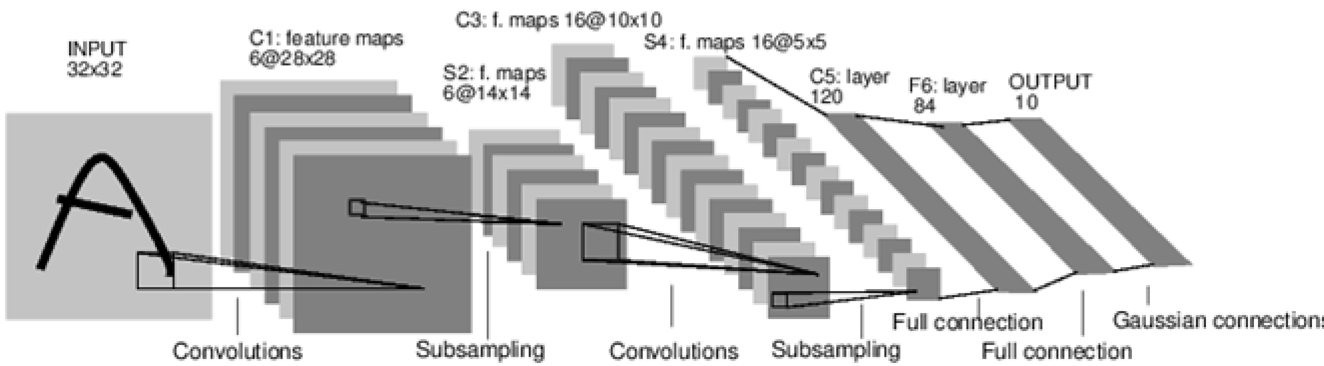
Bayesian Optimization

Brian Trippe & Paweł Budzianowski, MLG, 2016

Example - Picking Hyperparameters

Designing Deep Neural Networks



A Full Convolutional Neural Network (LeNet)

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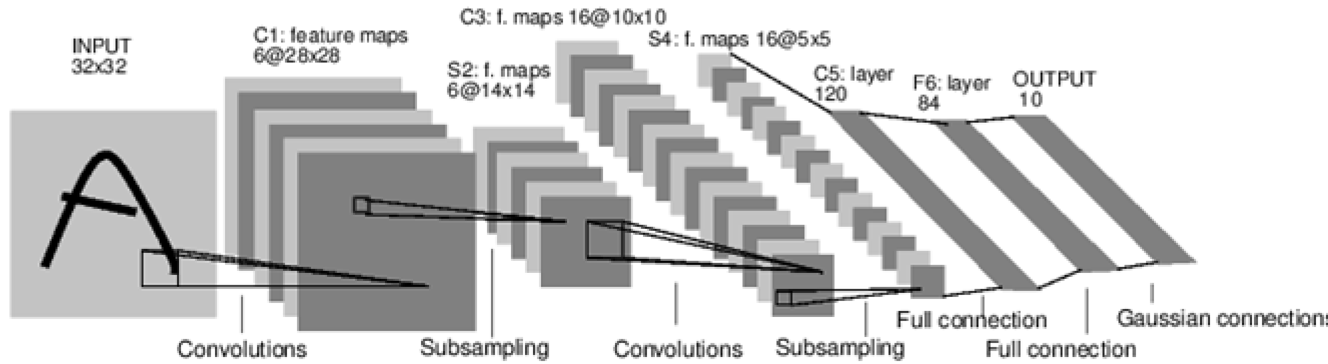


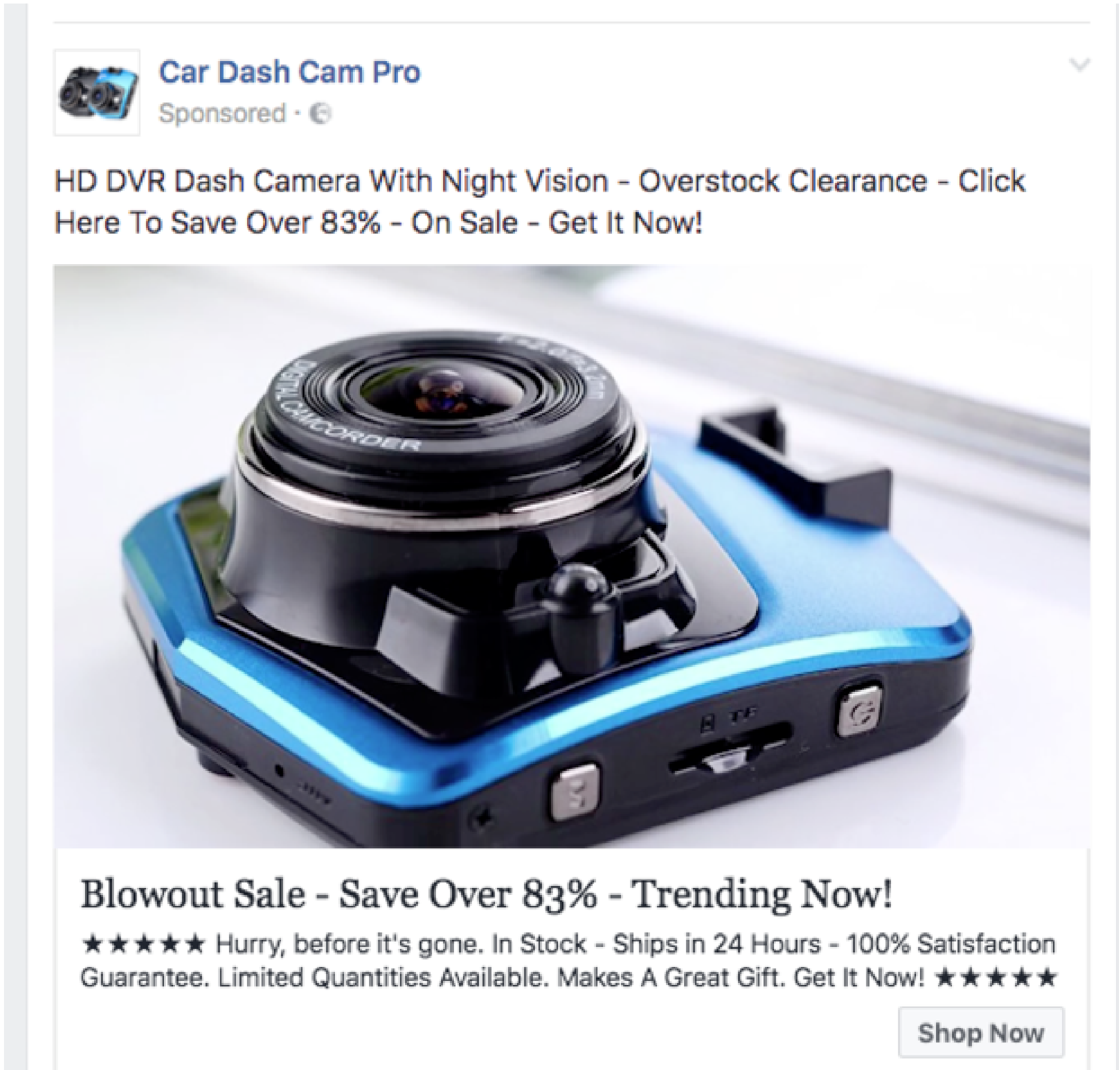
A Full Convolutional Neural Network (LeNet)

Validation accuracy is a function of hyperparamters

- learning rate, regularizations
- batch size, number/size of layers, convolution sizes
- Nonlinearity, Loss function

Example - A/B Testing

Tuning features of an Advertisement



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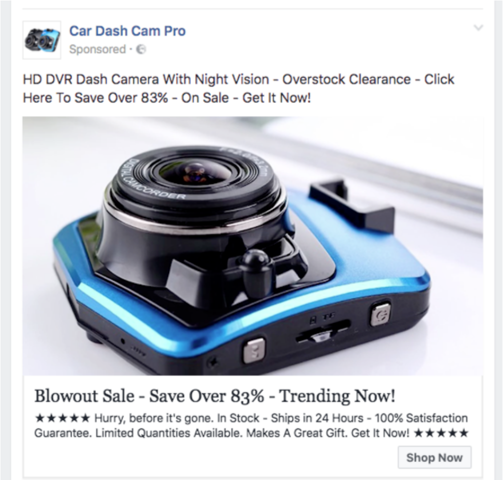
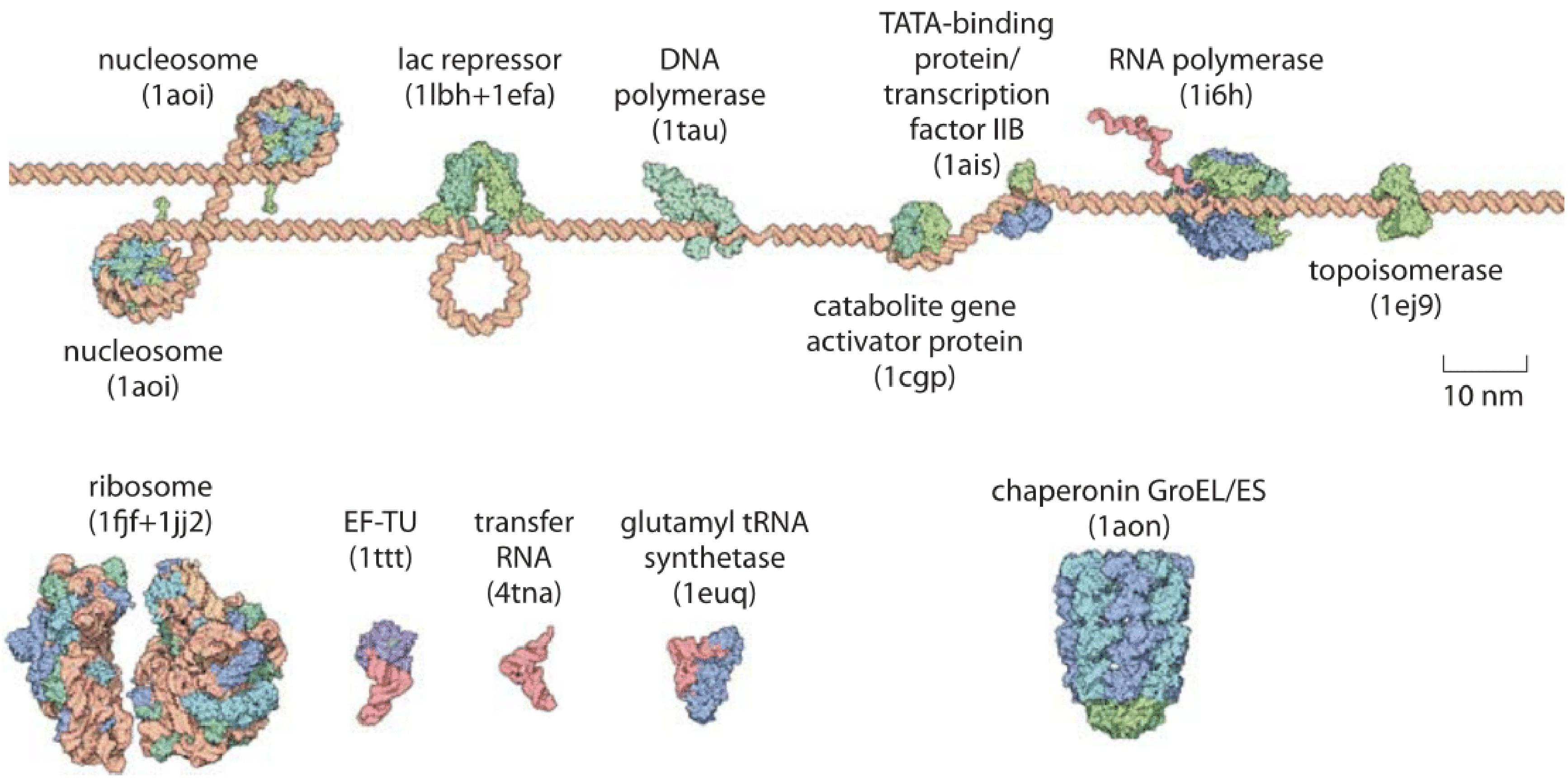


Click rates are a function of Advertiser's choices.

- Target Consumer Demographics and Interests
- Characteristics of what is displayed

Example - Gene design

Choosing Regulatory Sequences for Genetic Engineering



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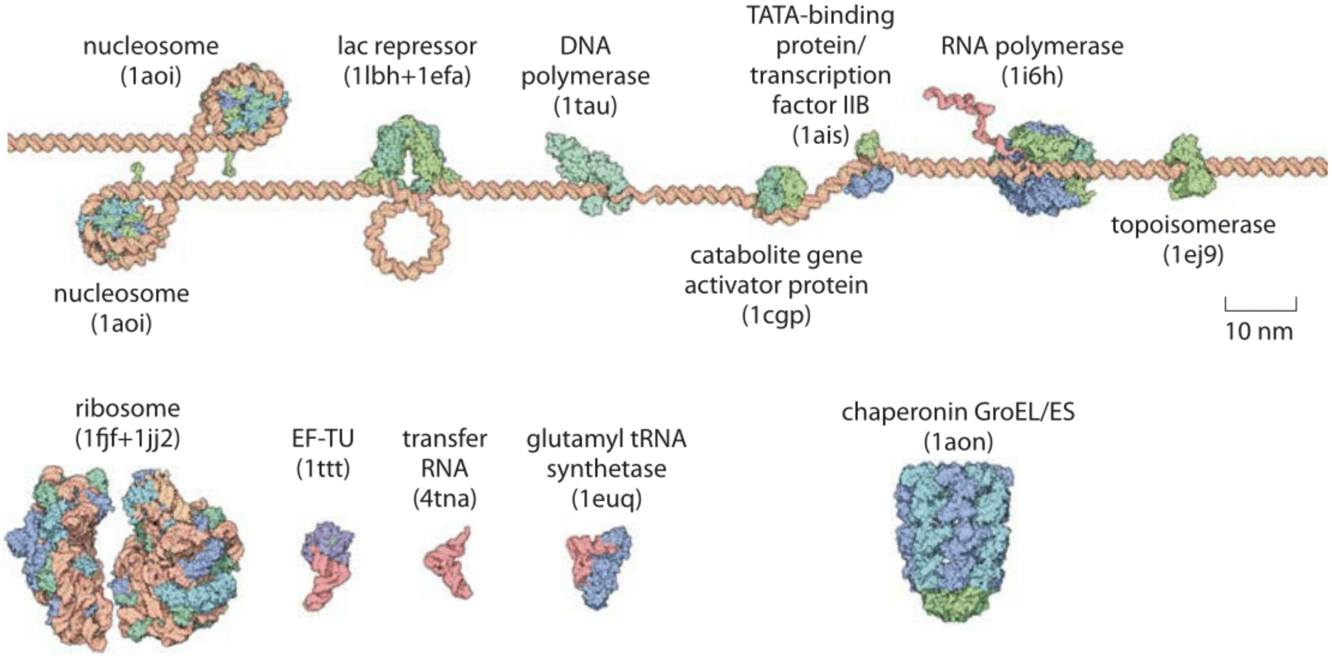


