

Bayesian Optimization

Partially based on Ryan Adams' Tutorial

<http://tinyurl.com/botutorial>

Recommended reading:

Brochu et al. (2009) [1], Shahriari et al. (2016) [18]

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Machine Learning Meta-Challenges

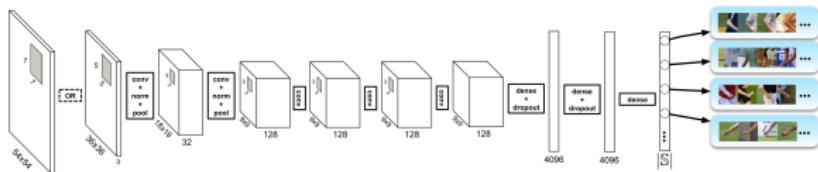
- Machine learning models are getting more and more complicated
 - ▶ Usually more parameters (e.g., deep neural networks)
- Non-convex optimization methods have many parameters to tune
- ▶ Generally hard to apply modern techniques or reproduce results

Machine Learning Meta-Challenges

- Machine learning models are getting more and more complicated
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Automate the selection of critical hyper-parameters
(see also: [Automated Machine Learning \(AutoML\)](#))

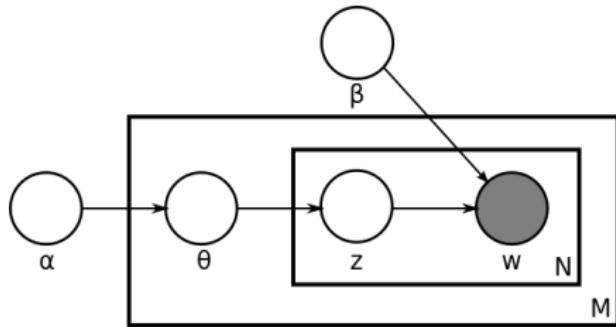
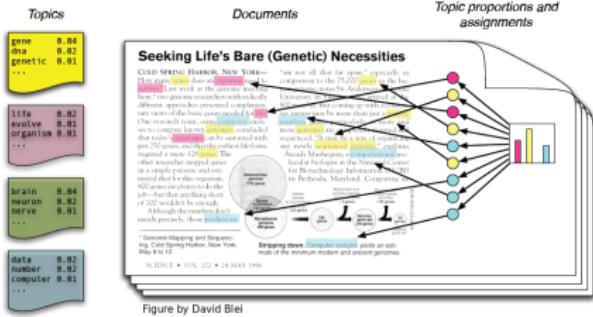
Example: Deep Neural Networks



Huge interest in large neural networks

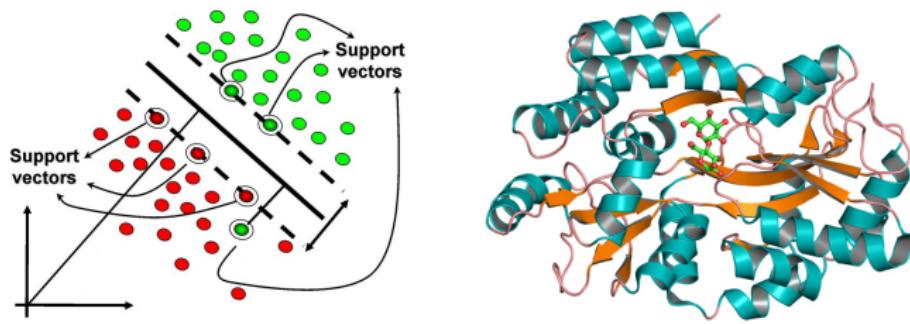
- When well-tuned, very successful for visual object identification, speech recognition, computational biology, ...
- Huge investments by Google, Facebook, Microsoft, etc.
- Many choices:** number of layers, weight regularization, layer size, which nonlinearity, batch size, learning rate schedule, stopping conditions

Example: Online Latent Dirichlet Allocation



- Hoffman et al. (2010): Approximate inference for **large-scale text analysis with Latent Dirichlet Allocation**
- Good empirical results when well tuned
- **Hyper-parameters** tricky to set: Dirichlet parameters, number of topics, learning rate schedule, batch size, vocabulary size, ...

