STAT GR6103: Applied Statistics III (Fall 2024)

Instructor: John Cunningham **Coordinates:** 903 School of Social Work, Tu/Th 10:10 – 11:25

TL;DR: PhD-level course on bayesian optimization, from the underlying gaussian processes to cutting-edge BO papers. Designed for statistics and machine learning students. In person attendance, required reading/writing/code, discussion, and a substantial course project.

Description:

Why and how can we use statistical modeling for optimization? Why: modern data sciences – machine learning, protein design, robotic control, and more – often require adaptation and experimentation over large, expensive, and/or black-box objective functions. How: bayesian optimization, which posits a model to reason about and carry out experimental design, has in the last four years seen a major shift in its capabilities and performance, and is now widely used throughout industry and academia.

This course will first cover the statistical roots of this literature, its connection to bayesian decision theory, and the required mechanics with gaussian processes, kernel methods, and optimization. Second, the course will study the fundamentals of adaptive experimentation and bayesian optimization. The third part of the course will cover very recent advances in the literature including trust region optimization, diverse optimization, latent space optimization, etc. Applications will include large scale machine learning systems, molecular design, and more.

The first two components of the course will center around the recent book Bayesian Optimization by Garnett, and current papers will fill out the remainder. Software will focus on BOTorch and related projects, and while the course does not expect any experience in BOTorch, some PyTorch familiarity is needed. Students interested in bayesian statistics, modern machine learning, and/or optimization will find this content relevant and challenging.

Requirements:

- In person attendance at (almost) every class
- Short reader reports and/or code implementations before each class
- Substantial final course project

References:

- Textbook: Roman Garnett, *Bayesian Optimization*, Cambridge, 2023. https://bayesoptbook.com/
- Software: Ax ax.dev and BOTorch botorch.org and GPyTorch gpytorch.ai
- Papers: linked in the outline below (subject to change!)

Prerequisites:

- PhD-level expertise in machine learning (roughly second year), such as at the level of GR6701.
- Facility with PyTorch at the level of https://pytorch.org/tutorials/beginner/introyt.html, up to roughly the "What is torch.nn really?" section. Another good resource is GR5245.

Outline:

- The table below contains a tentative topic/reading list; it is subject to change.

Date	Topic	Reading and/or Code
Sep 03 (Tu)	Logistics and intro to BO	Garnett Ch. 1 (no report due)
Sep 05 (Th)	Gaussian Processes (GP)	Garnett Ch. 2
Sep 10 (Tu)	GP kernels	Garnett Ch. 3
Sep 12 (Th)	GP model selection	Garnett Ch. 4 (ex. 4.6)
Sep 17 (Tu)	Cholesky and CG	Garnett Ch 9-9.1, TBD
Sep 19 (Th)	GPyTorch	Tutorials 0, 1
Sep 24 (Tu)	Bayesian Decision Theory	Garnett Ch. 5
Sep 26 (Th)	Utility, Exploration/Exploitation	Garnett Ch. 6 (7.7, 8.7)
Oct 01 (Tu)	Acquisition Functions	Garnett Ch. 7
Oct 03 (Th)	BO	Garnett Ch 8-8.9 (also Tutorial §1-4.3)
Oct 08 (Tu)	Scaling GP	BBMM and SVGP
Oct 10 (Th)	Ax and BOTorch	Basic Ax/BOTorch Tutorial
Oct 15 (Tu)	Accelerating BO	Inducing point BO
Oct 17 (Th)	Large Batch BO	MC acquisitions (also the paper)
Oct 22 (Tu)	Local BO	TuRBO
Oct 24 (Th)	Constrained BO	SCBO
Oct 29 (Tu)	Multi-objective BO	MORBO
Oct 31 (Th)	Diverse BO	ROBOT and DGEMO
Nov 05 (Tu)	No class	(election day holiday)
Nov 07 (Th)	Approximation aware BO	EULBO
Nov 12 (Tu)	discuss projects	due: project proposals
Nov 14 (Th)	High-dimensional BO	SAASBO (maybe also LOLBO)
Nov 19 (Tu)	Sparse BO	SEBO
Nov 21 (Th)	Mixed continuous/discrete	Probabilistic Reparam
Nov 26 (Tu)	Gray Box BO	Composite Objectives (plus refs therein)
Nov 28 (Th)	No class	(thanksgiving holiday)
Dec 03 (Tu)	Multifidelity BO	MFBO
Dec 05 (Th)	TBD (eg BO with derivatives)	TBD (eg COBALT)
Dec 10 (Tu)	No class	
Dec 12 (Th)	No class	due: final projects