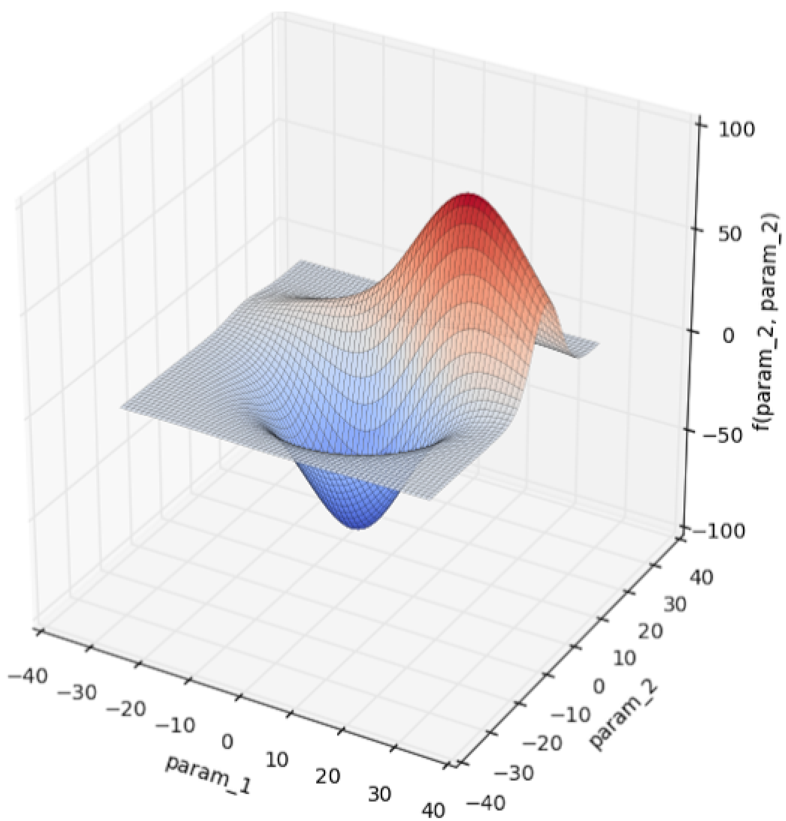
Transcription rate is a function of DNA sequence

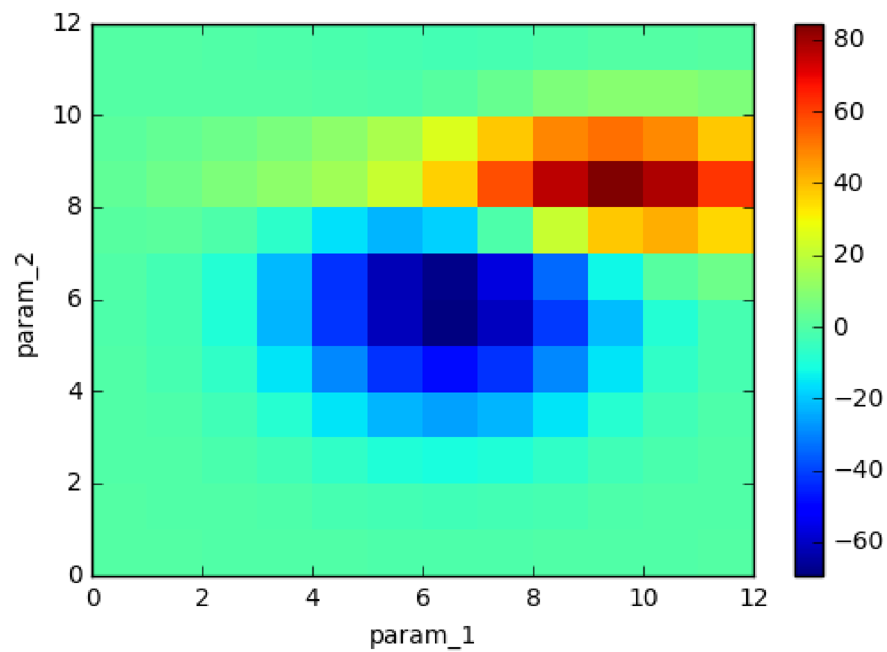
- regulatory motifs
- stability signals

González, Javier, et al. "Bayesian optimization for synthetic gene design." arXiv preprint arXiv:1505.01627 (2015).

How do we perform optimization?

We can use grid-search





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- What if we are in a high dimensional space?
  - The number of grid points will increase exponentially with the number of dimensions, $O(c^n)$
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- What if there is noise?

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By being Bayesian!

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By being Bayesian!

- Propose p(f)
- We can work with uncertainty and noise
- Make smarter choices about next points to query
- Use information from other problems to inform priors
- Hopefully, we get a good idea of the space with far less than an exponential number of points

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Assume that f is a **black-box** function - we can query it at any point but its derivatives are unavailable.

General algorithm

General algorithm

Algorithm 1 Bayesian optimization

Input: a black-box function f

1: **for** $n = 1, \ldots, N$ **do**

2: select $\mathbf{x}_n = \arg\max_{\mathbf{x} \in \mathcal{X}} \alpha_{n-1}(\mathbf{x})$

3: query f at $\mathbf{x}_n$ to obtain y_n

4: augment data $\mathcal{D}_n = \mathcal{D}_{n-1} \cup \{(\mathbf{x}_n, y_n)\}$

return $\widetilde{\mathbf{x}}_N = \arg\max_{\mathbf{x} \in \mathcal{X}} \mu_N(\mathbf{x})$

Two ingredients

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1. Probabilistic framework

$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f)p(f)}{p(\mathcal{D})}$$

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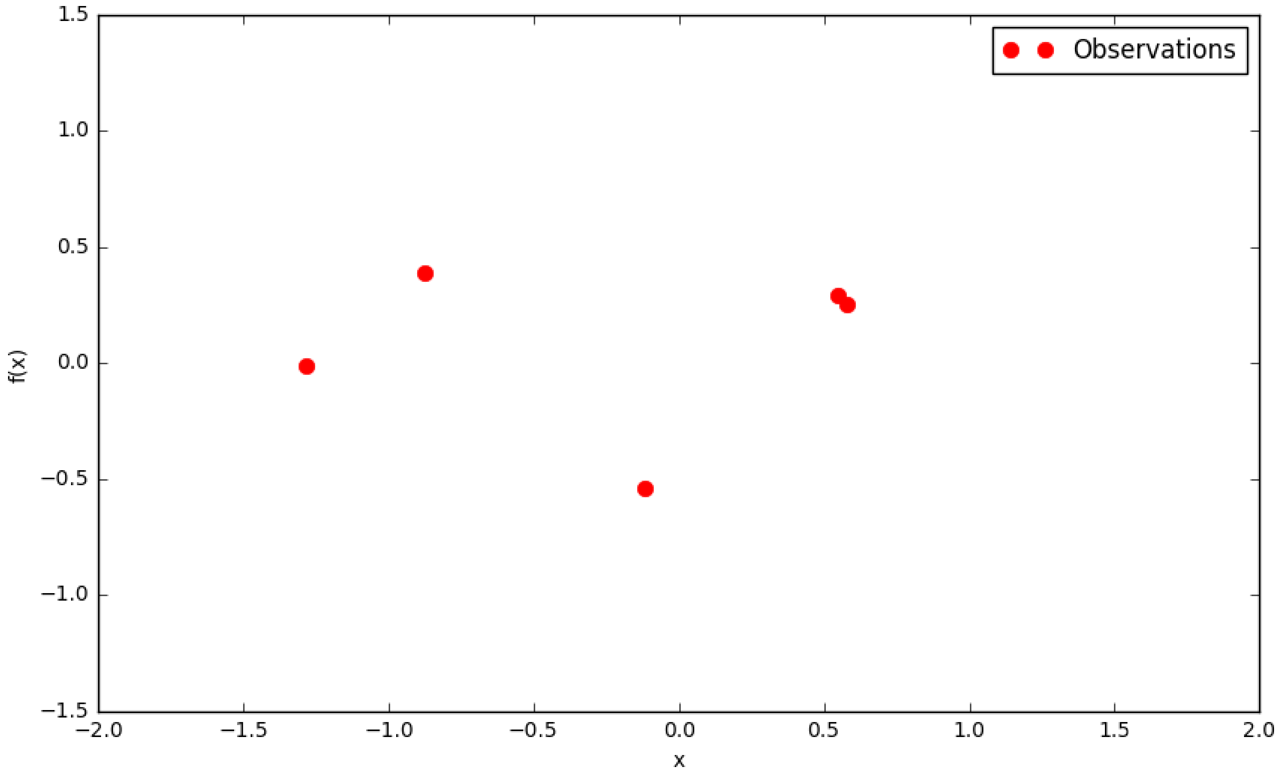
2. Acquisition function

$$U : \mathbb{R}^d \times \mathbb{R} \mapsto \mathbb{R}$$

$$\alpha(\mathbf{x};\ \mathcal{D}_n) = \mathbb{E}_{f(\mathbf{x})|\mathbf{x}}[U(\mathbf{x}, f(\mathbf{x}))]$$

A Concrete Example



- How do we pick the next point?
- We need a prior over functions

Gaussian Processes

The Gausian process provides a distribution over functions, $f : \mathbb{X} \to \mathbb{R}$

$$f \sim GP(\mu_0, k)$$

for $\mathbf{x} := (x_1, x_2, ..., x_n)$, $\mathbf{f} = (f(x_1), f(x_2), ..., f(x_n))$

$$\mathbf{f}|\mathbf{x} \sim \mathcal{N}(\mathbf{m}, \mathbf{K})$$

where $m_i = \mu_0(x_i)$ and $K_{i,j} = k(x_i, x_j)$

Often we have noisy observations $\mathbf{y} := (y_1, y_2, ..., y_n)$

$$y|f, \sigma^2 \sim \mathcal{N}(f, \sigma^2\mathbf{I})$$

Gaussian Processes

The posterior predictive distribution at an unseen point, x_{n+1} is Gaussian.

$$y_{n+1} \sim \mathcal{N}(\mu_n(x_{n+1}), \sigma_n(x_{n+1})^2)$$

The predictive mean and variances have a closed form.

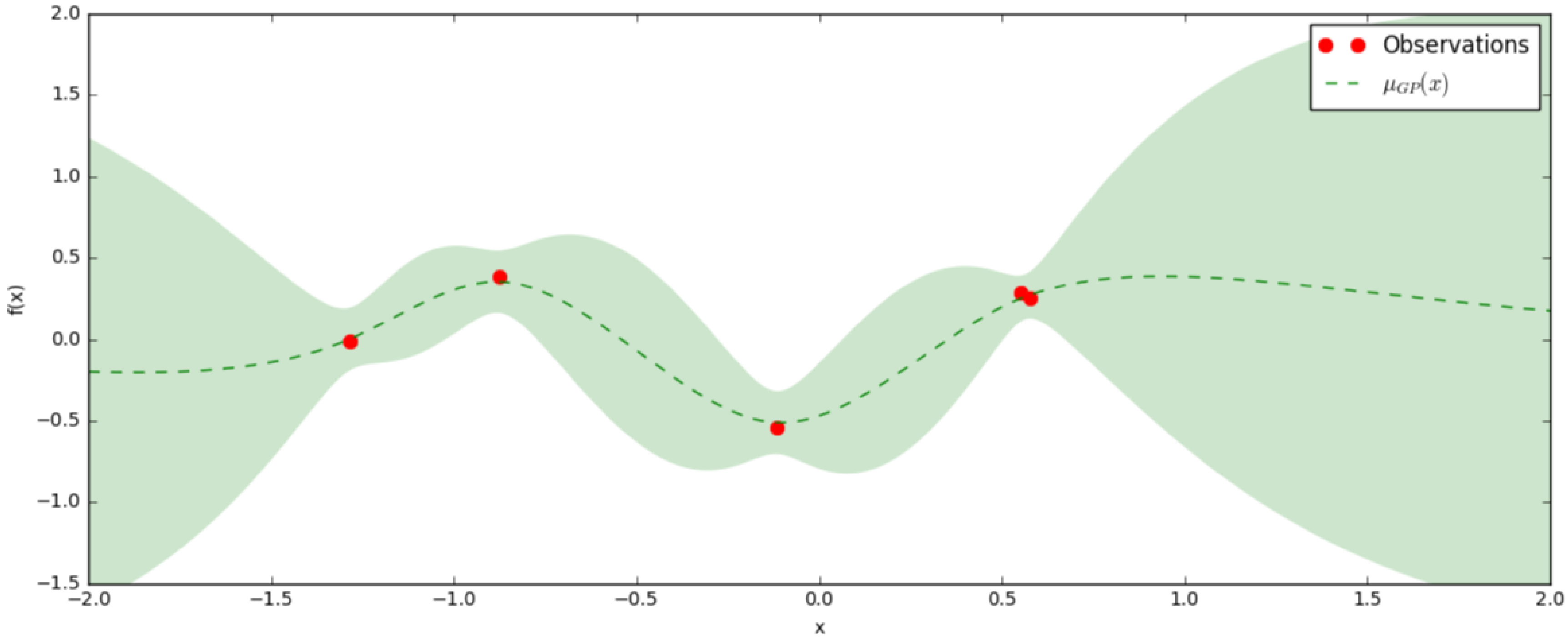
$$\mu_n(x_{n+1}) = \mu_o(x_{n+1}) + k(x_{n+1})^T(K + \sigma^2 I)^{-1}(\mathbf{y} - \mathbf{m})$$

$$\sigma_n^2(x_{n+1}) = k(x_{n+1}, x_{n+1}) - \mathbf{k}(x_{n+1})^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{k}(x_{n+1})$$

where $\mathbf{k}(x_{n+1})$ is a vector of covariance terms with other observations.

