examples

Active learning / Bayes Opt

- Given $D = \{x_i, f(x_i)\}_{i=1}^{N}$ propose x_{N+1}

  to solve $x_{N+1} = \max_{x} f(x)$

  Denote $f_N^M = \max_{i=1...N} f(x_i)$

- By building a GP surrogate, we model

  ~~$f(x) \sim N($~~

$$p(f(x) \mid D) = N(\mu^*, \Sigma^*)$$

- Define acquisition function to maximize

① (Easiest to interpret) Upper Confidence Bound (UCB)

$$a_{UCB}(x; \lambda) = \underbrace{\mu(x)}_{\text{exploitation}} + \lambda \underbrace{\sigma(x)}_{\text{exploration}}$$

② Expected improvement (EI)

Define improvement $u(x) = \max(f(x) - f_N^M, 0)$

$$a_{EI}(x) = \mathbb{E}[u(x) \mid D] = \int_{f_N^M}^{\infty} (f(x) - f_N^M)\, N(f)\, df$$

$$\mathbb{E}[u(x)|D] = \int_{f_N^m}^{\infty} (f(x) - f_N^m)\, N(f; \mu^*, \Sigma^*)\, df$$

Rewrite $\quad f(x) = \mu^* + \sigma^* z$

$z \sim N(0,1)$ $\qquad \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}$

$$z_0 = \frac{f(x_N^m) - \mu}{\sigma} \qquad = \int_{z_0}^{\infty} (\mu + \sigma z - \cancel{\ } f_N^m)\, \phi(z)\, dz$$

$$= (\mu - f_N^m) \underbrace{\int_{z_0}^{\infty} \phi(z)\, dz}_{1 - \text{CDF}} + \sigma \int_{z_0}^{\infty} z\, \phi(z)\, dz$$

$$= (\mu - f_N^m) \underbrace{\left[1 - \Phi_z(z_0)\right]}_{\Phi(-z_0)} + \frac{\sigma}{\sqrt{2\pi}} \int_{z_0}^{\infty} z e^{-\frac{z^2}{2}}\, dz$$

u substitution

$$= (\mu - f_N^m)\, \Phi(-z_0) + \frac{\sigma}{\sqrt{2\pi}} e^{-z_0^2}$$

$$= (\mu - f_N^m)\, \Phi\left(\frac{\mu - f_N^m}{\sigma}\right) + \sigma\, \phi\left(\frac{\mu - f_N^m}{\sigma}\right)$$

To encourage more exploration $\mu \Rightarrow \mu - \xi$

ex 2 Multifidelity

Assume access to $D_L = \{(x_i^L, y_i^L)\}_{i=1}^{N_L}$

$D_H = \{(x_i^H, y_i^H)\}_{i=1}^{N_H}$

$N_H << N_L$.

e.g. we can do many low quality experiments, a few good ones, but we assume a systemic bias between the two $\rightarrow f_H(x) = \rho f_L(x) + \delta$

$\uparrow$ indep of f_L

$$\Sigma = \begin{pmatrix} K_l(x_l, x_l') + \sigma_l^2 I & \rho K_l(x_l, x_h') \\ \rho K_l(x_h, x_l') & \rho^2 K_l(x_h, x_h') + K_h(x_h, x_h') + \sigma_h^2 I \end{pmatrix}$$

Break for Gaussian process code demo

Exam Coverage

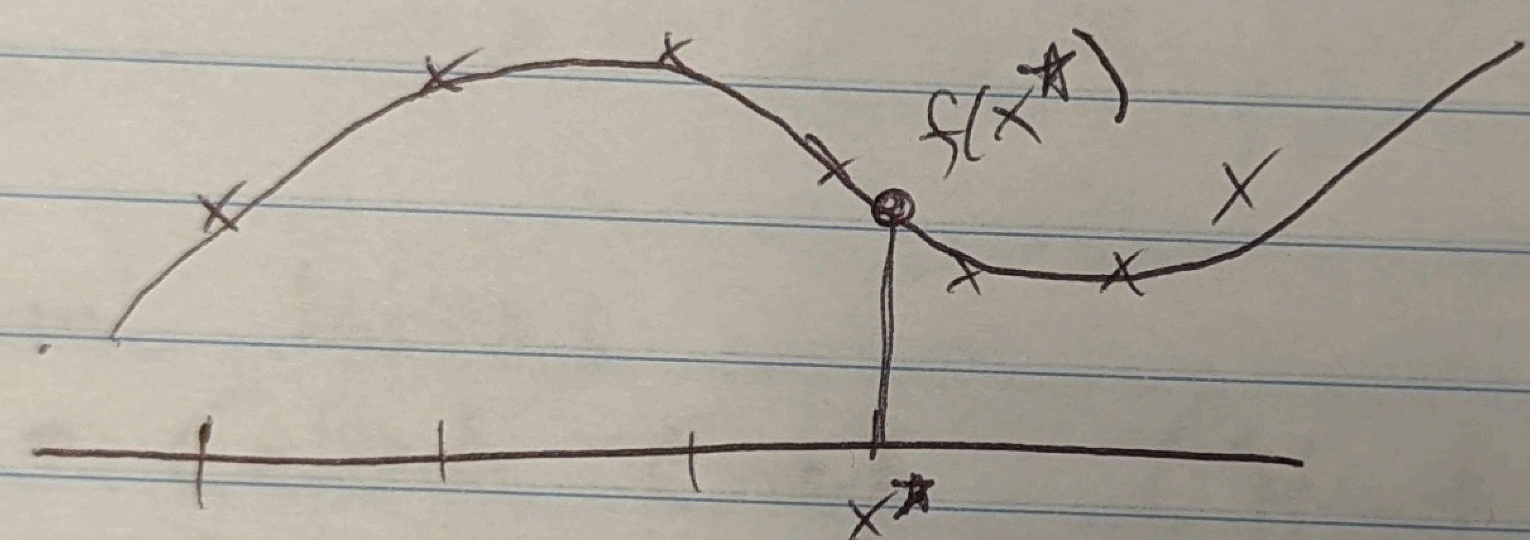
- Bring 1 page notes
- Simple true/false / multiple choice
- Some simple probability calculations
  → Be comfortable with
    - def of distributions
    - expectation, covariance
    - Chain rule
    - law of total prob
    - Gaussian tricks
    - Bayes Rule
- Regression → how to pull a linear system out of an MLE for polynomial fitting, Lagrange multipliers
- FEM → derive weak form
  → understand interpolant
  → how does approx compare to DNN
- VAE → Manipulations of ELBO
  → Understand reconstruction, KL
- Overall advice - go through notes, check that you can reproduce derivations