Example: Classification of DNA Sequences



- ▶ Objective: Predict which DNA sequences will bind with which proteins.
- ▶ Miller et al. (2012): [Latent Structural Support Vector Machine](#)
- ▶ **Hyper-parameters:** margin/slack parameter, entropy parameter, convergence criterion

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- ▶ Define an objective function
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 - ▶ Random search (very simple, works surprisingly well)
 - ▶ Manual tuning
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- ▶ Standard search procedures:
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 - ▶ Manual tuning
 - ▶ Black magic
- ▶ Painful:
 - ▶ Training may be very expensive (e.g., time or money)
 - ▶ Many training cycles
 - ▶ Possibly noisy

Alternative Approach: Bayesian Optimization

Setting

Globally optimize an objective function that is expensive to evaluate
(e.g., cross-validation error for a massive neural network)

- Build a **probabilistic proxy model** for the objective using outcomes of past experiments as training data

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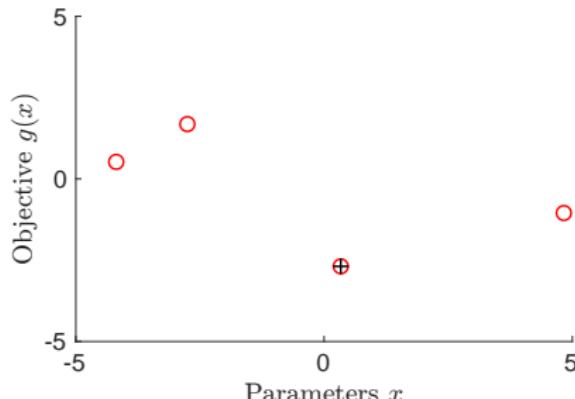
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- Standard proxy: **Gaussian process**

Setting (2)

- Objective: Find global minimum of objective function g :

$$\mathbf{x}_* = \arg \min_{\mathbf{x}} g(\mathbf{x})$$

- We can evaluate the objective g pointwise, but do not have an easy functional form or gradients; observations may be noisy
- Evaluating g is costly (e.g., train a massive deep network)



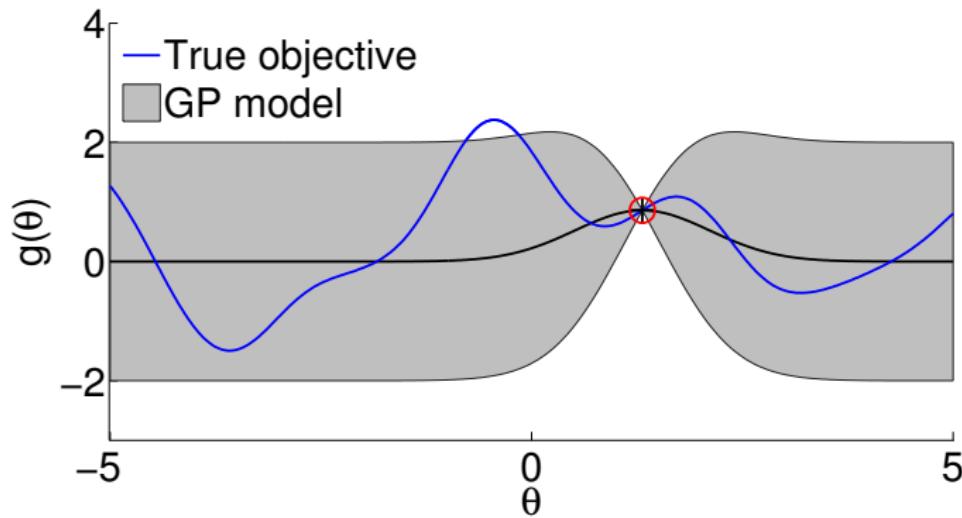
Key Steps

- To avoid evaluating g an excessive number of times, approximate it using a **proxy function** \tilde{g} (which is cheap to evaluate)
- Find a **global optimum** $\tilde{g}(\mathbf{x}_*)$ of proxy function \tilde{g}
- Evaluate true objective g at \mathbf{x}_*
- Overall: Evaluate g only once