Gaussian Processes

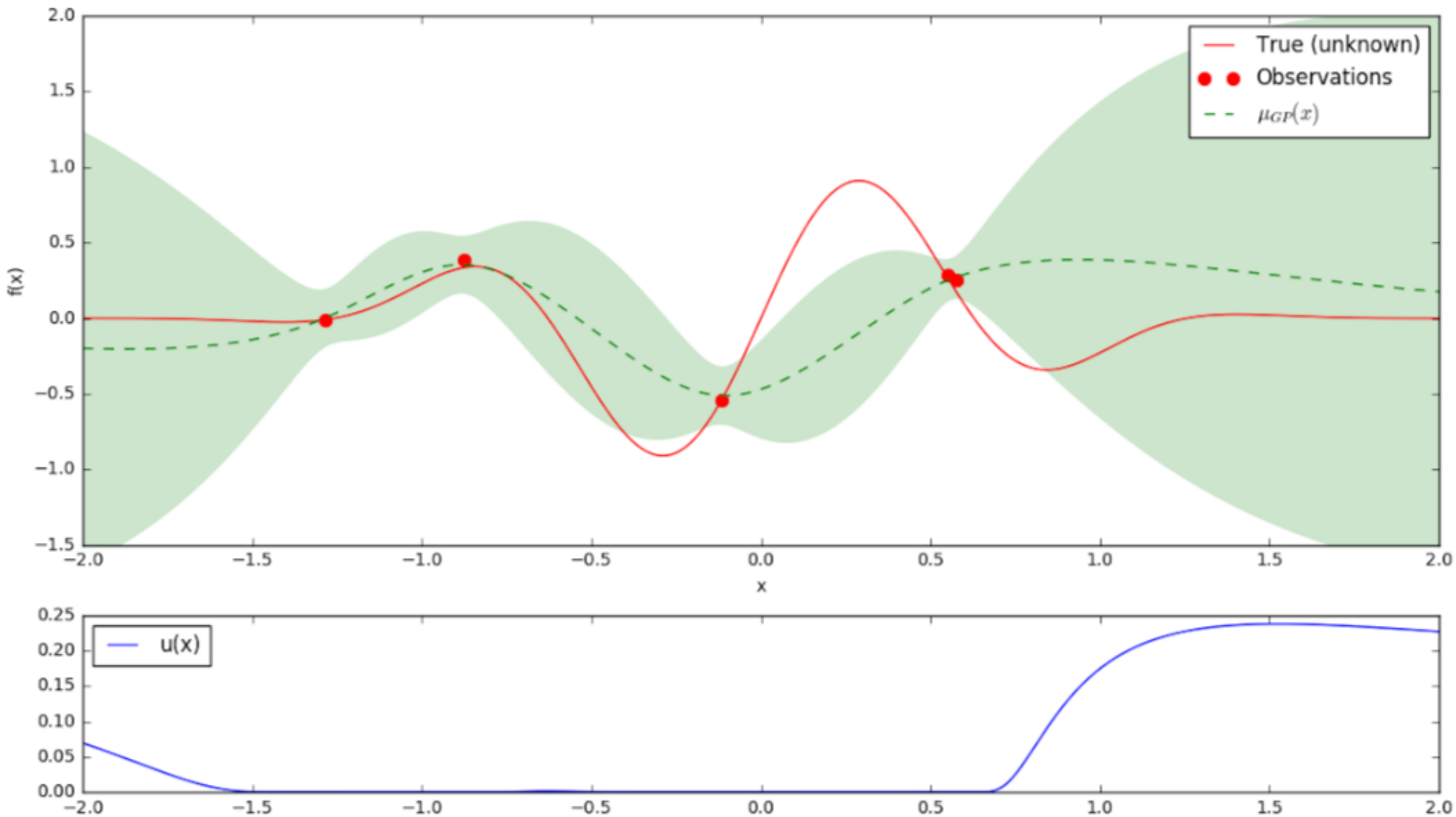
We fit a Gaussian process, picking hyperparameters by maximizing marginal likelihood.



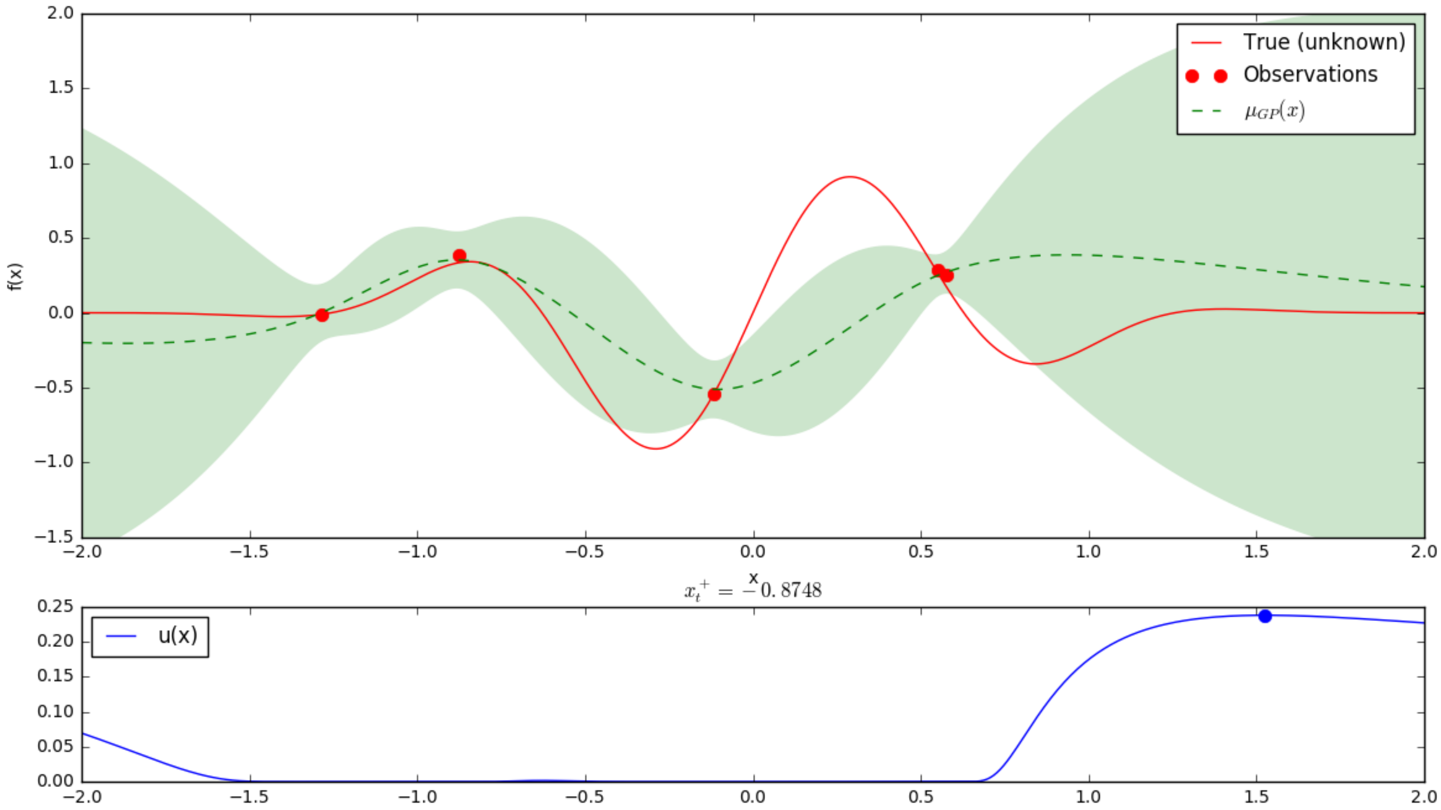
Acquisition Functions

Probability of Improvement

$$\alpha_{PI}(x;\mathcal{D}_n) = p(f_n(x) > y^*) = \Phi(\frac{\mu_n(x)-y^*}{\sigma_n(x)})$$



Bayesian Optimization in Action



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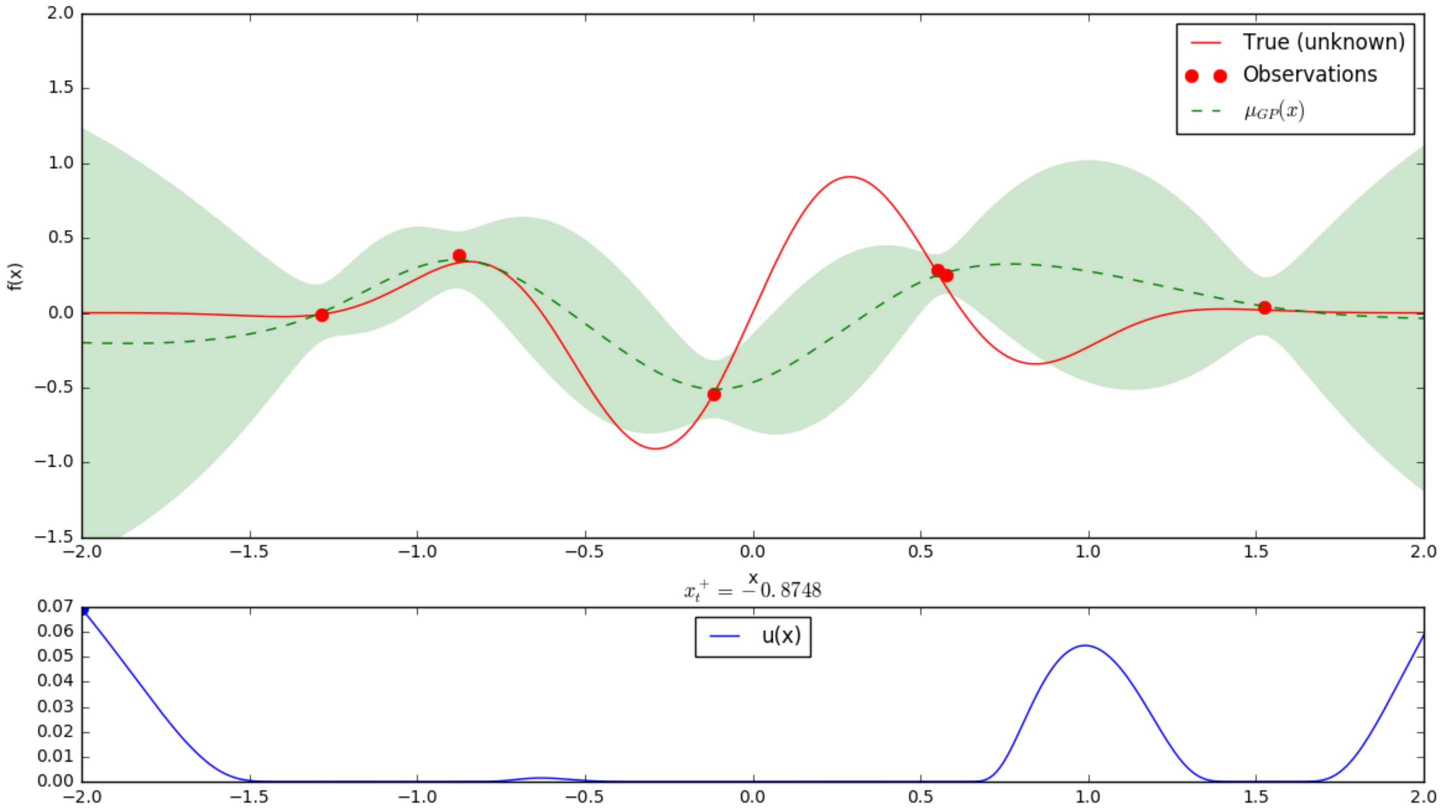

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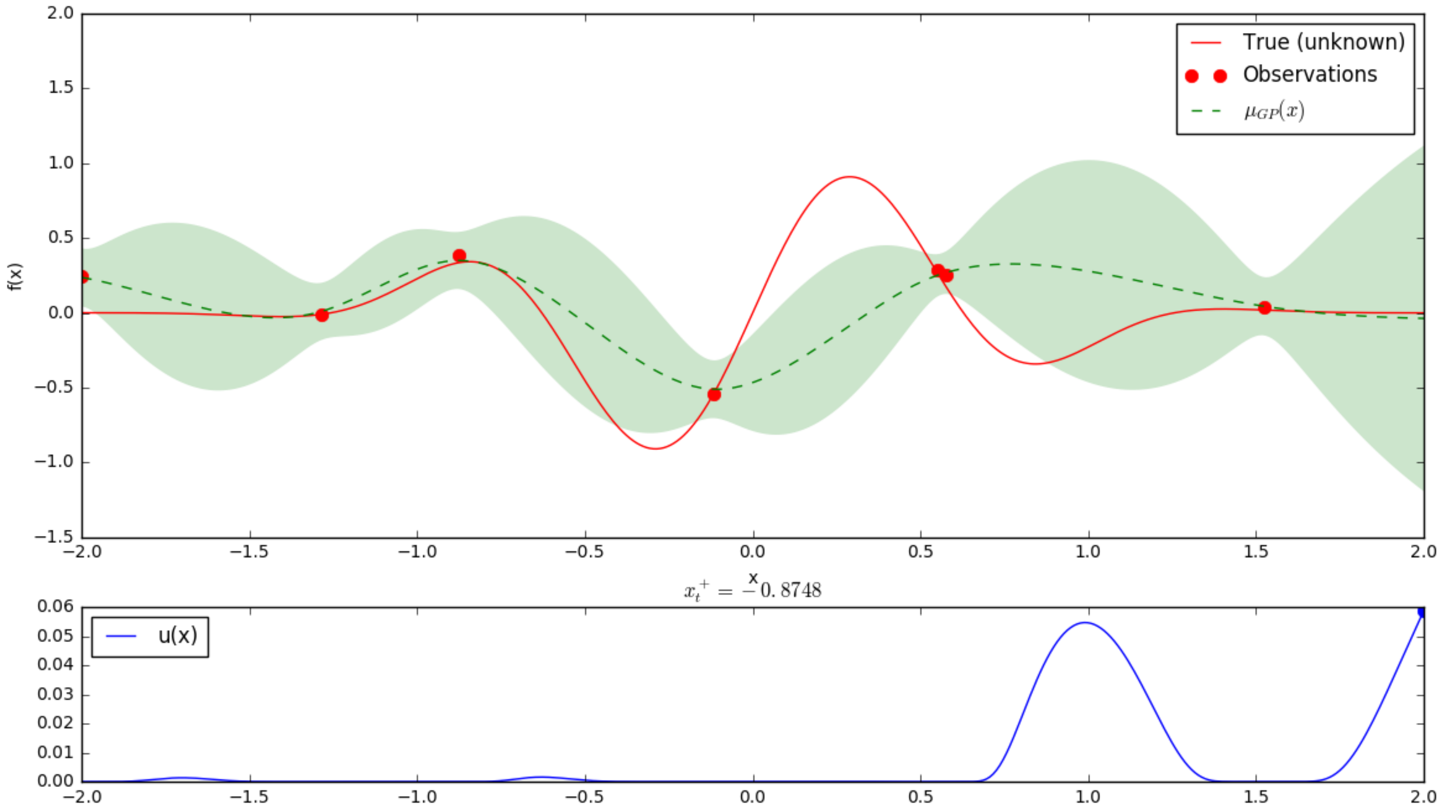