Operator learning

Previously studied regression

→ Given $x_1, \ldots x_N$
$f(x_1), \ldots f(x_N)$

For a new x^*, predict $f(x^*)$



Operator regression

Given <u>functions</u> $u_1(x), \ldots u_N(x)$

and observations of how an operator acts on those functions
$\mathcal{L}[u_1](x), \ldots \mathcal{L}[u_N](x)$

Given a new u^*, predict $\mathcal{L}[u^*](x)$

<u>ex1</u> infer dynamics $\frac{du}{dt} = \mathcal{L}[u]$

<u>ex2</u> PDE solver $\mathcal{L}[u](x) = \mathcal{F}^{-1} \circ f(x)$

3 techniques

- Fourier neural operators
- DeepONets
- Reduced order modeling ← note

not really opreg
but the classical
competitor

(slides for pictures)

FNO

Several Works
- Caltech Group (Stuart, Anandkumar)
- Ravi Patel
- Donghin Xiu

Def Fourier transform

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x) \exp(-i 2\pi \xi x)\, dx$$

Inverse transform

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi) \exp(i 2\pi \xi x)\, d\xi$$

Def Discrete Fourier series

$$f(x) = \sum_n c_n \exp\left(-i 2\pi \frac{nx}{P}\right) \qquad x \in \left[-\frac{P}{2}, \frac{P}{2}\right]$$

Differential Operators in Fourier space

$$\widehat{f'(\xi)} = \mathcal{F}\left[\frac{d}{dx} f(x)\right]$$

$$= \int_{-\infty}^{\infty} \frac{df}{dx} \exp(-2\pi i \xi x)\, dx$$

IBP

$$= -\int_{-\infty}^{\infty} f(x) \frac{d}{dx}\exp(-2\pi i \xi x)\, dx$$

$$= -\int_{-\infty}^{\infty} f(x) (-2\pi i \xi) \exp(-2\pi i \xi x)\, dx$$

uv

$\int u\,dv = -\int v\,du$

$$= (2\pi i \xi) \int_{-\infty}^{\infty} f(x) \exp(-2\pi i \xi x)\, dx$$

$$= (2\pi i \xi)\ \hat{f}(\xi)$$

☆ in Fourier space derivatives are multiplication!

Other nice parameterizations of
eigenvalues
convolutions

More generally $\widehat{\sum_n c_n \frac{d^\alpha}{dx^\alpha} f} = \underbrace{\sum_n c_n (i2\pi\xi)^n}_{\text{Symbol of differential operator}} \hat{f}$

Architecture

$$\mathcal{L} = \underset{\text{Inverse FFT}}{\boxed{\Pi^{-1}}} \leftarrow \underset{\text{symbol}}{\overset{\overset{k}{\downarrow}}{\boxed{g_\theta(k)}}} \leftarrow \underset{\text{FFT}}{\boxed{\Pi}} \leftarrow \underset{\text{nonlinearity}}{\boxed{h_\theta}} \leftarrow u(x)$$

Architecture

$$\mathcal{L} = \underset{\text{Inverse FFT}}{\boxed{\Pi^{-1}}} \leftarrow \underset{\text{symbol}}{\boxed{g_\xi(k)}} \leftarrow \underset{\text{FFT}}{\boxed{\Pi}} \leftarrow \underset{\text{nonlinearity}}{\boxed{h_\xi}} \leftarrow u(x)$$

k