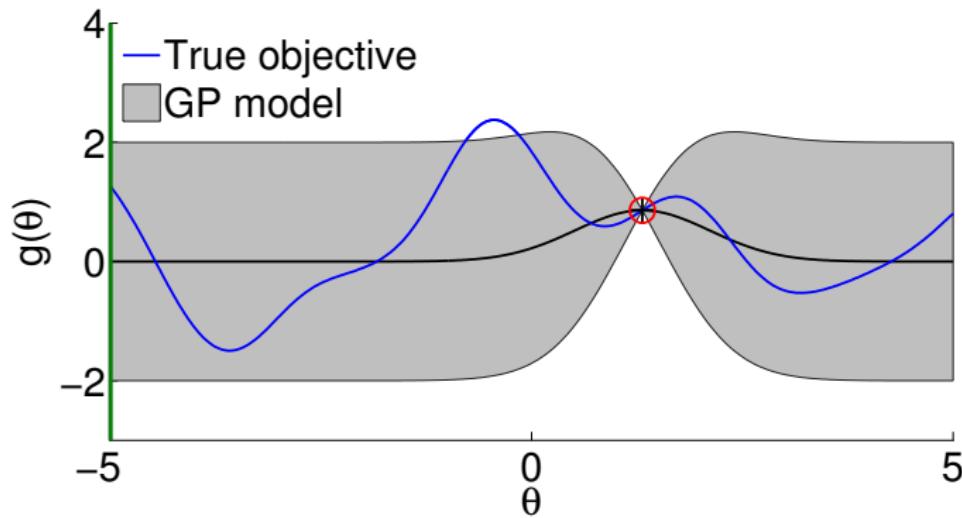
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- Overall: Evaluate g only once
- Works well if $\tilde{g} \approx g$.
- Usually not the case ➤ Repeat this cycle and keep updating \tilde{g}