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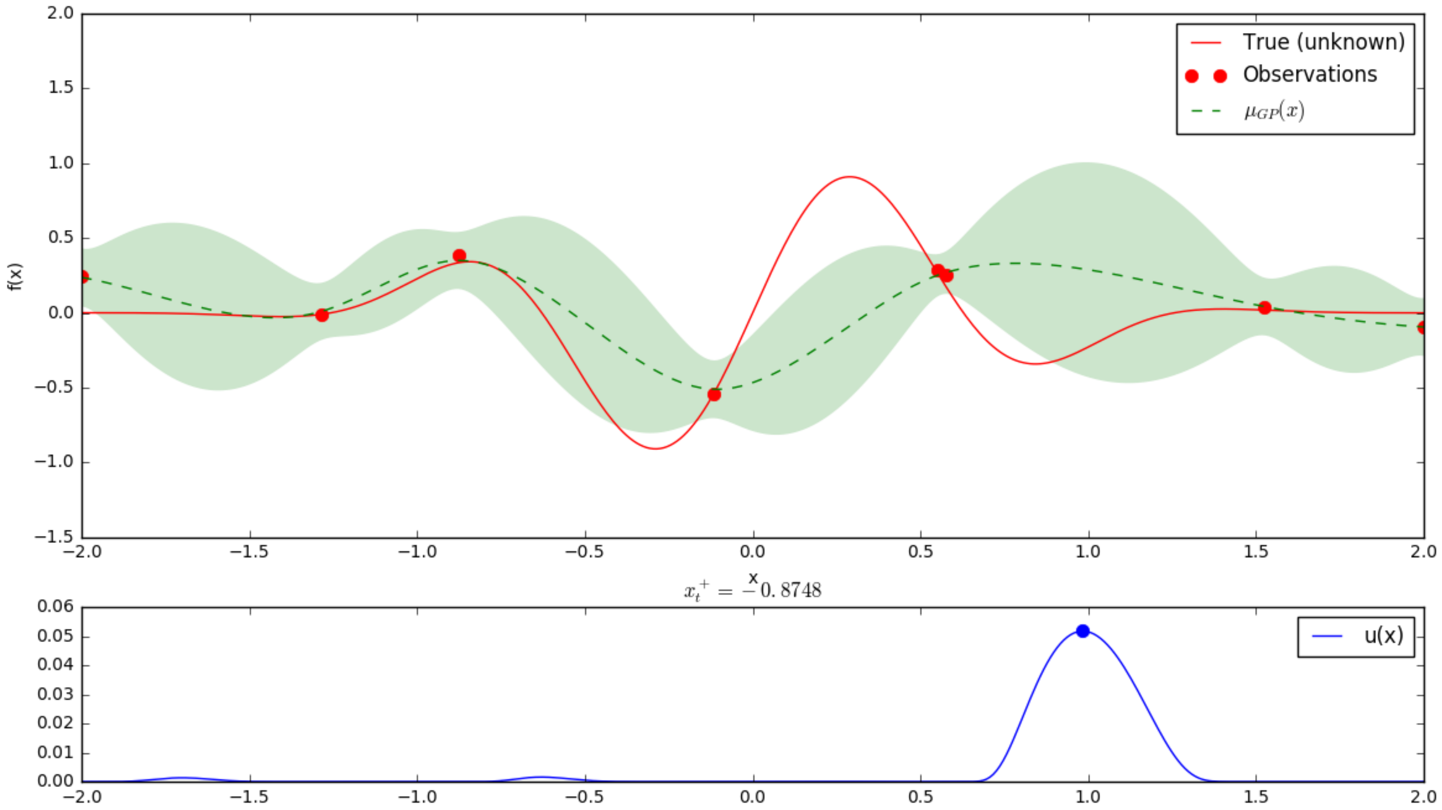

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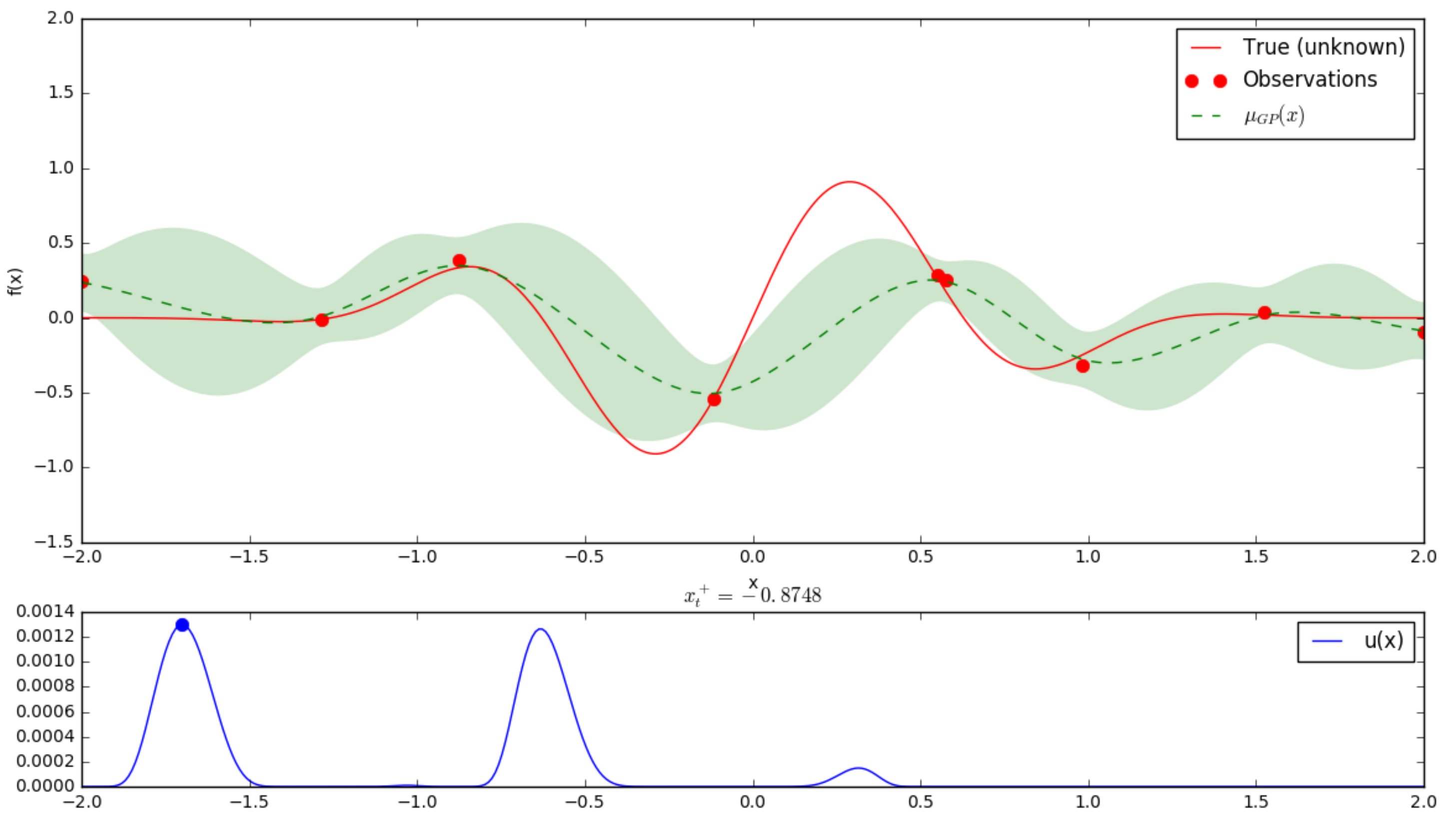

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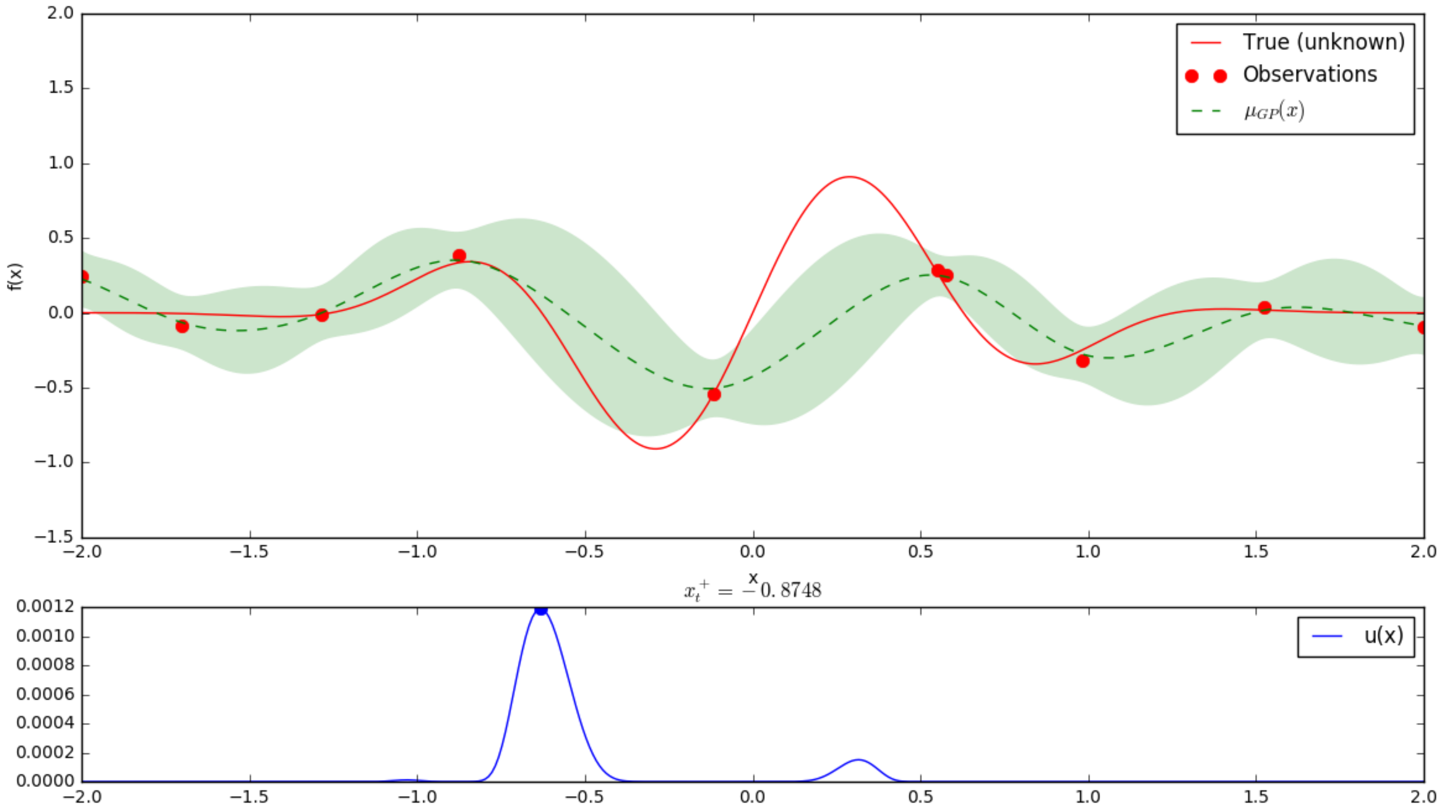

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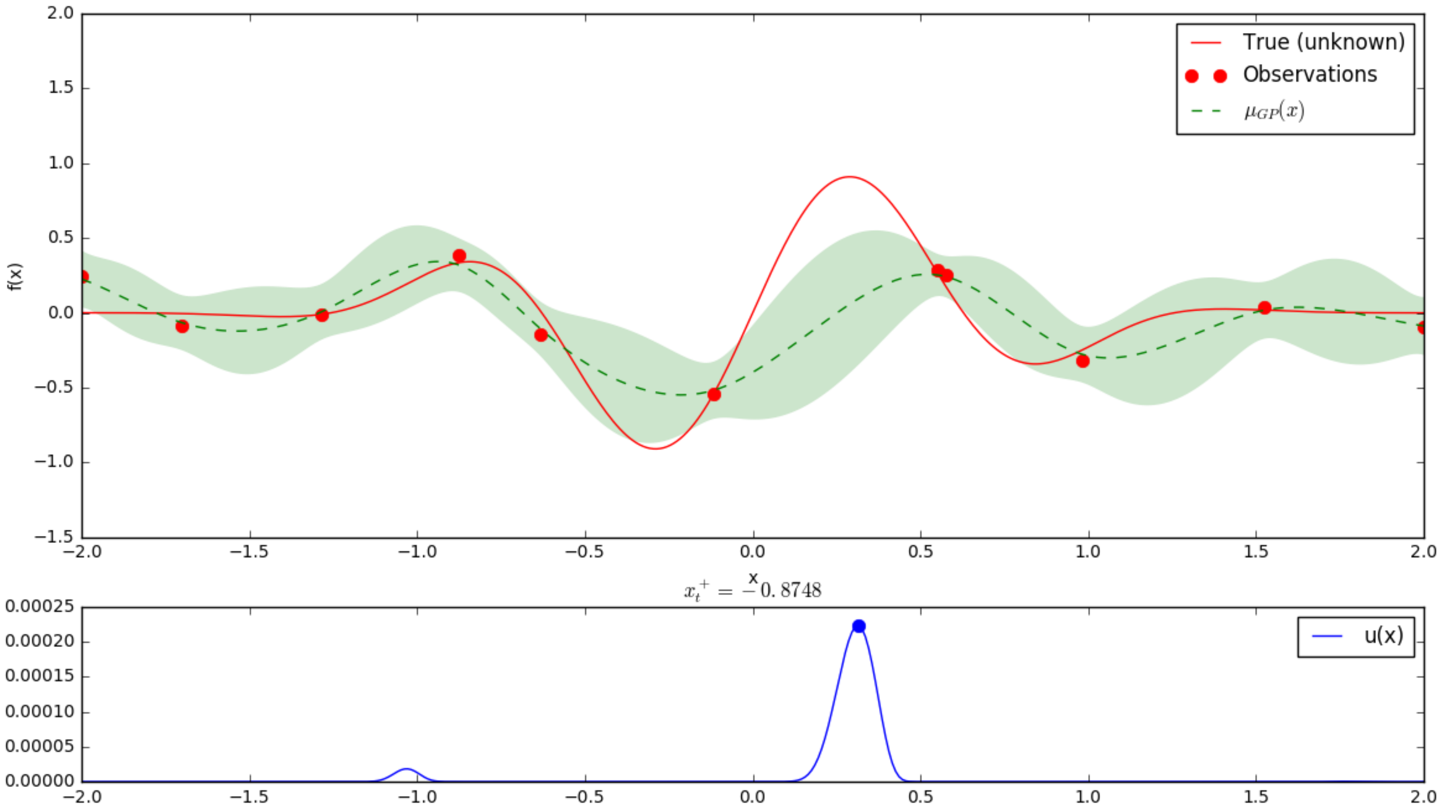

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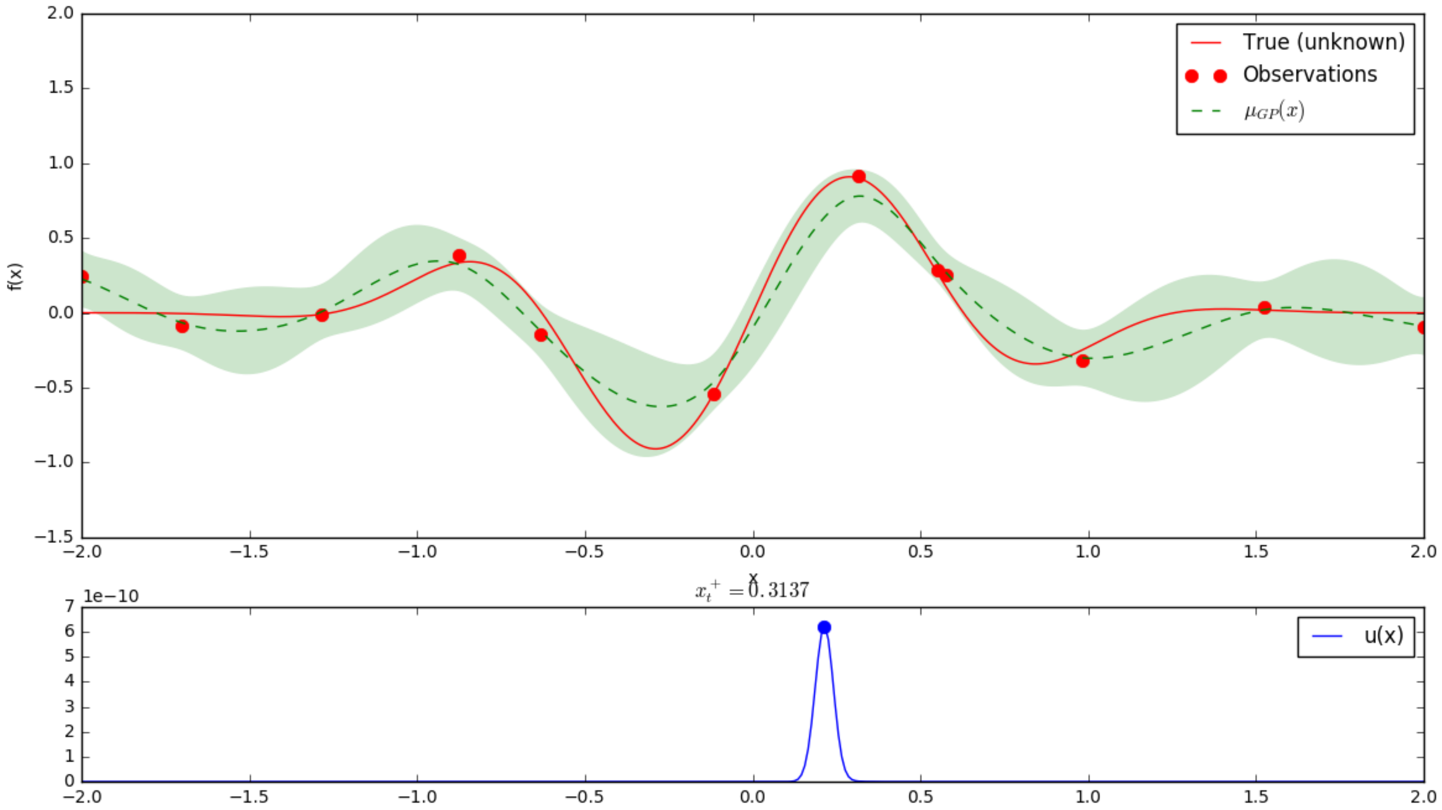

