Part 1 - A Useless Tutorial for using KG

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Plan

Overview

A presentation in multiple parts that:

1. Adds to our toolbox of acquisition functions: UCB, PI, EI (Expected Improvement) with another acronym
2. (potentially some theory) Sequential sampling policies with KG
3. Applications (covariance emulation)

Some references

1. A Tutorial on Bayesian Optimization (Frazier, 2018)
2. Maximizing Acquisition Functions for BO (Wilson et al., 2018)
3. BO for noisy experiments (Letham et al., 2019)

Bayesian Optimization

1. Derivative-free optimization method for black box functions $d^* \in \arg\max_d f(d, \xi)$ or (OUU variant): $d^* \in \arg\max_d \mathbb{E}(f(d, \xi))$
2. Two ingredients: Probabilistic surrogate model (99 % of times this is a GP):
3. Maximize an acquisition function quantifying the utility of a given design point:

A Vast and Unending Field

Impossible to enumerate everything that goes on here, some examples:

1. Plenty of exotic variants e.g. (Eriksson et al., 2020; Miller and Mak, 2024; Astudillo and Frazier, 2019; Brochu et al., 2011) and new findings e.g. (Hvarfner et al., 2024)
2. Plenty of software (some good, some beta)

   e.g. GPyTorch (https://github.com/cornellius-gp/gpytorch), BoTorch (https://botorch.org), vanilla BO (https://github.com/bayesian-optimization/BayesianOptimization)
3. To achieve fame and success - find your own acquisition function, write software to do domain-agnostic BO, tailor acquisition to very hard problems!

Plan

KG Definition

Why KG right now? We are interested in this acquisition for (potentially) selecting model subsets for pilot sampling / multifidelity estimation and thought this a good opportunity to explore the formulation.

KG Definition

Acquisition and Updates

Acquisition and updates

Comparisons with EI

Preview for Part II

References I

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References II

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Thank you!