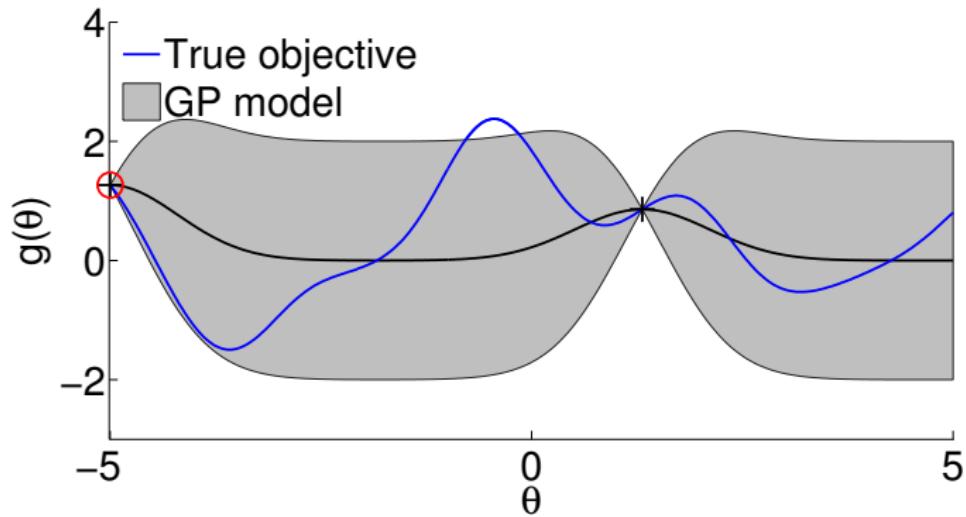
Bayesian Optimization: Illustration



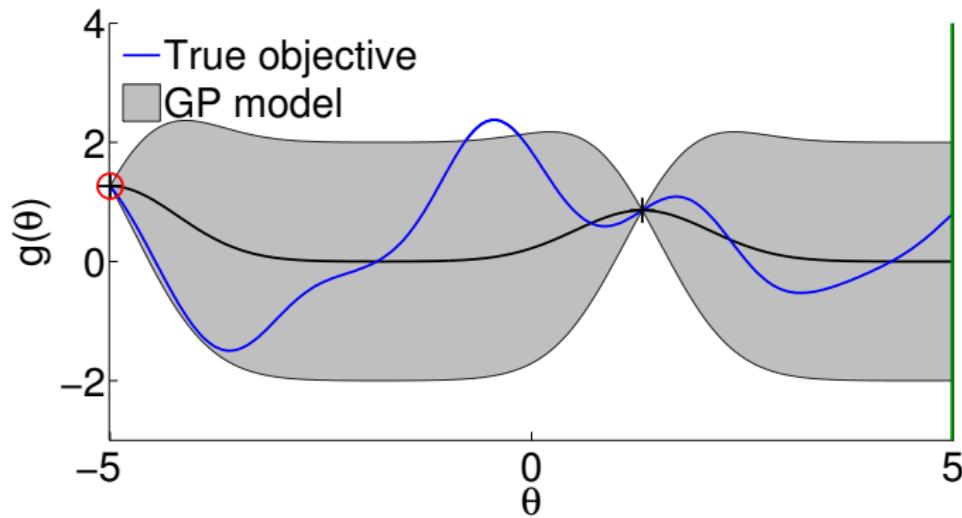
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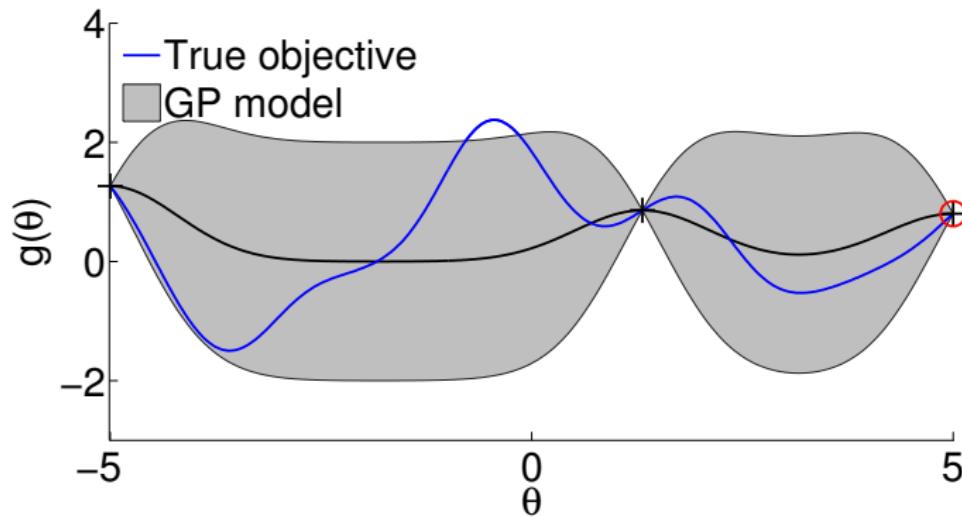