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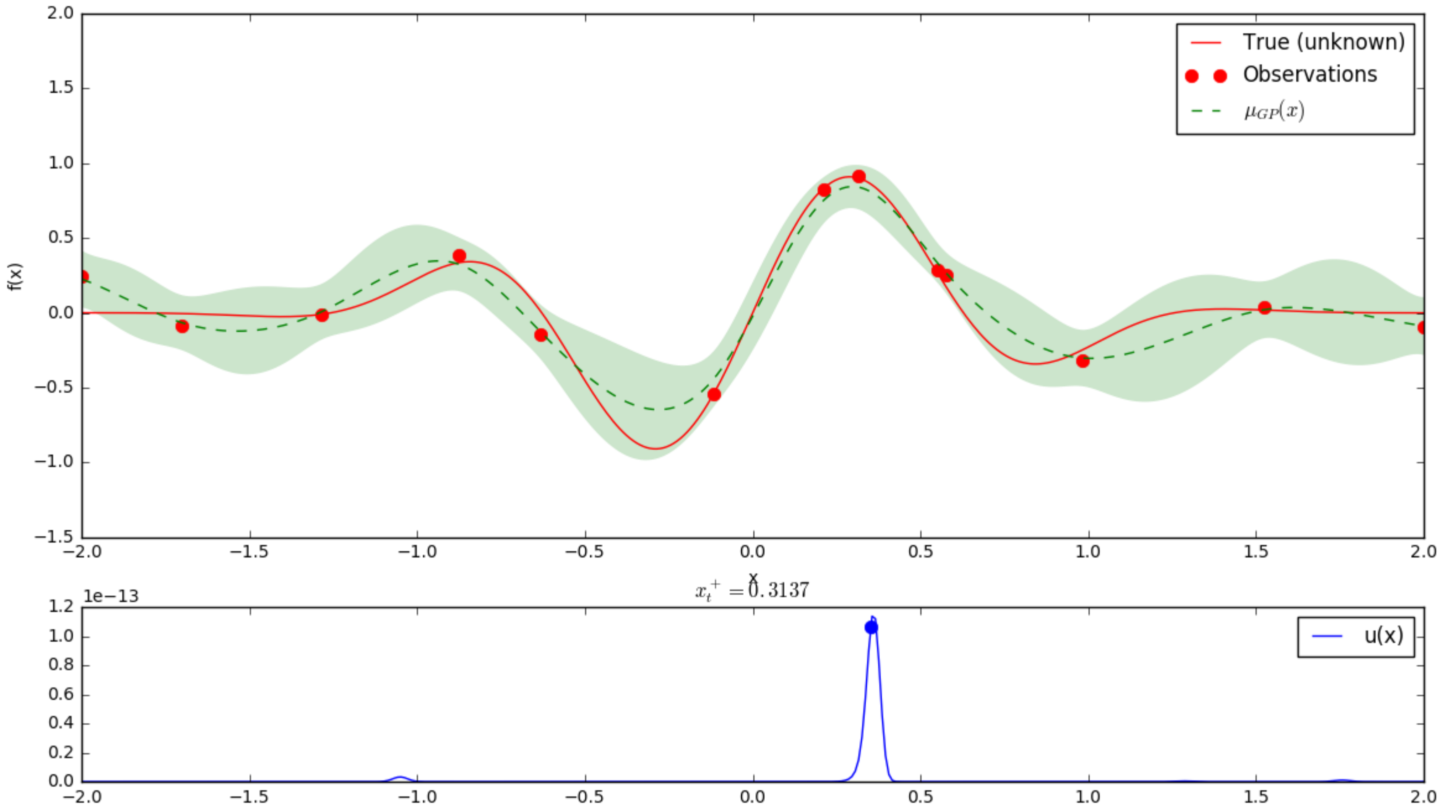

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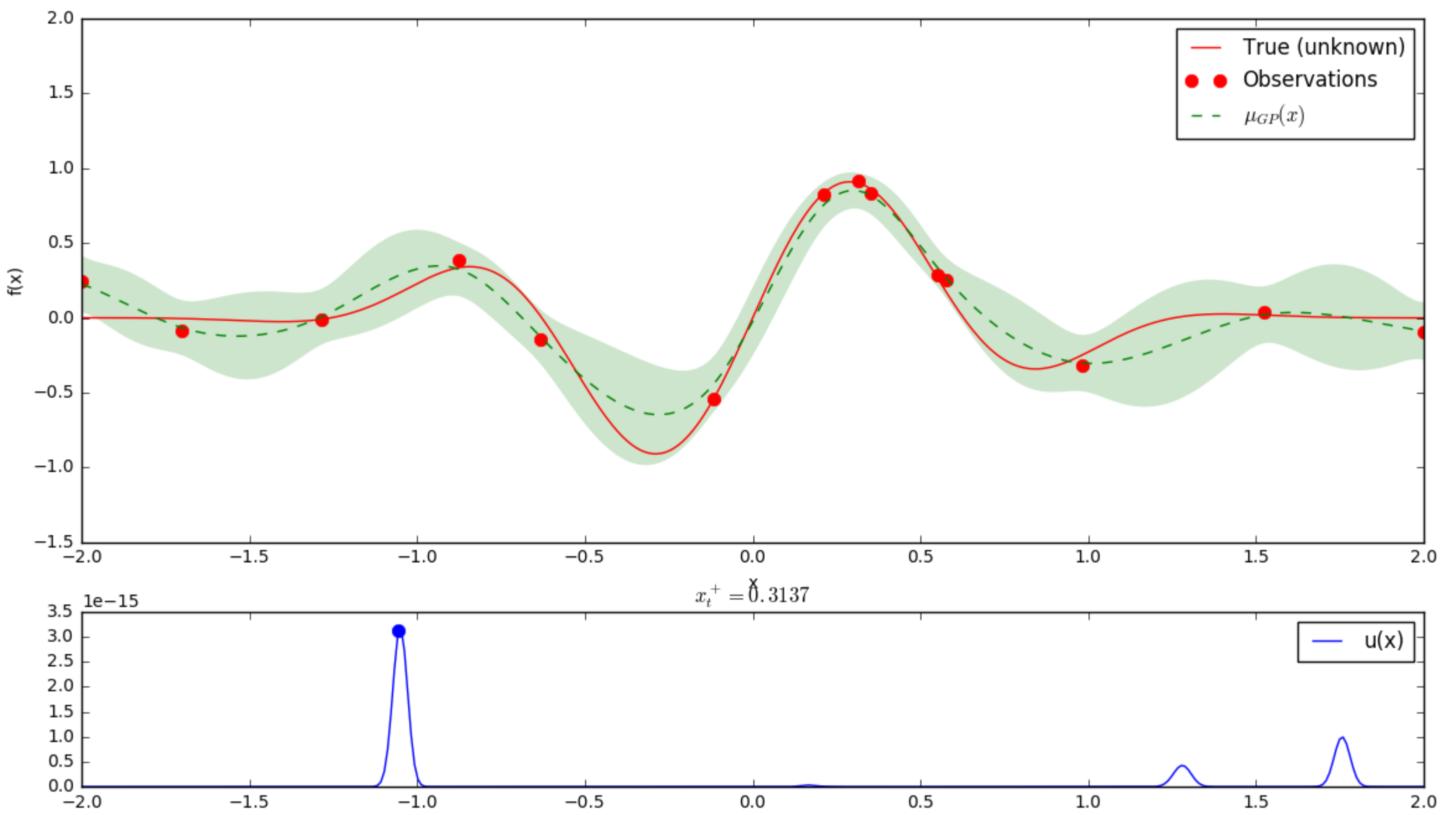

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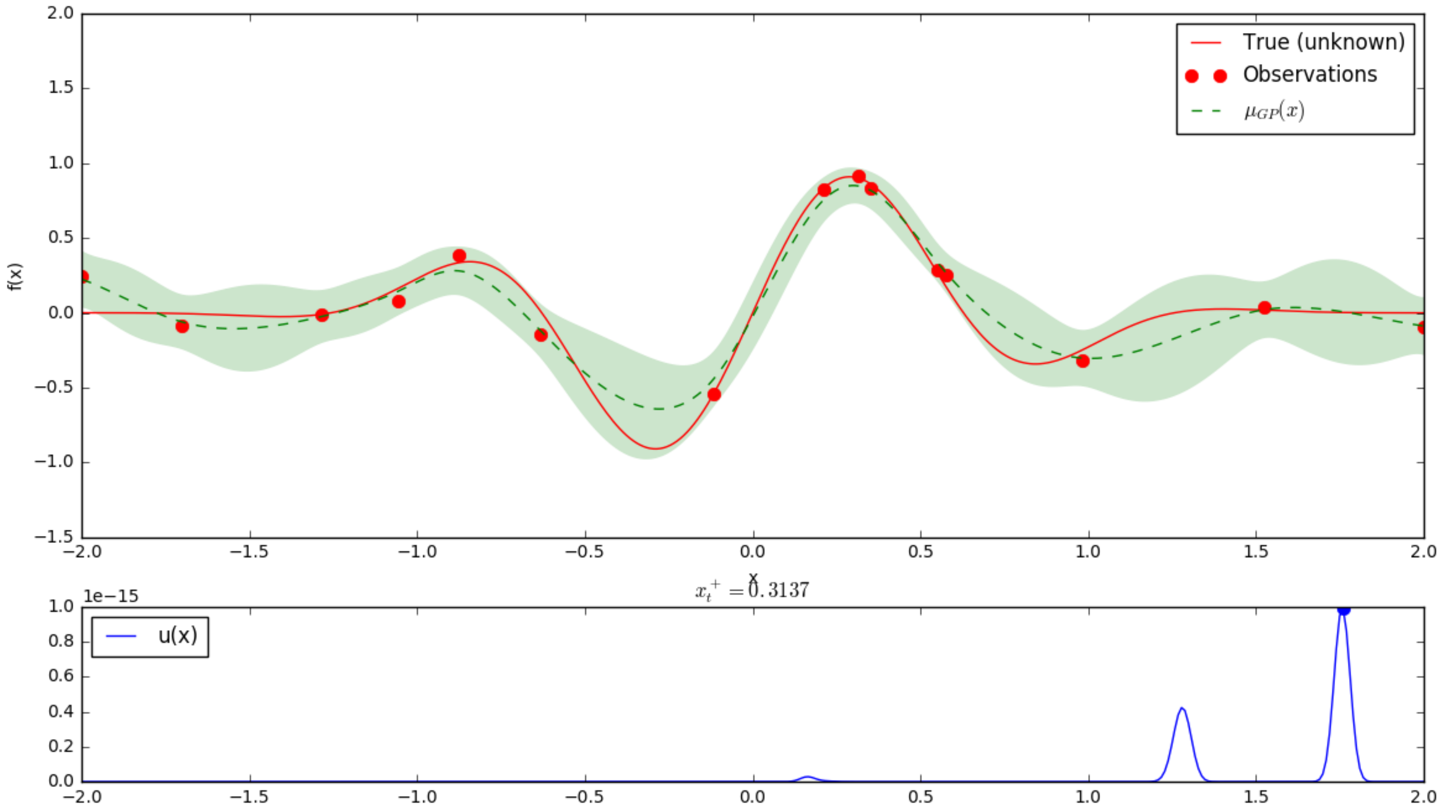

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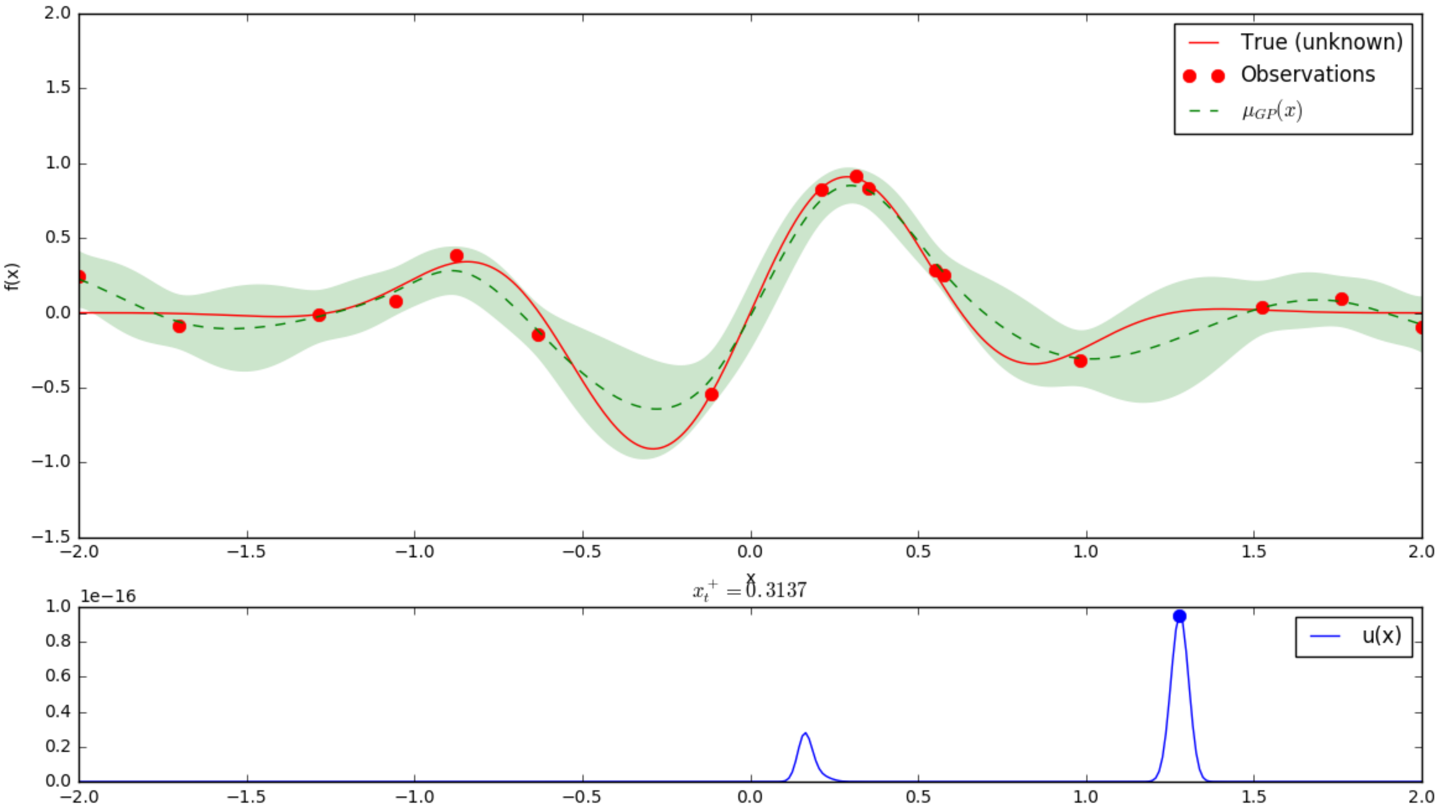

