

Bayesian Optimization for Hyperparameter Tuning in the Fully Connected Layers of VGG16

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Abstract

Optimization of neural network hyperparameters is a costly process usually pervaded by uncertainty. This report combines Bayesian optimization with Gaussian processes to find optimal hyperparameters for the VGG16 image classification network when training on the CIFAR10 dataset.

1 Introduction

Humans are slow and faulty. This means that work costs heaps of money and mistakes happen often. To help mitigate this, machine learning can learn the task at hand in order to optimize the performance at a much lower cost. While effective for many applications, machine learning has one glaring issue that requires skill and tonnes of computing power to overcome; hyperparameter optimization. Optimizing the hyperparameters usually devolves into random guessing, though new methods are on the rise like Bayesian optimization, which greatly reduces the effort involved in finding the parameters with use of an acquisition function and probabilistic model.

In this paper, Bayesian optimization with Gaussian processes as probabilistic model and expected improvement, upper confidence bound and probability of improvement as acquisition function will be used to find the hyperparameters of the VGG16 classifier network when training to classify on the 10 classes of the CIFAR10 dataset, optimizing for the validation accuracy.

2 Methods

Gaussian process and Bayesian optimization...

Three different acquisition functions + random...

Gaussian Process

Acquisition Functions

In the following section three different acquisition functions will be presented. All of these acquisition functions are implemented by using the GPyOpt library.

Probability of Improvement

Probability of improvement evaluates f , the objective function, at the point most likely to improve the minimum value. In this project, the objective function returns the negative validation accuracy. Probability of improvement then evaluates at the point most likely to obtain a higher accuracy, since the the function is given the negative accuracy. Mathematically PI can be expressed as,

$$PI(\mathbf{x}) = P(f(\mathbf{x}) \geq f(\mathbf{x}^+) + \xi) = \Phi\left(\frac{\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi}{\sigma(\mathbf{x})}\right)$$

where ξ is a hyperparameter which can be set by the user. The hyperparameter is a trade off between exploration and exploitation. Φ is the cumulative distribution function of the Gaussian distribution.

Expected Improvement

The expected improvement tries to quantify the improvement instead of the probability of improving as Probability of Improvement does. It is possible to quantify the average value of improvement if we sample the objective function at x . The acquisition function then computes the expected value of the improvement function at a certain x . Mathematically EI can be expressed as,

$$EI(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+)) \Phi(Z) + \sigma(\mathbf{x}) \phi(Z) & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) < 0 \end{cases}$$

Here the variable $Z = \frac{\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi}{\sigma(\mathbf{x})}$

Gaussian Process Upper Confidence Bound

The idea behind the GP-UCB is to directly use the mean and variance from the Gaussian distribution. These two parameters are used as the exploration / exploitation trade off. The function UCB (Upper Confidence Bound) can be formulated as the following,

$$UCB(x) = \mu(x) + \kappa \sigma(x)$$

Where κ is a user defined variable used to control the trade off between exploration and exploitation.

	Hidden units	Dropout probability	Activation function	Accuracy
EI	1300	0.3748	Sigmoid	0.664
MPI	3500	0.5982	Sigmoid	0.654
LCB	2900	0.5835	Sigmoid	0.651
GridSearch	2000	0.66	Sigmoid	0.653

3 Results

Comparison of aquisition functions and random...
 Results and plots...

4 Discussion

Which one is better...

5 References

<https://gpyopt.readthedocs.io/en/latest/index.html>