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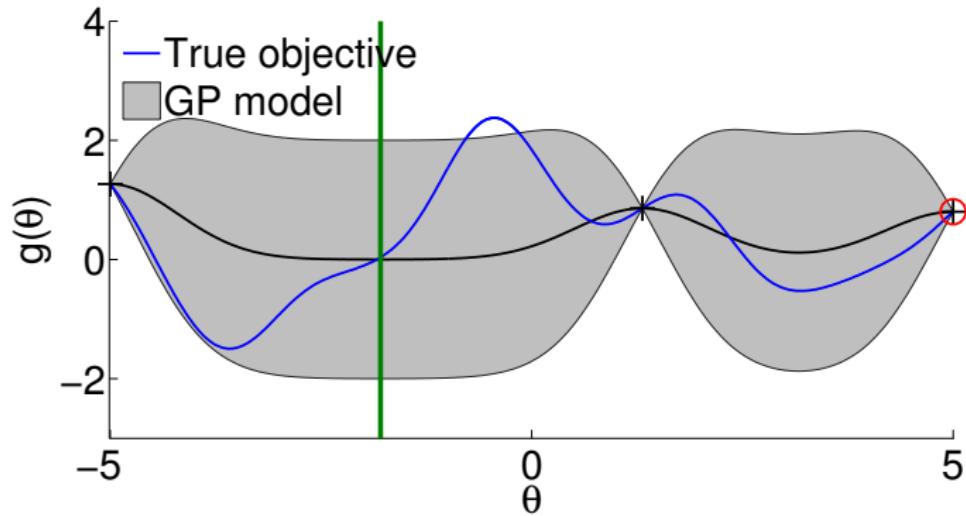
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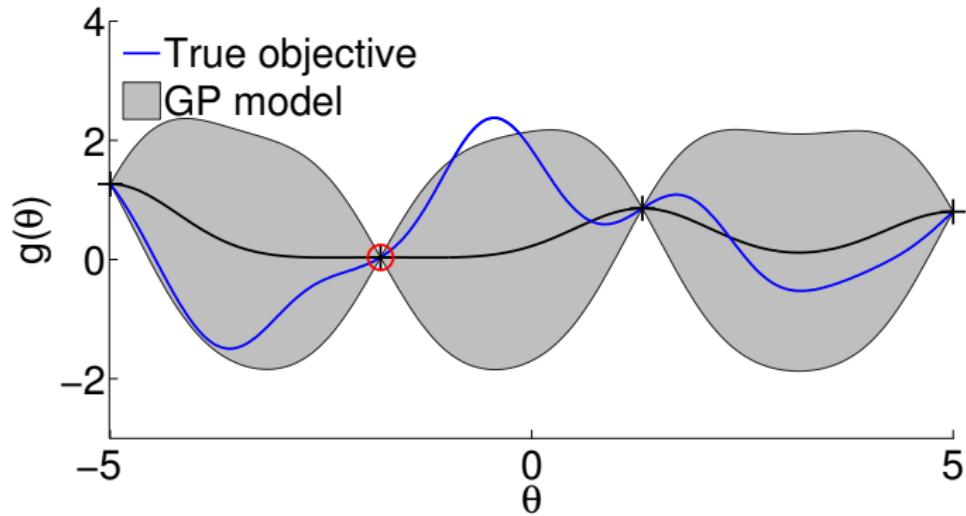
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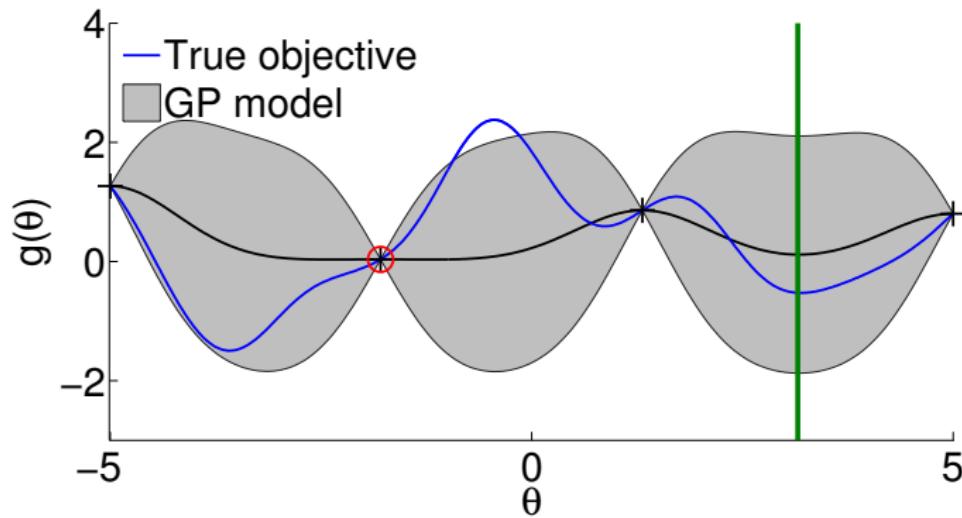