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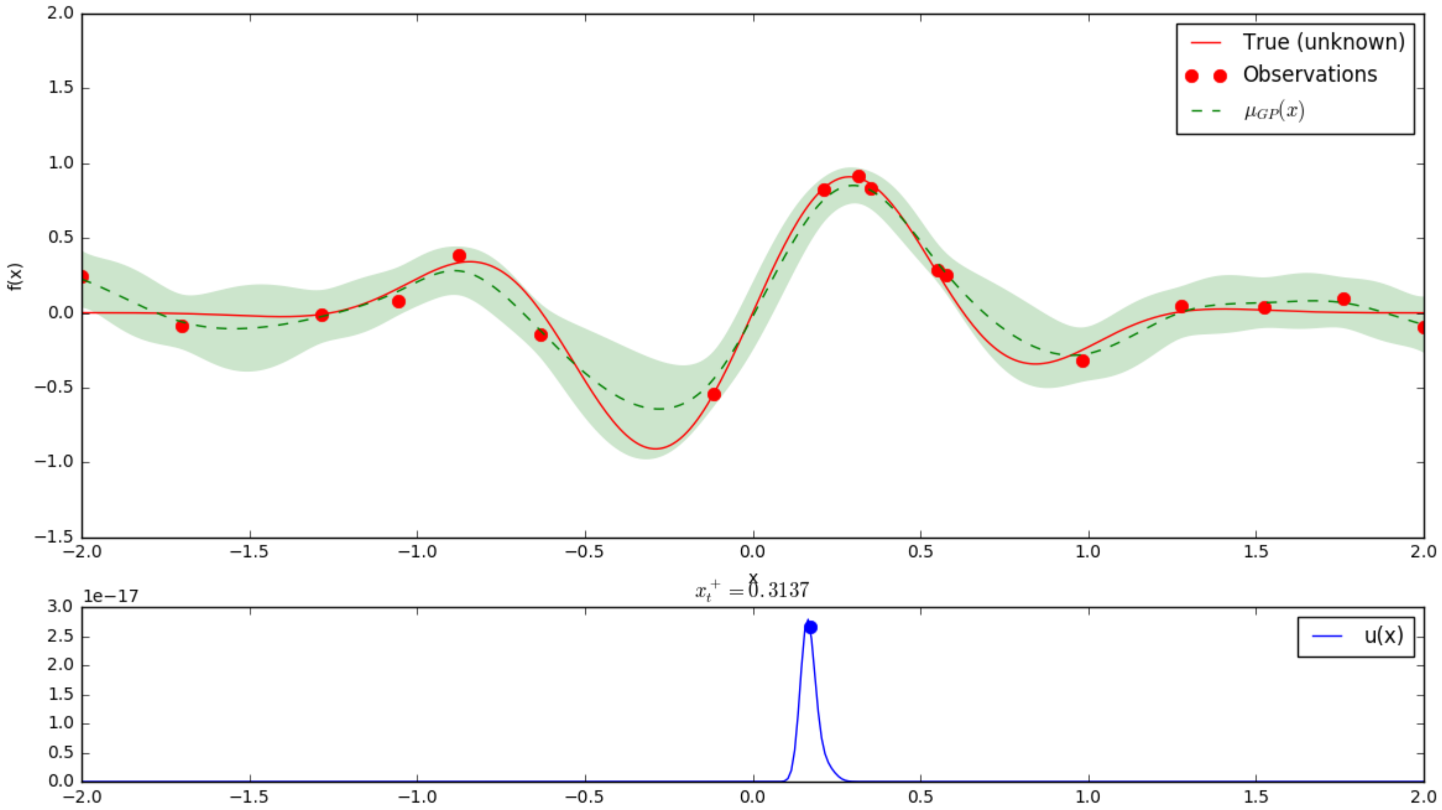

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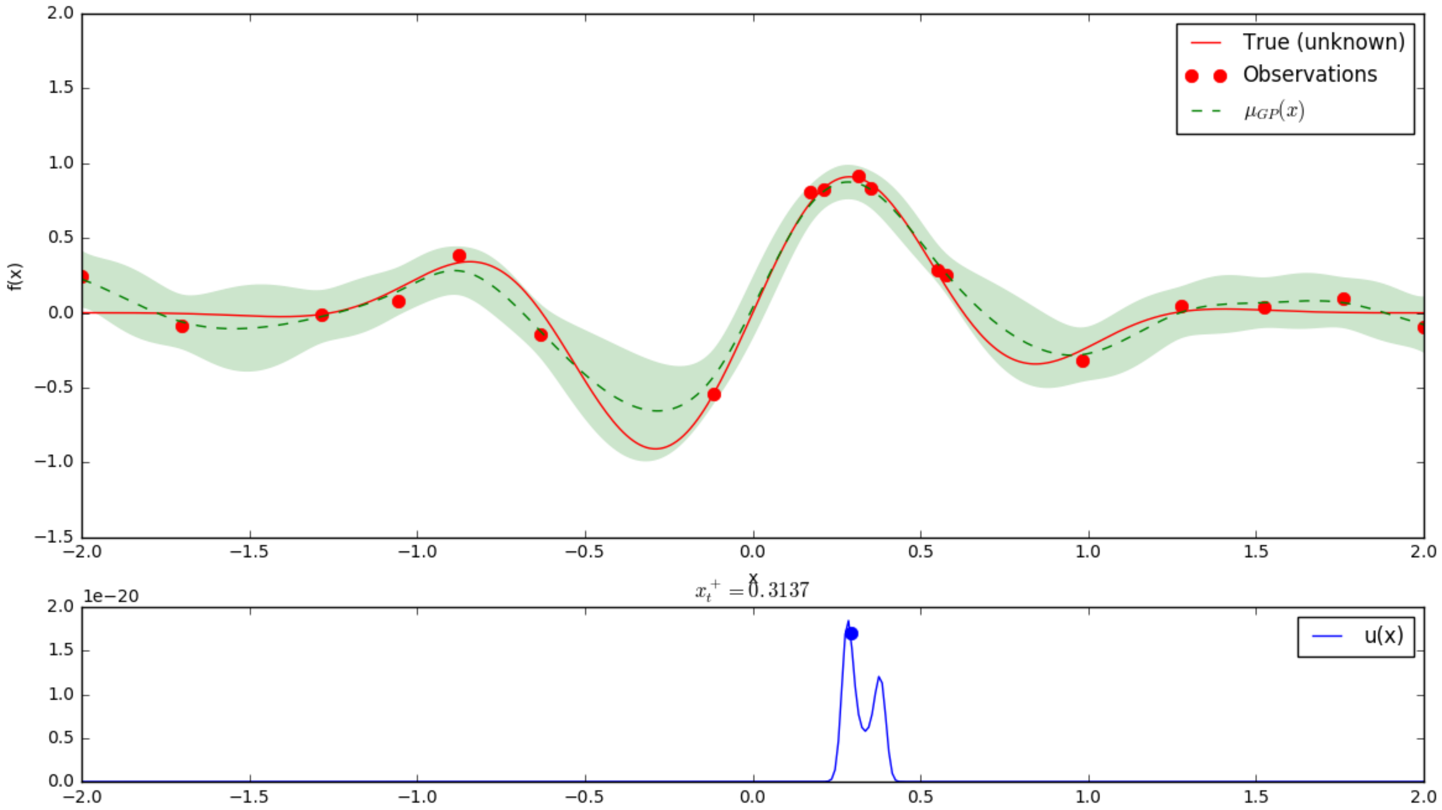

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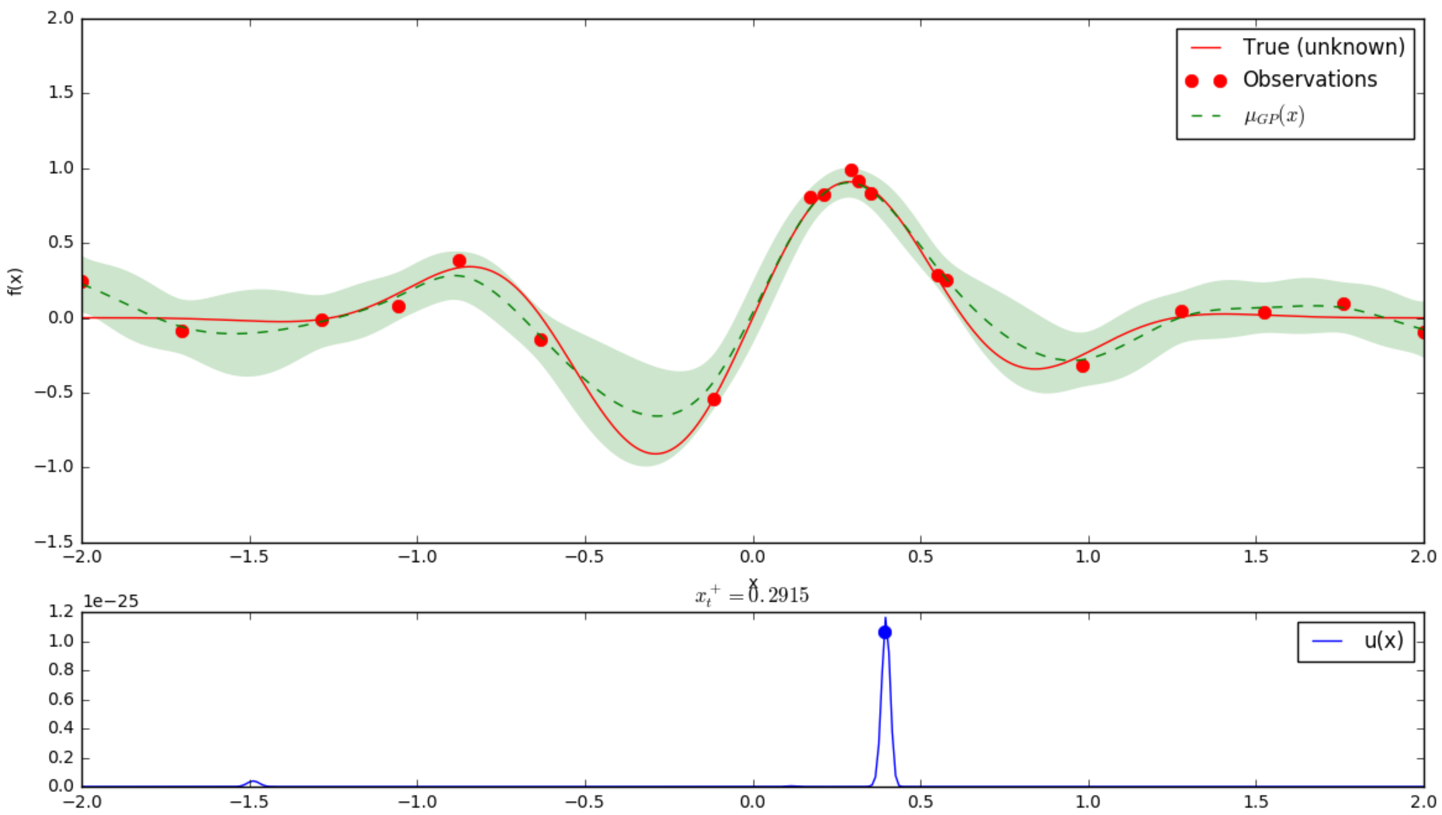


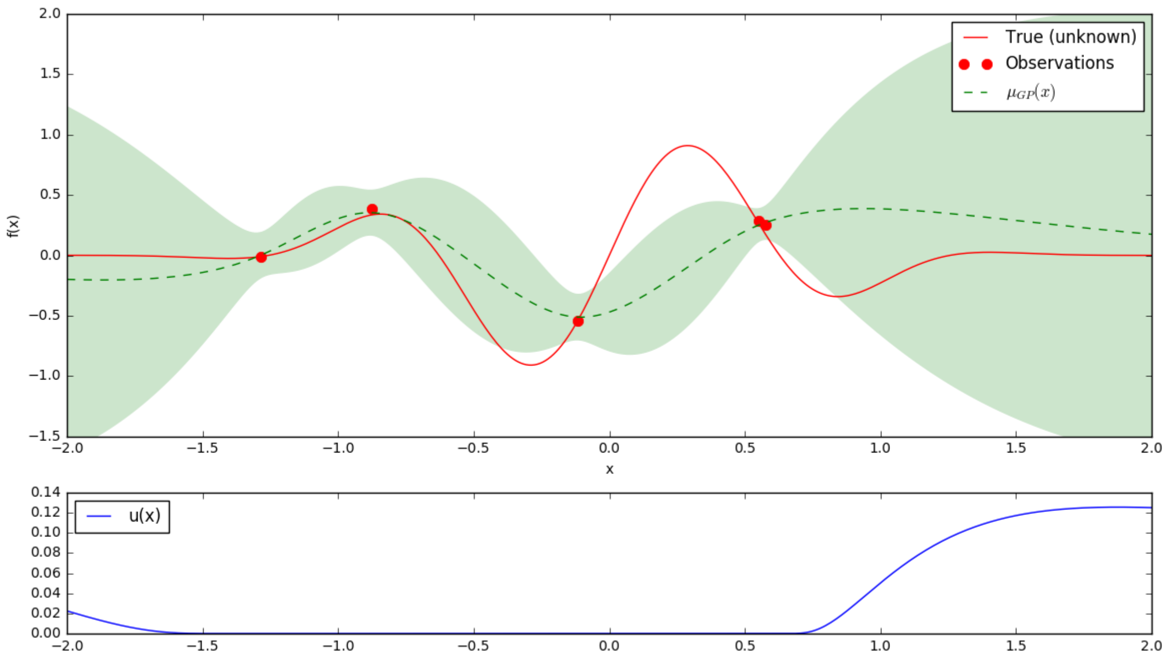
Acquisition Functions

Expected Improvement (EI)

$$\alpha_{\mathrm{EI}}(x|\mathcal{D}_n) = \mathbb{E}_{y\sim p(y|\mathcal{D}_n,x)}[I(x,y)]$$

