Sequential Decision-Making under Uncertainty (Active Learning, Bayesian Optimization, Bandits)

Piyush Rai

Topics in Probabilistic Modeling and Inference (CS698X)

April 15, 2019

Outline for today

- An overview of three problems
  - Bayesian Active Learning
  - Bayesian Optimization
  - Multi-armed Bandits and Contextual Bandits
- All of these can be framed as sequential decision-making problems
- Leveraging uncertainty is the key in all these problems!

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- How to identify the hardest inputs?
- Estimate of uncertainty in f helps in that (and Bayesian methods provide that naturally)

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- Some popular (Bayesian) ways to identify the most useful (hardest) inputs $\boldsymbol{x}$

†Bayesian Active Learning for Classification and Preference Learning (Houlsby et al,2011), †Deep Bayesian Active Learning with Image Data (Gal et al, 2017)

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- Some popular (Bayesian) ways to identify the most useful (hardest) inputs $\boldsymbol{x}$
  - Inputs $\boldsymbol{x}$ whose posterior predictive distribution has the largest uncertainty/entropy

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- Bayesian Active Learning[‡] shown to be very successful for many deep learning models that require lots of labeled data when learned "passively"

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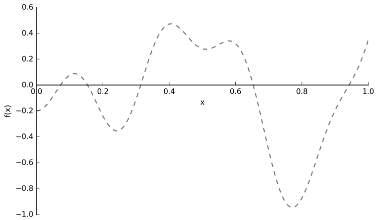
Bayesian Optimization

Bayesian Optimization: The Basic Formulation

- Consider finding the optima x_* (say minima) of a function $f(x)$



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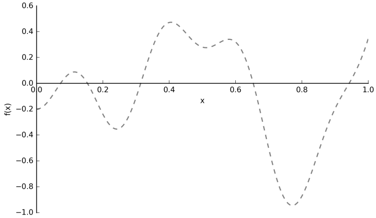

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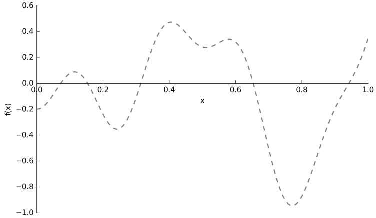

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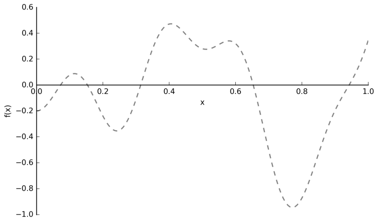
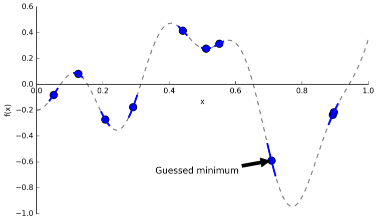


- Caveat: We don't know the form of the function; can't get its gradient,Hessian, etc
- Suppose we can only query the function's values at certain points (i.e., only black-box access)
- Several applications, such as drug design, hyperparameter optimization, etc.

Bayesian Optimization

- We would like to locate the minima using the queries we made



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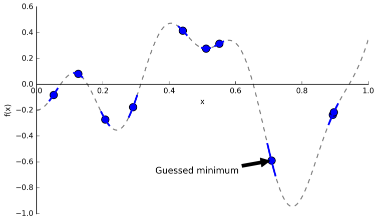

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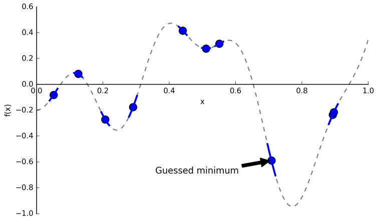

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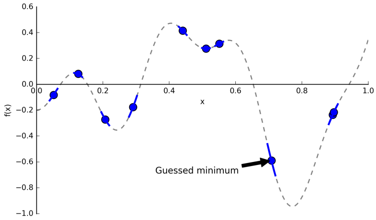

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- Reason: Each query may be costly
- The cost may be time, money, or both

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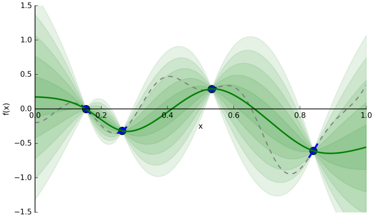

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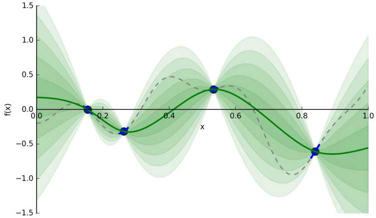

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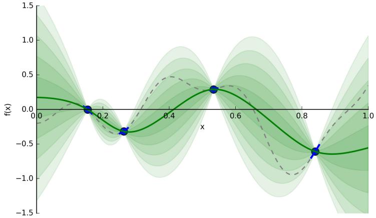