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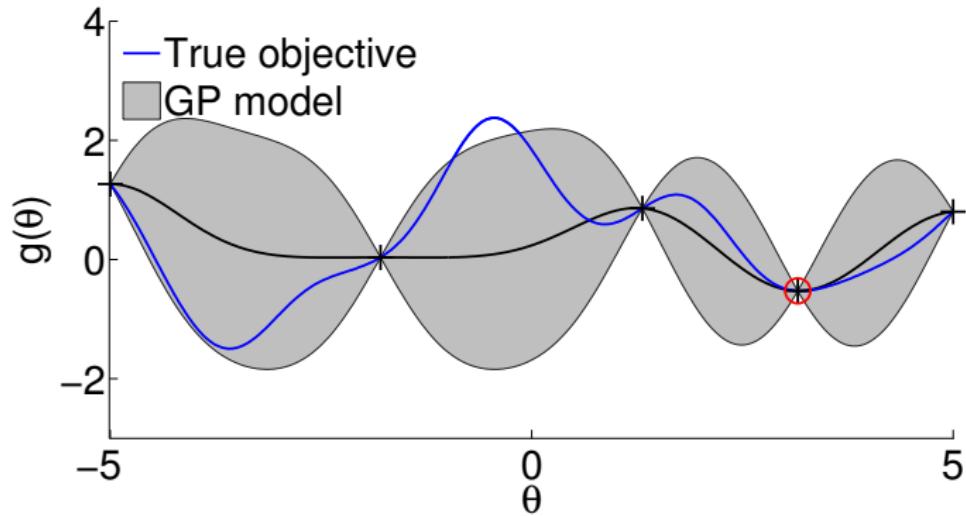
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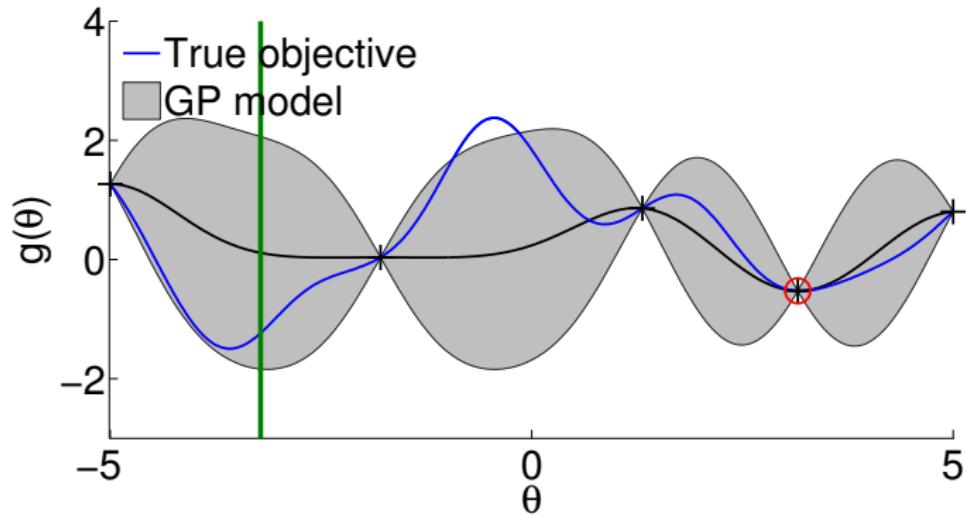
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