

Lecture 9

Course overview

Bayesian optimization

OH 1:30-2:25

This Wed
only

Overview

- EDF $\hat{F}$ and consistency of means
- MC integration $\leftarrow$ Application
- How to sample
 - F^{-1}
 - importance s.
 - rejection s.
- $\rightarrow$ • Bootstrap $\leftarrow \text{Var}(\hat{\theta}) \approx ?$
- Imputation (fill missing data)
- MCMC (Markov chain MC)

"Bayesian" Optimization

Bayesian Estimation ← Sampling

Active Learning

$$\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \dots\} \quad |\mathcal{D}| = n \leftarrow \text{standard}$$

1. start with $\mathcal{D}_0$, $|\mathcal{D}_0| = n_0$, learn model $\hat{f}$ from $\mathcal{D}_0$ (train) (Active learning)

a. for $i = n_0 + 1, \dots$

sample $x_i \sim P_{\text{active}}(\mathcal{D})$

get y_i

$\mathcal{D} \leftarrow \mathcal{D} \cup \{(x_i, y_i)\}$

update model f (a predictor)

Bayesian Opt.

Pb

Wanted

$$x^* = \underset{x}{\operatorname{argmax}} f(x) \quad \leftarrow \text{unknown}$$

promising local optimum



next x_i

Ex: cost of industrial process f = efficiency
 x = process parameters

• new battery efficient, environmental, cheap = f
 x = materials, technology

Alg 1 (greedy)

for $i = \text{not} + 1, \dots$ ^{estimated}

$$x_i = \underset{x}{\operatorname{argmax}} f(x)$$

$$\text{get } y_i = \underbrace{f(x_i)}_{\text{true}} + \text{noise}$$

re-estimate (update) $\hat{f}$

Alg 2 Naive sampling

for $i = \text{not} + 1, \dots$

$$x_i \sim g(x)$$

$$g(x) \propto \hat{f}(x)$$

$$\text{get } y_i = \underbrace{f(x_i)}_{\text{true}} + \text{noise}$$

re-estimate (update) $\hat{f}$

Alg 3 B.O

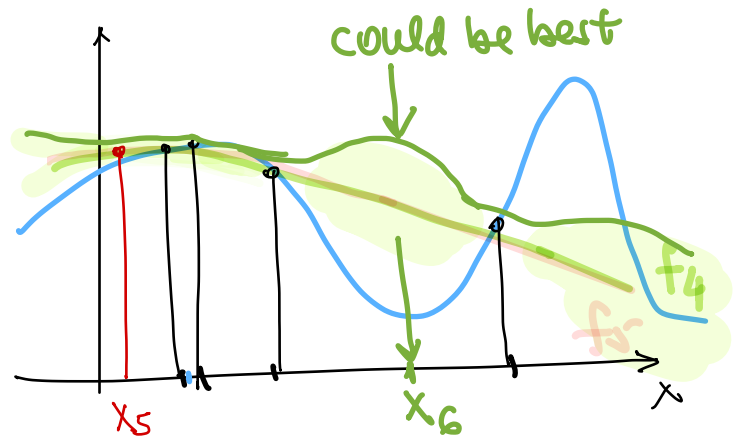
$\dots$

$$x_i \sim g_{\text{BO}}(x)$$

$$g_{\text{BO}}(x) \propto \hat{f}(x) + \hat{\sigma}(x) \cdot c$$

get y_i

update $\hat{f}$, $\hat{\sigma}(x) = \text{uncertainty}$
 $\hat{\sigma}(x) = \sqrt{\hat{\text{Var}} \hat{f}(x)}$



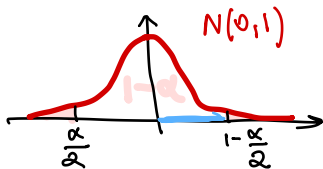
~~Example: Variance of the Median~~

Bootstrap = resampling method

estimates $\rightarrow$ $\widehat{\text{Var}} \hat{\theta}$
param of interest

Assume $\hat{\theta} \sim N(\theta, \widehat{\text{Var}} \hat{\theta})$

Want $1-\alpha$ CI for $\hat{\theta}$



Bootstrap
 $\text{CI for } \theta: [\hat{\theta} \pm z_{1-\alpha/2} \sqrt{\widehat{\text{Var}} \hat{\theta}}]$

$1-\alpha$ = confidence level (e.g. 95%)