

Bayesian Optimization Botorch

Wednesday, January 15, 2025 10:05 AM

<https://github.com/cornellius-gp/gpytorch/issues/1137>

Iteratively improve an overall GP regression quality by adding training points where are necessary #1137

<https://github.com/pytorch/botorch/discussions/2132>

<https://github.com/VlachosGroup/nextorch>

[https://chemrxiv.org/engage/api-](https://chemrxiv.org/engage/api-gateway/chemrxiv/assets/orp/resource/item/60c773d3842e65ea88db4b52/original/nex-torch-a-design-and-bayesian-optimization-toolkit-for-chemical-sciences-and-engineering.pdf)

[gateway/chemrxiv/assets/orp/resource/item/60c773d3842e65ea88db4b52/original/nex-torch-a-design-and-bayesian-optimization-toolkit-for-chemical-sciences-and-engineering.pdf](https://chemrxiv.org/engage/api-gateway/chemrxiv/assets/orp/resource/item/60c773d3842e65ea88db4b52/original/nex-torch-a-design-and-bayesian-optimization-toolkit-for-chemical-sciences-and-engineering.pdf)

Handling categorical variables in BO?

<https://github.com/pytorch/botorch/discussions/1450>

<https://medium.com/@whyamit404/a-practical-guide-to-sampling-from-a-categorical-distribution-in-pytorch-a03a638c9cdb>

<https://github.com/svedel/greattunes>

Easy-to-use Bayesian Optimization across continuous, categorical and integer variables (as well as any combination of variables) made available for either closed-loop or user-driven (manual) optimization of either known or unknown objective functions. Drawing on PyTorch (GPyTorch), BOTorch and with proprietary extensions.

<https://medium.com/henkel-data-and-analytics/bayesian-optimisation-on-mixed-domains-597ccd64e429>

<https://github.com/pytorch/botorch/issues/2398>

ModelListGP.fantasize does not support MultiTaskGP, but
other ModelListGP methods do #2398

<https://github.com/pytorch/botorch/issues/2138>

Acquisition function for a multitask multioutput GP

<https://github.com/pytorch/botorch/issues/2416>

https://github.com/wjmaddox/mtgp_sampler/blob/master/mtgp_experiments/constrained_mobo.py

<https://github.com/pytorch/botorch/issues/2138>

<https://github.com/pytorch/botorch/issues/325>