Expressive Priors for Gaussian Processes in Bayesian Optimization

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Introduction

Bayesian Optimization (BO) is a time effective method of automating accelerator tuning for LCLS because we sample as few points as possible to find input values that achieve a good optimum. A problem with this BO application is that its performance worsens exponentially in higher dimensions due to poor scaling. A good prior mean in Gaussian Processes (GPs) can help with scaling. Therefore, this study’s objective is to explore cheap and more expressive (non-constant) prior means for Gaussian Processes to optimize Bayesian Optimization for tuning the injector.

Objective Function

- We use BO during accelerator tuning to find input values to the injector that minimize \( \text{emittance} \times \text{bmag} \) (maximize \(-\text{emittance} \times \text{bmag}\)).
- The objective function employs a Neural Net (NN) surrogate model of the accelerator injector to prototype this optimization approach.

Implementing Custom Priors

- Using a NN model prior mean that includes prior information of the objective function, BO should be able to find better optima faster.
- The GP’s predictive mean fits through ground truth points and then returns to the prior mean in areas with no data samples.

Gaussian Processes

The GP and predictive mean function (blue line) are defined as:

\[ f(x) = \mathcal{GP}(m(x), k(x,x')) \]
\[ \mu = m(x') + K(x, X)^{-1}(y - m(X)) \]

where
\[ K = R + \sigma_n I \]

Neural Net Accuracies

Correlation with ground truth: 0.889

Model1

Correlation with ground truth: 0.547

Model2

Next Steps

- We will explore methods of improving BO performance during the fine-tuning stage.
- We will perform an experimental demonstration with the real accelerator.

Conclusions

- Our goal was to determine how accurate a model must be as a prior mean in order to get a performance gain in BO.
- Including prior information in the GP’s prior mean always leads to an improvement in BO performance during coarse tuning.
- During fine tuning, we need a more accurate model to give better BO performance.

References


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