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- Somewhat similar to Active Learning but BO also uses past queries to decide where to query next

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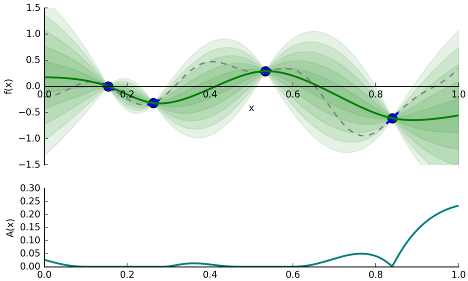

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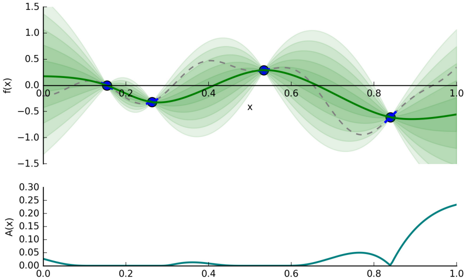

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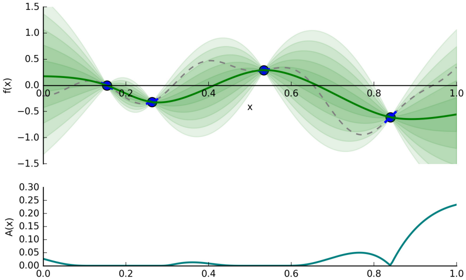

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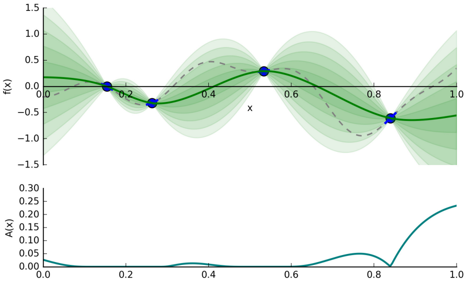

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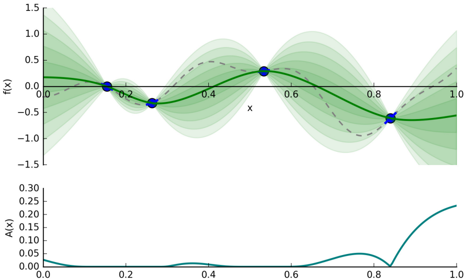

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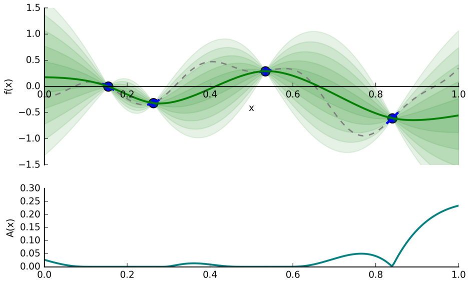

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- Important: The regression model must also have estimate of function's uncertainty, e.g.,
  - Gaussian Process, Bayesian Neural Network, or any nonlinear regression model with uncertainty

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- Note that BO involves optimizating the acquisition function to find the next query point x (this optimization to be cheaper than the original problem)

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  - Prefer points with low predictive mean (exploitation) and large predictive variance (exploration)

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- Used when the regression model is a Gaussian Process (GP)
- Assuming the posterior predictive for a new point x to be $\mathcal{N}(\mu(x), \sigma^2(x))$, the LCB is

$$A_{LCB}(x) = \mu(x) - \kappa\sigma(x)$$

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Bayesian Optimization: Further Resources

- Some survey papers:
  - A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning (Brochu *et al.*, 2010)
  - Taking the Human Out of the Loop: A Review of Bayesian Optimization (Shahriari *et al.*, 2015)
- Some open source software libraries

Software	Regr. Model	Acq. Function
Spearmint	Gaussian Process	Exp. Improv
MOE	Gaussian Process	Exp. Improv
Hyperopt	Tree Parzen Est.	Exp. Improv
SMAC	Random Forest	Exp. Improv

- Another one: SIGOPT (`https://sigopt.com/research`)

Multi-armed Bandits and Contextual Bandits

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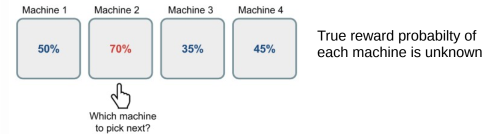

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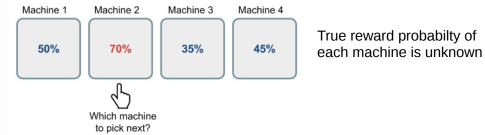

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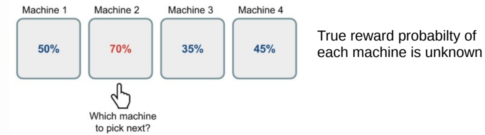