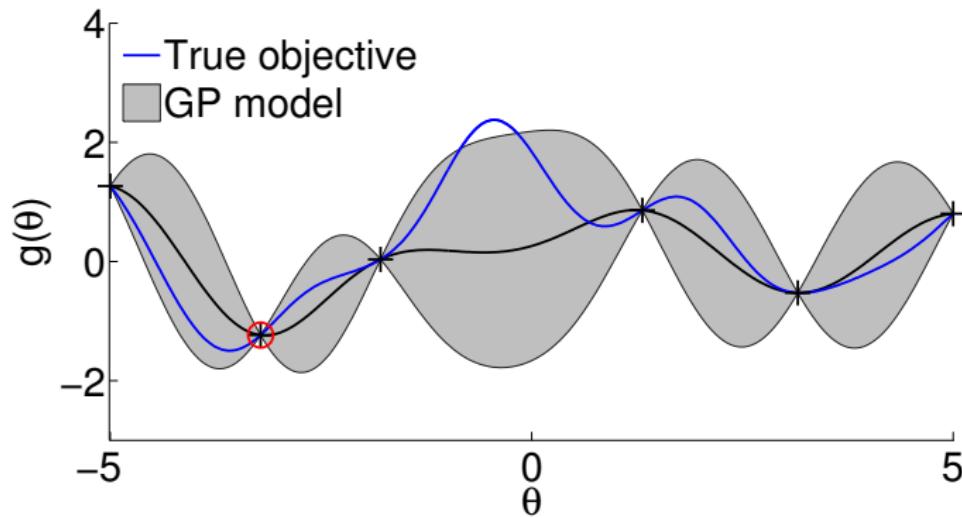
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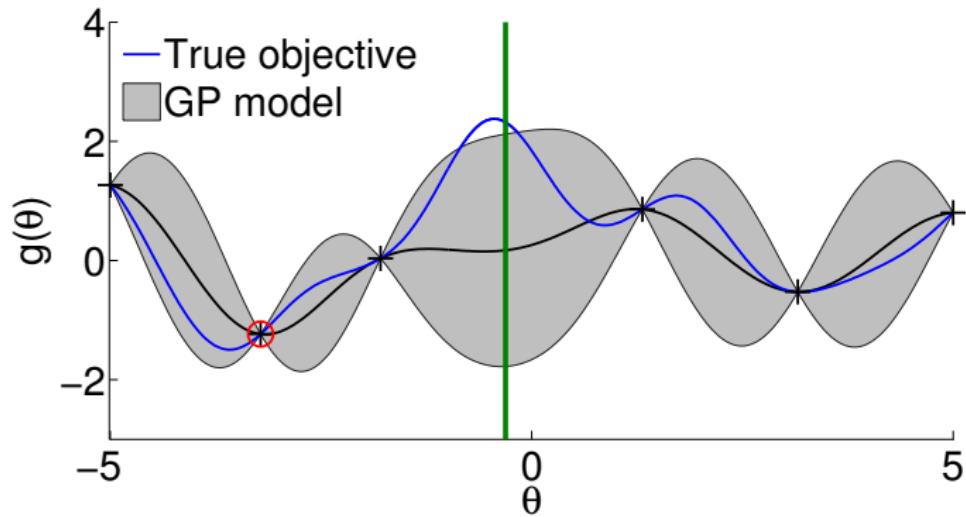
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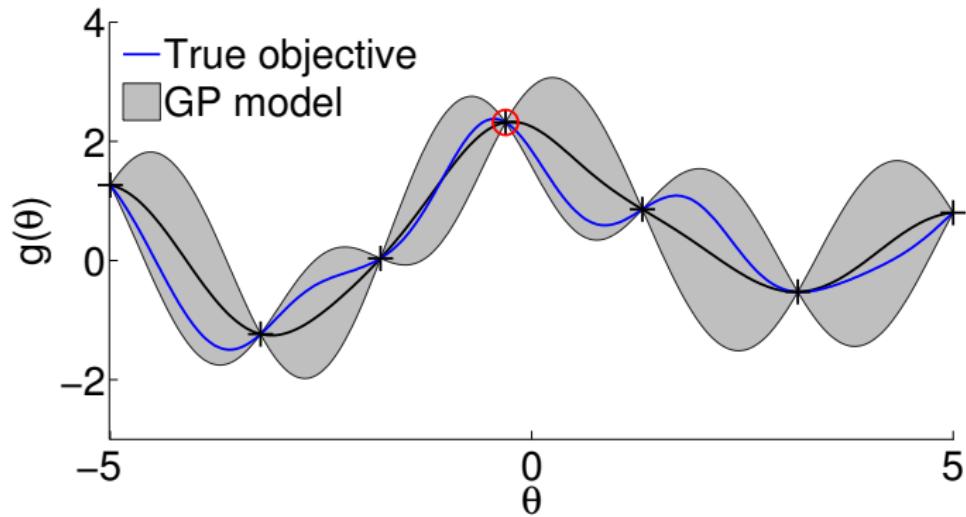
