Uncertainty Quantification for Machine Learning

Stat 991 (Spring 2022), U Penn, Wharton Department of Stats & Data Science

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Example of Emerging Course in Data Science,
Statistics Curriculum Retreat, SPH, U Michigan, May 2024

Context of Course

- Prediction/Generation accuracy of ML increasing
  - AlphaFold, GPT, skin cancer classification based on images, etc
- But, consequential failures
  - Tesla self-driving crash
  - Misleading/controversial/racist generations
  - …
- ML methods designed for **straightforward prediction**

Prediction and Uncertainty

- ML: Given x, predict y

	x	y
AlphaFold	Protein sequence	3D structure
GPT	Text prompt	Answer
Skin cancer	Skin image	Cancer type
Self-driving car	3D environment, location, ...	Control signal

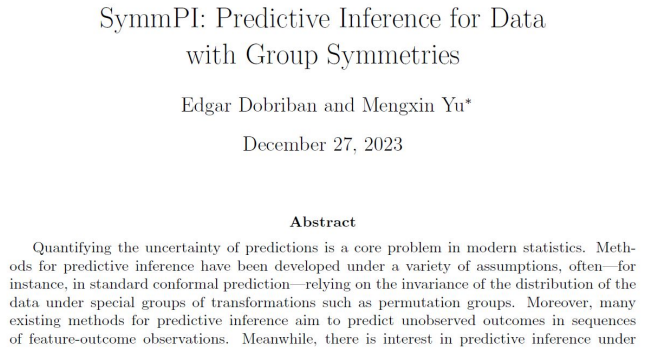
- Given x, the answer y is often **not uniquely determined**
  - GPT: given text prompt, ...?
  - Self-driving cars: given 3D environment, location, ...?
  - skin cancer classification: given skin image, ...?
- Standard ML pipeline (Empirical Risk Minimization) **does not provide a solution**

Goals/Aims of the UQ-ML Course

- **Audience**: Aimed at PhD students in year 2+, from all depts (Stats, Biostats, CS, EE, Applied Math …), open by permission to others (30 students)
- **Style**: First third by instructor, remaining student presentations
  - Based on previous good experiences with similar deep learning course
- Introduce **major approaches to handling uncertainty** that are currently popular in ML (and applicable to SotA DL methods)
  - Bayesian approaches (Bayesian NN, MC Dropout, …)
  - Conformal prediction
  - Calibration
- Understand their strengths and weaknesses
- Allow students to explore a topic of their choice through **90-min presentation**
- Identify **research directions** (Fast growing research areas!)

More on the UQ-ML Course

- **First course on this** broad set of topics anywhere?
  - Motivated by my own desire to learn
- "create an engaging, fun, but rigorous intellectual environment, where we will all learn and develop" — intense critical discussions
  - Some research topics identified
  - Problem **NOT** solved
- Most materials **available online** github.com/dobriban/Topics-In-Modern-Statistical-Learning
  - Some social media attention



SymmPI: Predictive Inference for Data with Group Symmetries

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Abstract

Quantifying the uncertainty of predictions is a core problem in modern statistics. Methods for predictive inference have been developed under a variety of assumptions, often—for instance, in standard conformal prediction—relying on the invariance of the distribution of the data under special groups of transformations such as permutation groups. Moreover, many existing methods for predictive inference aim to predict unobserved outcomes in sequences of feature-outcome observations. Meanwhile, there is interest in predictive inference under

Future of UQ-ML course

- Aim to offer it again (Spring ‘25?)
- Need to update it with **UQ for foundation models** (LLMs, diffusion models)
- Need to **polish materials** (lecture notes, Colab notebooks)
    - Equivalent materials for undergrad/Masters