where $I(x,y) = (y - y^*)\mathbb{I}[y > y^*]$

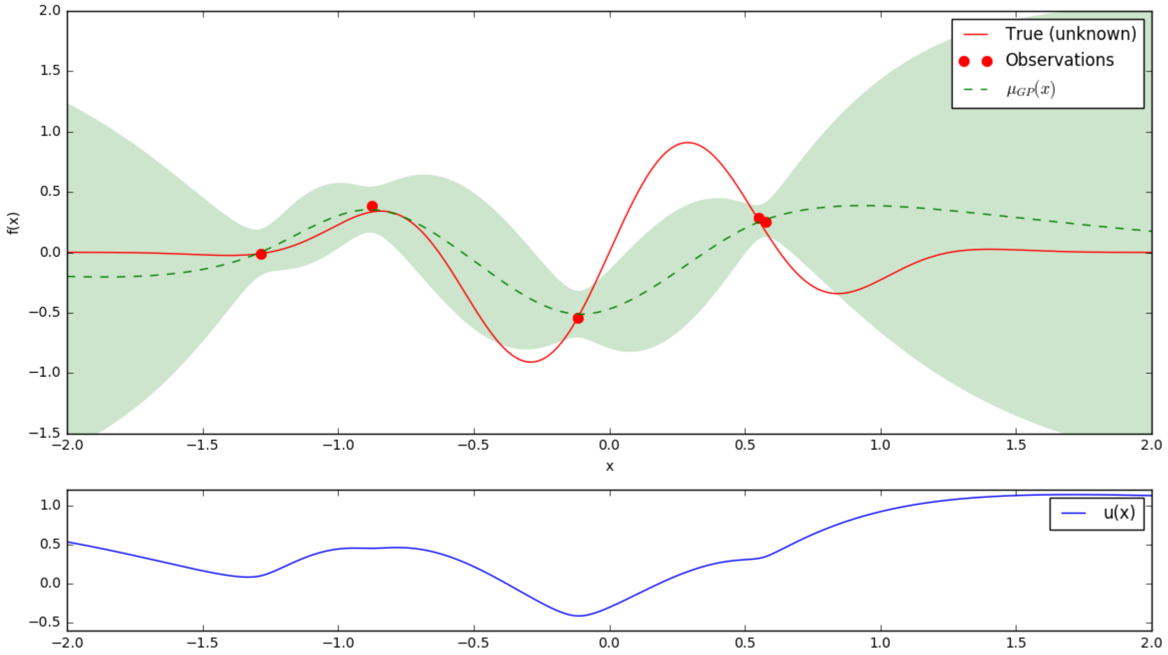
$$= (\mu_n(x) - y^*)\Phi(\frac{\mu_n(x)-y^*}{\sigma_n(x)}) + \sigma_n(x)\phi(\frac{\mu_n(x)-y^*}{\sigma_n(x)})$$



Acquisition Functions

Upper Confidence Bound (UCB)

$$\alpha_{\mathrm{UCB}}(x|\mathcal{D}_n) = \mu_n(x) + \beta_n \sigma_n(x)$$



Information theoretic approach

Entropy search

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Information theoretic approach

Entropy search

Consider posterior over the unknown maximizer:

$$p(\mathbf{x}_*|\mathcal{D}_n).$$

We aim on reducing the uncertainty in the location of $\mathbf{x}_*$:

$$\alpha_{\mathrm{ES}}(\mathbf{x}) := H\left[p(\mathbf{x}_*|\mathcal{D}_n)\right] - \mathbb{E}_{p(y|D_n,\mathbf{x})}\left[H\left[p(\mathbf{x}^*|\mathcal{D}_n \cup \{\mathbf{x}, y\})\right]\right].$$

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This leads to the new form of the acquisition function:

$$\alpha_{\mathrm{PES}}(\mathbf{x};\mathcal{D}_n) := H\left[p(y|\mathcal{D}_n,\mathbf{x})\right] - \mathbb{E}_{p(\mathbf{x}_*|\mathcal{D}_n)}\left[H\left[p(y|\mathcal{D}_n,\mathbf{x},\mathbf{x}_*)\right]\right]$$

Sampling from $p(\mathbf{x}_* | \mathcal{D}_n)$

We will use Monte Carlo approximation to compute the expectation.

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A natural approach is to produce sample from posterior:

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A natural approach is to produce sample from posterior:

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However, this would cost $\mathcal{O}(m^3)$ where m is the number of function evaluations.

Thus, we need the analytic approximation of $\mathbf{f}$.

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where $\theta \sim \mathcal{N}(\mathbf{0}, \mathbf{1})$. This can be maximized to obtain:

$$\mathbf{x}_*^{(i)} = \arg\max_{\mathbf{x} \in \mathcal{X}} f^{(i)}(\mathbf{x}).$$

Approximating $p(y|\mathcal{D}_n, \mathbf{x}, \mathbf{x}_*)$

Let's note that:

$$p(y|\mathcal{D}_n, \mathbf{x}, \mathbf{x}_*) = \int p(y|f(\mathbf{x}))p(f(\mathbf{x})|\mathcal{D}_n, \mathbf{x}_*)\mathrm{d}f(\mathbf{x})$$

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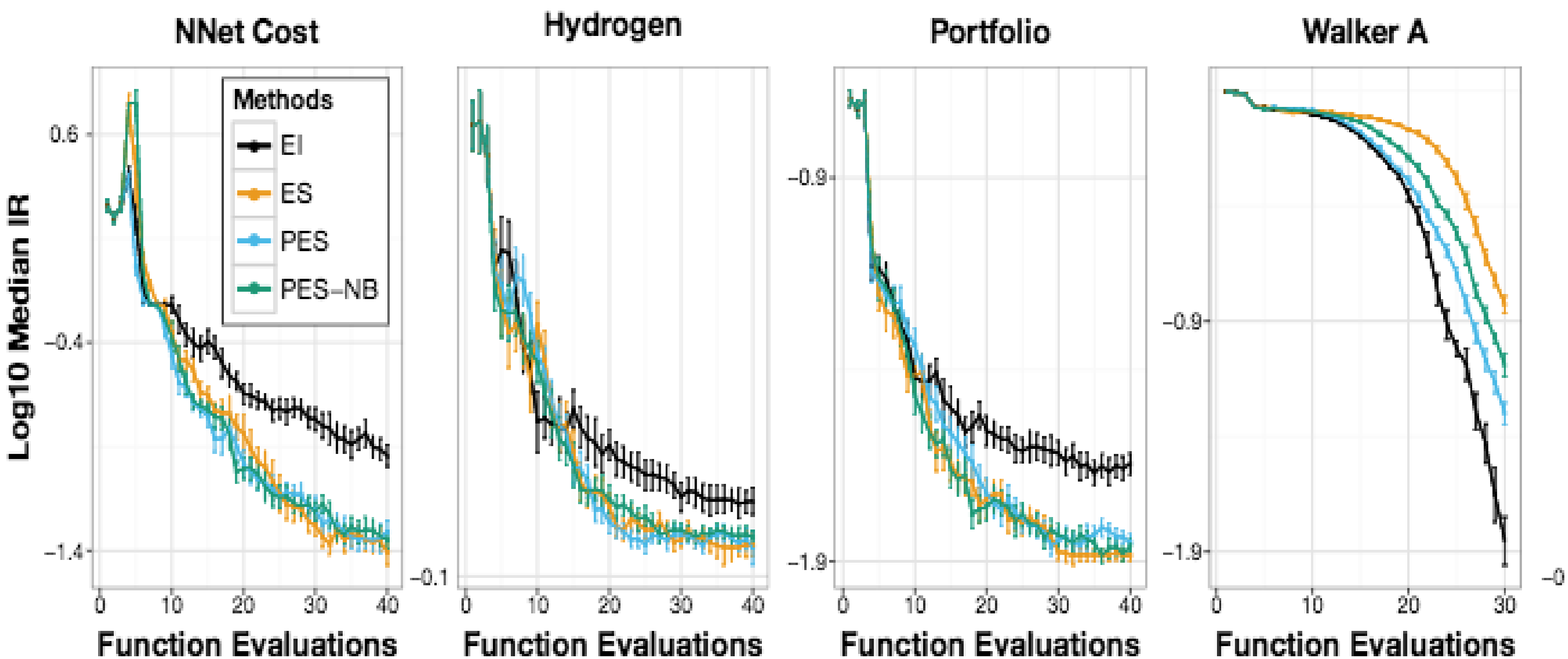
You can find more in Hernandez-Lobato et al. 2014.

How does it work?



Probabilistic Frameworks

Using GPs

How do we choose a kernel and hyper-parameters?

- A common approach is by empirical Bayes
  - $\theta^* = \operatorname{argmax}_\theta p(\mathcal{D}_n|\theta)$
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  - $\alpha(x) = \ \mathrm{E}_{f|\theta^*}[U(f(x))]$
- Alternatively we can be more Bayesian
  - $\theta \sim p(\theta|\lambda)$
  - $\alpha(x) = \ \mathrm{E}_{\theta|\mathcal{D}_n,\lambda}[\mathrm{E}_{f|\theta}[U(f(x))]]$

Shortcomings of GPs

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- Scalability with Dimensionality

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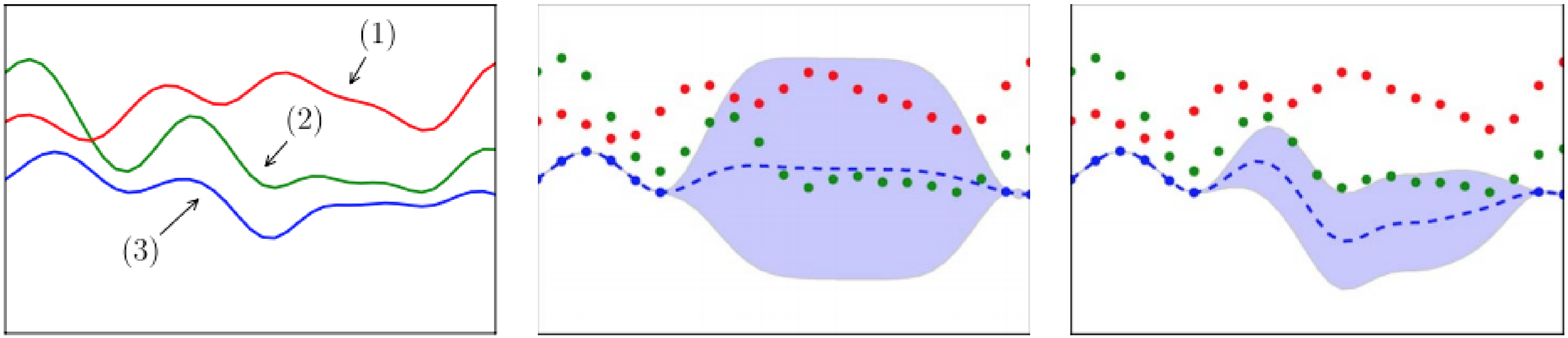
We use the *intrinisic model of coregionalization*

- $k((x,t),(x',t')) = k_{\mathbb{X}}(x,x')k_T(t,t')$

Matthias Seeger, Yee-Whye Teh, and Michael I. Jordan. Semiparametric latent factor models. In AISTATS, 2005.

Edwin V. Bonilla, Kian Ming A. Chai, and Christopher K. I. Williams. Multi-task Gaussian process prediction. In NIPS, 2008.

Multi-Task Bayesian Optimization



Transferring knowledge from other tasks, f_1 and f_2 informs our prior over f_3

We can better cope with the size of the space!

Swersky, Kevin, Jasper Snoek, and Ryan P. Adams. "Multi-task bayesian optimization." Advances in neural information processing systems. 2013.

Bayesian Neural Nets

Short intro

Bayesian Neural Nets

Let's denote by θ parameters of out network. We are interested in computing the posterior predictive distribution

$$p(y|\mathbf{x},\mathcal{D}_n).$$

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Using posterior distribution over parameters:

$$p(\theta|\mathcal{D}_n) \propto p(\theta)\prod_{i=1}^{n} p(y_i|\mathbf{x}_i,\theta)$$

we have:

$$p(y|\mathbf{x},\mathcal{D}_n) = \int p(y|\mathbf{x},\theta)p(\theta|\mathcal{D}_n)\mathrm{d}\theta$$

Approximations for $p(\theta|\mathcal{D}_n)$

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Approximations for $p(\theta|\mathcal{D}_n)$

1. Probabilistic backpropagation (PBP), Hernandez-Lobato and Adams, 2015,
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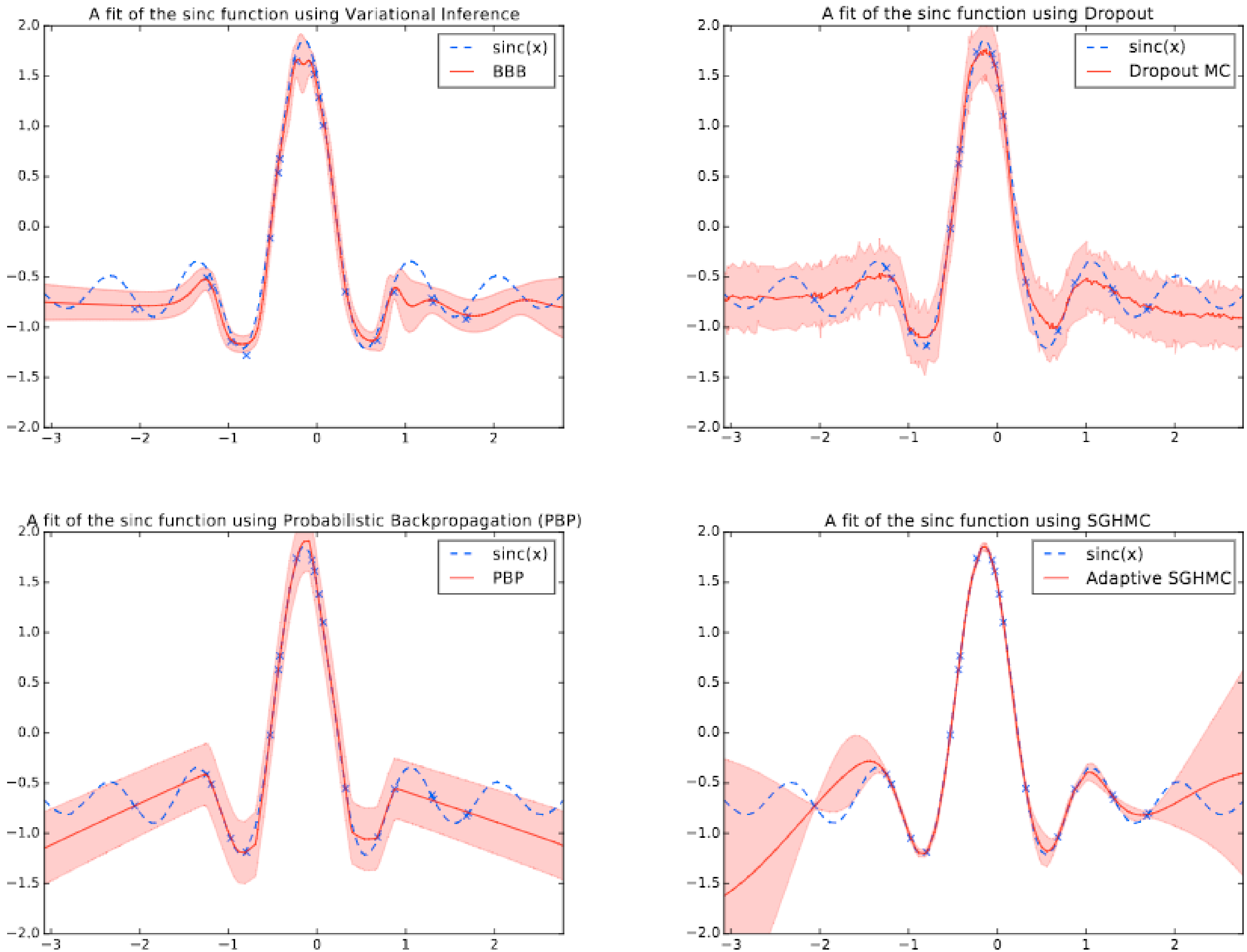
3. Dropout MC, Gal and Ghahramani, 2015

Comparison


A fit of the sinc function using Variational Inference
sinc(x)
BBB
A fit of the sinc function using Dropout
sinc(x)
Dropout MC
A fit of the sinc function using Probabilistic Backpropagation (PBP)
sinc(x)
PBP
A fit of the sinc function using SGHMC
sinc(x)
Adaptive SGHMC

MCMC methods for $p(\theta|\mathcal{D}_n)$

MCMC methods for $p(\theta|\mathcal{D}_n)$

Stochastic gradient Langevin dynamics (SGLD), Welling and Teh, 2011. This is just:

$$\theta_{t+1} = \theta_t + \epsilon_t/2\left(\nabla \log p(\theta_t) + \frac{N}{n}\sum_{i=1}^{n} \nabla \log p(\mathbf{x}_{ti}|\theta_t)\right) + \eta_t,$$

where $\eta_t \sim \mathcal{N}(0, \epsilon_t)$.

