty propogation 4
2.2 Exploiting additive structures within the function 4
2.2.1 Independent additive structures within the target function 4
2.2.2 Ideas 4
2.3 Other approaches 5
2.3.1 Elastic Gaussian Processes 5
2.3.2 Bayesian Optimization using Dropout 5
2.3.3 Ideas 5
2.4 Datasets for benchmarking 5

3 Benchmarking methods **9**
3.1 Methods from 9
3.1.1 First subsection in the first section 9

References **11**

Appendix A How to install LaTeX **13**

List of figures

1 This function in D=2 dimesions only has d=1 effective dimension. Hence, the 1-dimensional embedding includes the 2-dimensional function's optimizer. It is more efficient to search for the optimum along the 1-dimensional random embedding than in the original 2-dimensional space iv

List of tables

Chapter 1

Background

1.1

Lorem Ipsum is simply dummy text of the printing and typesetting industry (see

Chapter 2

Existing Approaches

This section will cover approaches taken so far to solve the problem. We will present algorithms that solve the approach, and the dataset that the algorithm was evaluated on, as well as their effectiveness.

2.1 Using a projection matrix

2.1.1 Active learning of linear subspace

[3] Assume f depends only on $u := xR^T$ with $R \in \mathbf{R}^{d \times D}$ where $d << D$. Learn an algorithm that learns $\hat{f}(u) = f(x)$ and R.

Steps include: 1.) Create a probability distribution over possible embeddings to learn R (Laplace approximation). 2.) Use this to create a probability distribution over f. 3.) Perform active selection over all possible points.

3.) is done using using Bayesian Active Learning by disagreement, where the utility function is the expected reduction in entropy (equal to the mutual information), as opposed to uncertainty sampling, which simply minimizes the entropy.

Tests are conducted on a real, and synthetic dataset with up to $D = 318$ and selecting $N = 100$ observations.

2.1.2 High dimensional Gaussian bandits

[1] Assume there exists a function $g : \mathbf{R}^k \implies [0,1]$ and a matrix $A \in \mathbf{R}d \times D$ with orthogonal rows, such that $f(x) = g(Ax)$. Assume $g \in \mathscr{C}^2$. Assume that $B = \mathbf{B}^D(1+\varepsilon)$. We want to

maximize $f : B \implies [0,1]$.

The SI-BO algorithm has a two-step approach: 1.) subspace identification. 2.) Bayesian Optimization on the learned subspace.

2.1.3 Random embeddings (REMBO)

[8] Let $x \in \mathbb{R}^D$ and $y \in \mathbb{R}^d$. Assume, that $f(x) = f(Ax)$. We can generate $A \in \mathbb{R}^{D \times d}$ by randomly generating this matrix.

2.1.4 Applications to high-dimensional uncertainty propogation

[7] Assume $f(x) \approx g(\mathbf{W}^T y)$ where $\mathbf{W} \in \mathbb{R}^{D \times d}$ and $D >> d$. We assume that $\mathbf{W}$ is orthogonal.

This algorithm does not require gradient-information (thus, easier to implement, and robust to noise). The standard-deviation, kernel parameters and $\mathbf{W}$ can be found iteratively. First we fix $\mathbf{W}$, and optimize over the standard-deviation, kernel parameters. Then we fix the standard-deviation, kernel parameters. and optimize over $\mathbf{W}$. We repeat this procedure until the change of the log-likelihood between iterations is below some ε_l.

2.2 Exploiting additive structures within the function

2.2.1 Independent additive structures within the target function

[2] Assume that $f(x) = \sum_{i=1}^{|P|} f_i(x[P_i])$, i.e. f is fully additive, and can be represented as a sum of smaller-dimensional functions f_i, each of which accepts a subset of the input-variables. The kernel also results in an additive structure: $f(x) = \sum_{i=1}^{|P|} k_i(x[P_i], x[P_i])$. The posterior is calculated usin ghte Metropolis Hastings algorithm. The two actions for the sampling algorithm are 'Merge two subsets', and 'Split one set into two subsets'. k models are sampled, and we respectively approximate $p(f_*|D,x^*) = \frac{1}{k}\sum_{j=1}^{k} p(f(x^*|D,x,M_j))$, where M_j denotes the partition amongst all input-variables of the original function f.

2.2.2 Ideas

We could have a function sth like: $f(x) = g(Ax_1) + g(Bx_2) + ...$ as this does not assume that the dimensions are directly correlated. We could also use PCA or anything similar to choose the axis (i.e. $A, B, C..$)

2.3 Other approaches

2.3.1 Elastic Gaussian Processes

[5] Use a process where the space is iteratively explored. The key insight here is that with low length-scales, the acquisition function is extremely flat, but with higher length-scales, the acquisition function starts to have significant gradients. The two key-steps is to 1.) additively increase the length-scale for the gaussian process if the length-scale is not maximal and if $||x_{init} - x^*|| = 0$. And 2.) exponentially decrease the length-scale for the gaussian process if the length-scale is below the optimum length-scale and if $||x_{init} - x^*|| = 0$.