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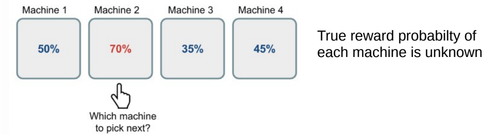

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- The problem setting called "Bandit" since we only get to know the reward for the chosen arm (don't get to know the rewards we would have got upon choosing other arms)

Multi-armed Bandits: Exploration vs Exploitation

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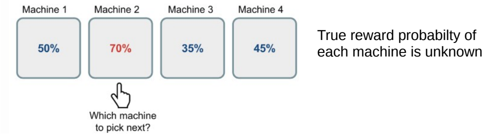

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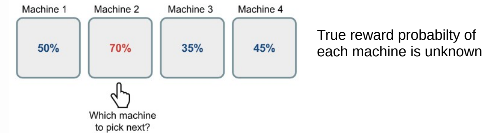

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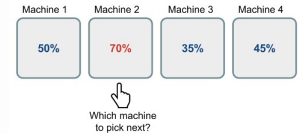

True reward probabilty of each machine is unknown

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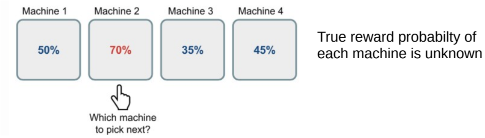

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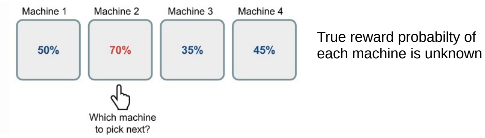

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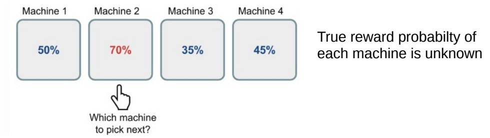

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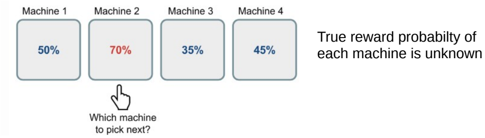

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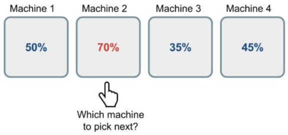

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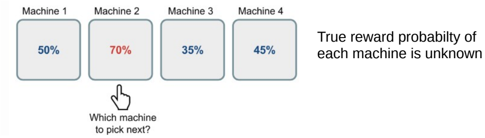

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- Just like the MAB case, performance is measured in terms of regret. For linear model

$$R(T) = \sum_{t=1}^{T} (\theta^\top \boldsymbol{x}_t^* - \theta^\top \boldsymbol{x}_t) \qquad (\text{assuming } f \text{ is linear model})$$

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- For selecting the next context, can use exploitation or exploitation+exploration as in MAB

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[†] Thompson Sampling for Contextual Bandits with Linear Payoffs (Agrawal and Goyal, 2013), Deep Bayesian Bandits Showdown: An Empirical Comparison of Bayesian Deep Networks for Thompson Sampling (Riquelme et al, 2018)

Contextual Bandits (Contd.)

- The goal is to learn the underlying reward function f to minimize the regret
- Assuming a linear model, i.e., $r_t = \theta^\top \boldsymbol{x}_t + \epsilon_t$, estimating θ is like solving linear regression
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- For selecting the next context, can use exploitation or exploitation+exploration as in MAB
  - Greedy, ϵ-Greedy, UCB, Thompson Sampling[†], etc
  - For exploration, we need an estimate of the uncertainty in f (e.g., using f's posterior, or some other uncertainty estimate)

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Thompson Sampling for Contextual Bandits

- Assume a linear model, i.e., $r_t = \theta^\top \boldsymbol{x}_t + \epsilon_t$ with $\epsilon_t \sim \mathcal{N}(0, \beta^{-1})$

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- Assume a linear model, i.e., $r_t = \theta^\top \boldsymbol{x}_t + \epsilon_t$ with $\epsilon_t \sim \mathcal{N}(0, \beta^{-1})$
- Assuming Gaussian prior $p(\theta) = \mathcal{N}(0, \mathbf{I})$, the posterior over θ (assuming hyperparams known)

$$p(\theta | \{\boldsymbol{x}_t, r_t\}_{t=1}^T) = \mathcal{N}(\mu_T, \Sigma_T)$$

where μ_T and Σ_T are the mean and covariance of the Gaussian posterior

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Example	Context	Action	Reward	
News site	User location	an article to display	1 if clicked, 0 otherwise	makes sense even w/o context $\Rightarrow$ bandits or contextual bandits
Dynamic pricing	Buyer's profile	a price p	p if sale, 0 otherwise	
Health advice	User health profile	what to recommend	1 if adopted, 0 otherwise	Context is essential $\Rightarrow$ contextual bandits
Chatbot	Stage of conversation	what to say	1 if task completed, 0 otherwise	Context is essential, depends on the past actions $\Rightarrow$ reinforcement learning

(Table credit: Alekh Agarwal)