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Methods based on hybrid Monte Carlo - many variations.

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We consider a joint system of θ and auxiliary momentum variables, r:

$$p(\theta, r|\mathcal{D}_n) \propto \exp\left(-\log p(\theta,\mathcal{D}_n) - \frac{1}{2}r^T M^{-1} r\right).$$

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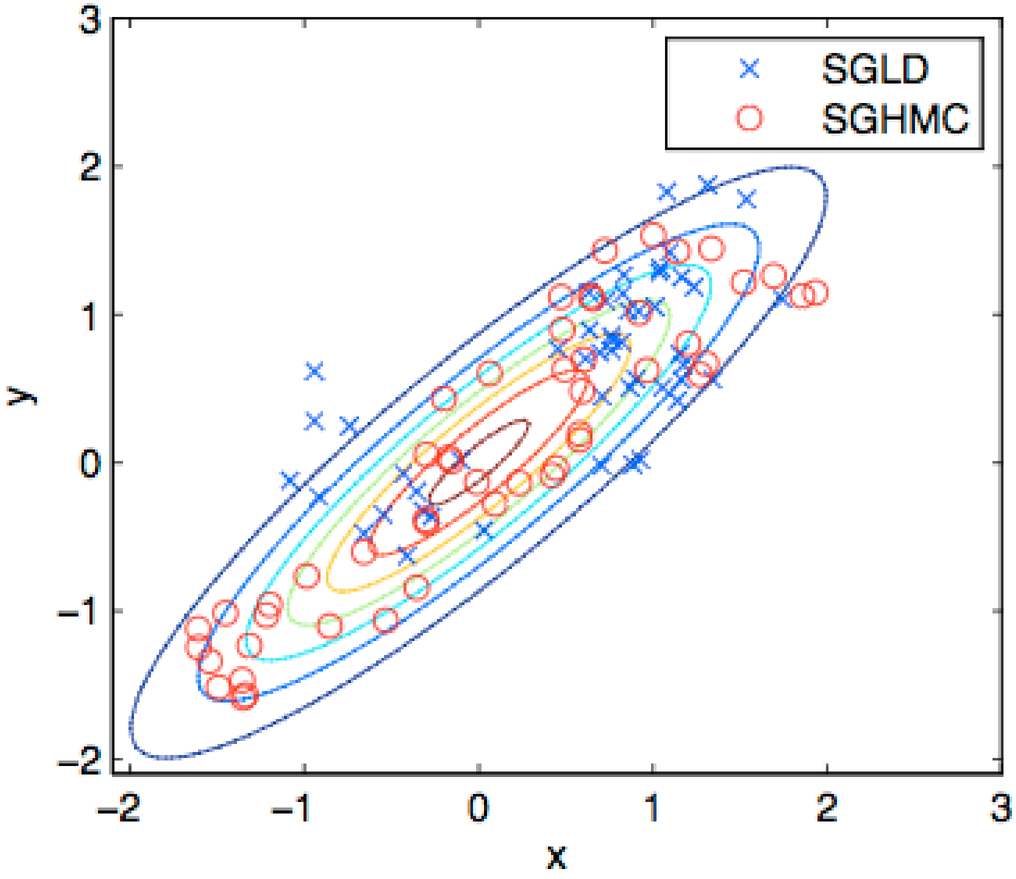
Stochastic gradient Hamiltionian Monte Carlo (SGHMC), Chen et. al. 2014.

SGLD vs SGHMC



Bayesian Optimization with Hamiltonian Monte Carlo Artificial Neural Networks (BOHAMIANN)

Springenberg et al., 2016

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In the context of BNN, our probabilistic model takes the form:

$$p(f_t(\mathbf{x})|\mathbf{x}, \theta) = \mathcal{N}(\hat{f}(\mathbf{x}, t; \theta_\mu), \theta_{\sigma^2})$$

where $\hat{f}(\mathbf{x}, t; \theta_\mu)$ is the output of a parametric model with parameters θ_μ and noise is assumed to be homoscedastic.

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We follow SGHMC algorithm to reach the posterior distribution - this requires running a chain for a 'long' time.

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At test time we use S samples θ^s generated using our chain which can be seen as samples from the posterior $p(\theta|\mathcal{D}_n)$.

What about acquisition function?

We managed to generate approximate samples $\theta_i \sim p(\theta|\mathcal{D}_n)$ from the posterior. For the EI we can obtain:

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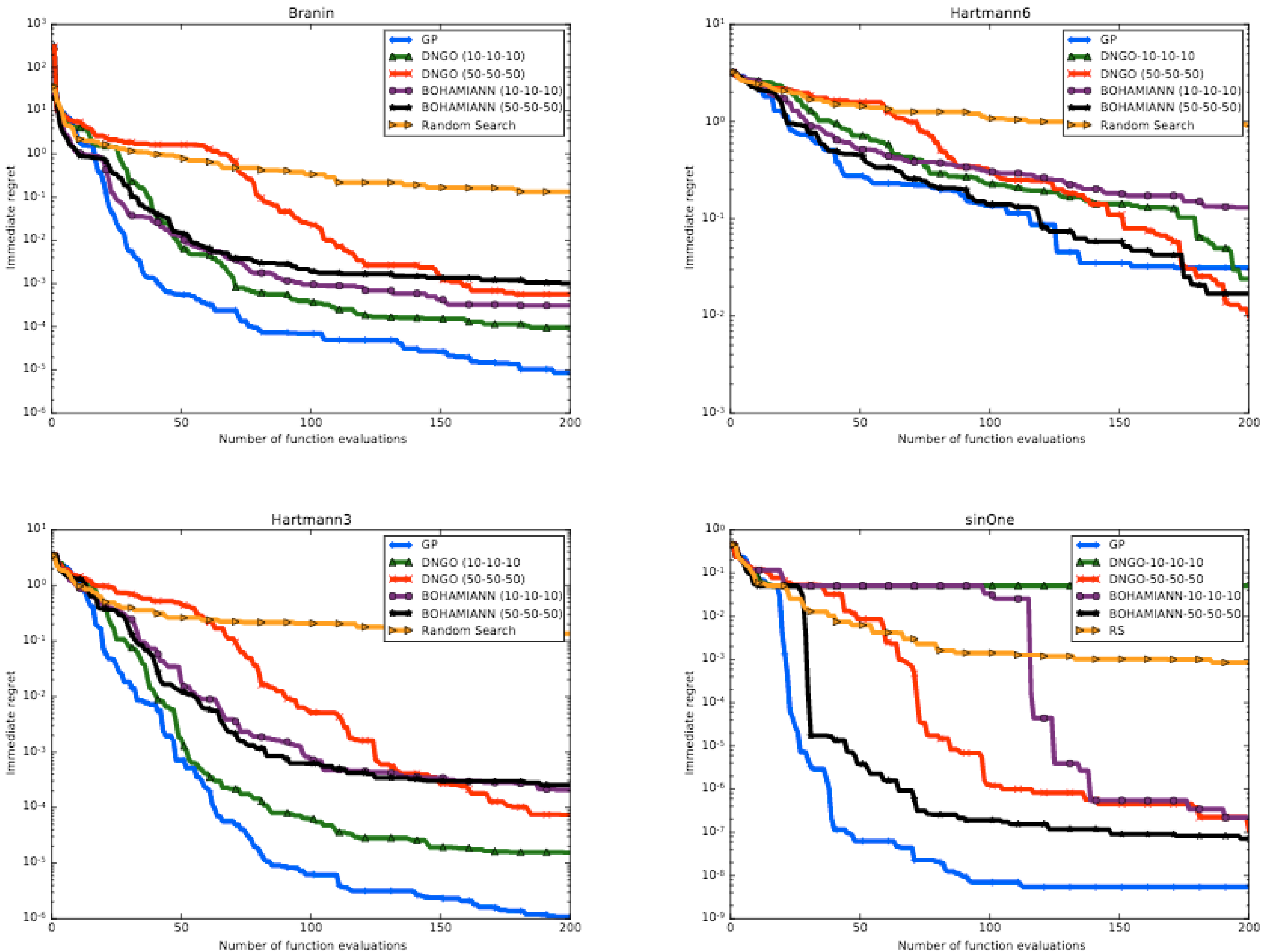
Note - we can compute partial derivatives of α_{EI} with respect to $\mathbf{x}$ which allows us to use standard gradient-based techniques to maximize acquisition function!

Final comparison



Open Questions and Problems

- Parallelization
    - Non-sequential samples
- Cost sensitivity
    - When we have variable cost for different queries (e.g. layer sizes)
    - Expected improvement per second

Snoek, Jasper, Hugo Larochelle, and Ryan P. Adams. "Practical bayesian optimization of machine learning algorithms." Advances in neural information processing systems. 2012.

Open Questions and Problems

- Exploration vs Exploitation tradeoff changes over time
  - 'Portfolios' of acquisition functions are often the best solution.
  - A meta criterion is used to pick the best solution across the portfolio

- Acquisition functions are often don't answer the questions we want to ask
  - Short-sighted
  - Don't consider utility of exploitation/exploration

Hoffman, Matthew D., Eric Brochu, and Nando de Freitas. "Portfolio Allocation for Bayesian

Optimization." UAI. 2011.

Active learning

Active learning

1. Contextual bandits,

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2. Thompson Sampling (1933),

Active learning

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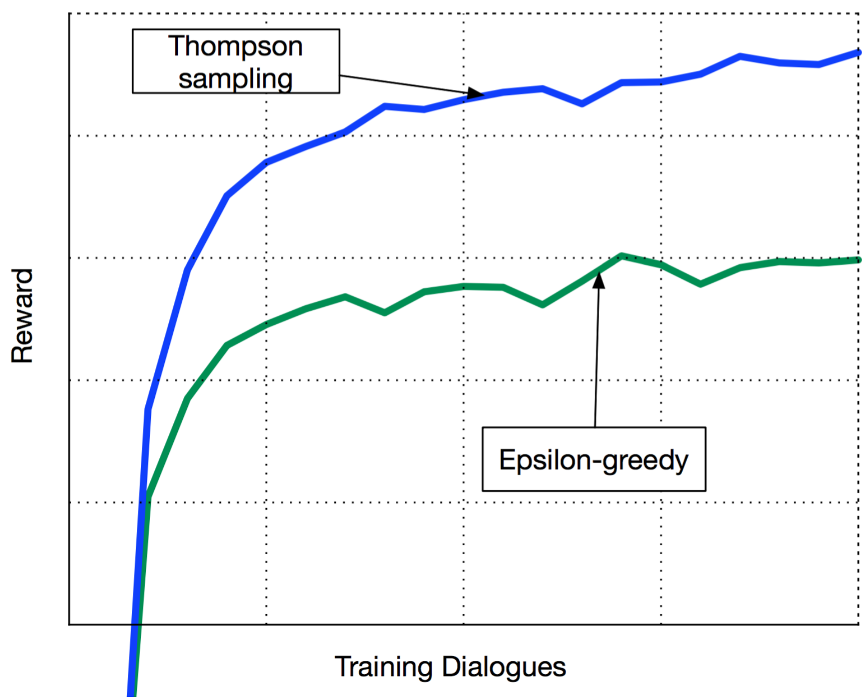
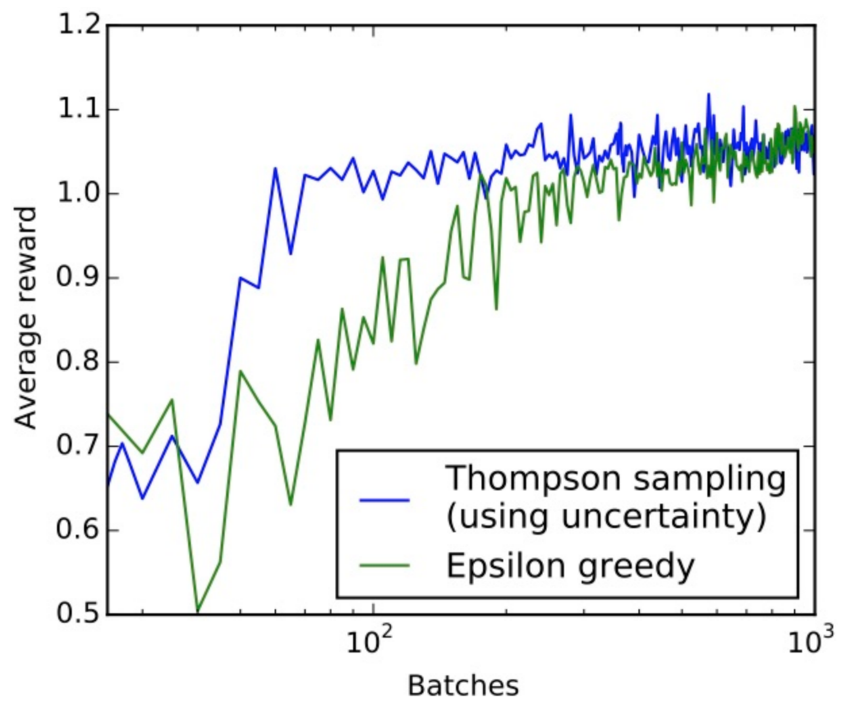
2. Thompson Sampling (1933),
3. Bayesian RL - Gasic et al. 2009, Gal 2016.

Thompson sampling vs ϵ-greedy approach





Thank you!