2.3.2 Bayesian Optimization using Dropout

[4] propose that the assumption of an active subspace is restrictive and often not fulfilled in real-world applications. They propose three algorithms, to iteratively optimize amongst certain dimensions that are not within the d 'most influential' dimensions: 1.) Dropout Random, which picks dimensions to be optimized at random, 2.) Dropout copy, which continuous optimizing the function values from the found local optimum configuration, and 3.) which does method 1. with probability p, and else method 2. The d 'most influential' dimensions are picked at random at each iteration.

2.3.3 Ideas

I think optimizing the hyper-parameters of Gaussian processes, and also the kernel is a valueable insight not much explored.

2.4 Datasets for benchmarking

1. [3] Synthetic in-model data matching the proposed model, with $d = 2,3$, and $D = 10,20$.
2. [3] (Synthetic) Braning function, $d = 2$, hidden in a higher dimensional space $D = 10,20$.
3. [3] Temperature data $D = 106$ and $d = 2$.
4. [3] Communities and Crime dataset $d = 2$, and $D = 96$.
5. [3] Relative location of CT slices on axial axis with $d = 2$ and $D = 318$.

6. [1] (Synthetic) Random GP samples from 2-dimensional Matern-Kernel-output, embedded within 100 dimensions
7. [1] Gabor Filters: Determine visual stimuli that maximally excite some neurons which reacts to edges in the image. We have $f(x) = \exp(-(\theta^T x - 1)^2)$. θ is of size 17x17, and the set of admissible signals is d.
8. [8] (Synthethic) $d = 2$ and $D = 1 * 10^9$.
9. [8] $D = 47$ where each dimension is a parameter of a mixed integer linear programming solver.
10. [8] $D = 14$ with d for a random forest body part classifier.
11. [7] (Synthetic) Use $d = 1, 10$ and $D = 10$.
12. [7] (Half-synthetic) Stochastic elliptic partial differential equation, where $D = 100$, and an assume value for d of 1 or 2.
13. [7] Granular crystals $X \in \mathbb{R}^{1000 \times 2n_p+1}$, and $y \in \mathbb{R}^{1000}$.
14. [2] (Synthetic) Styblinski–Tang function where D is freely choosable.
15. [2] (Synthetic) Michalewicz function where D is freely choosable.
16. [2] (Simulated) NASA cosmological constant data where $D = 9$.
17. [2] Simple matrix completion with $D = 3$.
18. [5] (Synthetic) Hertmann6d in [0, 1].
19. [5] (Synthetic) Unnormalized Gaussian PDF with a maximum of 1 in $[-1, 1]^d$ for $D = 20$ and $[-0.5, 0.5]^d$ for $D = 50$
20. [5] (Synthetic) Generalized Rosenbrock function $[-5, 10]^d$
21. [5] Training cascade classifiers, with $D = 10$ per group.
22. [5] Optimizing alloys $D = 13$.
23. [4] (Synthetic) Gaussian mixture function
24. [4] (Synthetic) Schwefel's 1.2 function.
25. [**?**] A list of optimiztation test functions can be found here.
26. [**?**] A more comprehensive list of general functions can be found here.

Enumeration

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Chapter 3

Benchmarking methods

3.1 Methods from

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And now to cite some more people **? ?**]

3.1.1 First subsection in the first section

. . . and some more

References

[1] Djolonga, J., Krause, A., and Cevher, V. (2013). High-Dimensional Gaussian Process Bandits.

[2] Gardner, J. R., Guo, C., Weinberger, K. Q., Garnett, R., and Grosse, R. (2017). Discovering and Exploiting Additive Structure for Bayesian Optimization.

[3] Garnett, R., Osborne, M. A., and Hennig, P. (2013). Active Learning of Linear Embeddings for Gaussian Processes.

[4] Li, C., Gupta, S., Rana, S., Nguyen, V., Venkatesh, S., and Shilton, A. (2018). High Dimensional Bayesian Optimization Using Dropout.

[5] Rana, S., Li, C., Gupta, S., Nguyen, V., and Venkatesh, S. (2017). High Dimensional Bayesian Optimization with Elastic Gaussian Process.

[6] Rolland, P., Scarlett, J., Bogunovic, I., and Cevher, V. (2018). High-Dimensional Bayesian Optimization via Additive Models with Overlapping Groups.

[7] Tripathy, R., Bilionis, I., and Gonzalez, M. (2016). Gaussian processes with built-in dimensionality reduction: Applications in high-dimensional uncertainty propagation.

[8] Wang, Z., Hutter, F., Zoghi, M., Matheson, D., and De Freitas, N. (2013). Bayesian Optimization in High Dimensions via Random Embeddings.

Appendix A

How to install LaTeX

Mac OS X

MacTeX - TeX distribution

1. Download the file from
   https://www.tug.org/mactex/
2. Extract and double click to run the installer. It does the entire configuration, sit back and relax.