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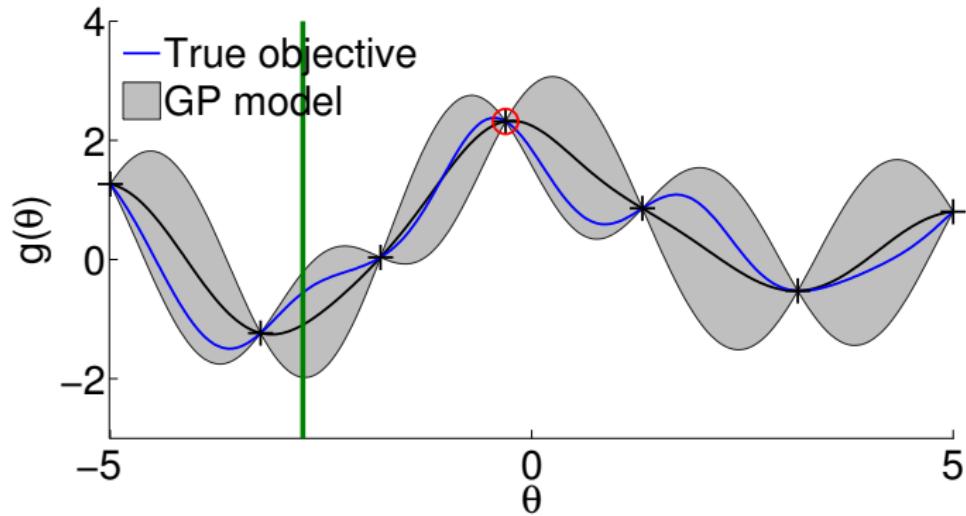
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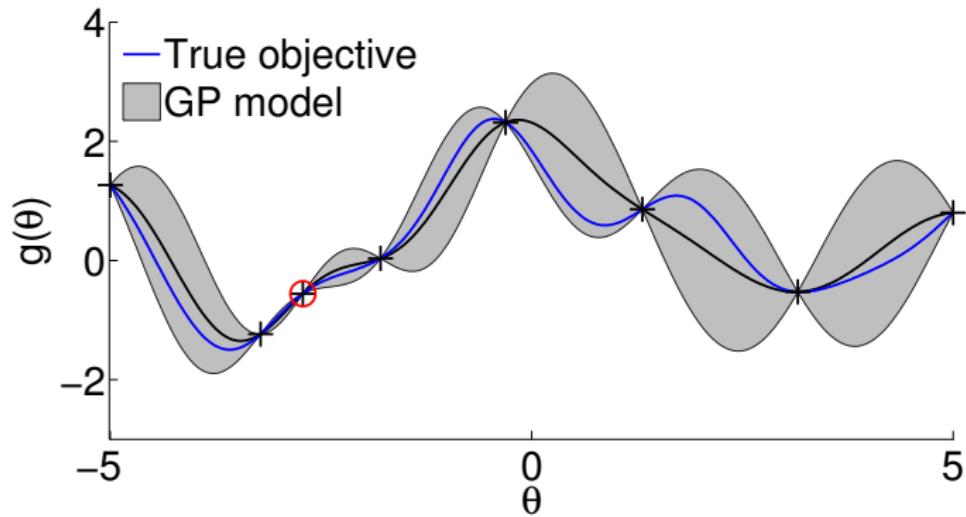
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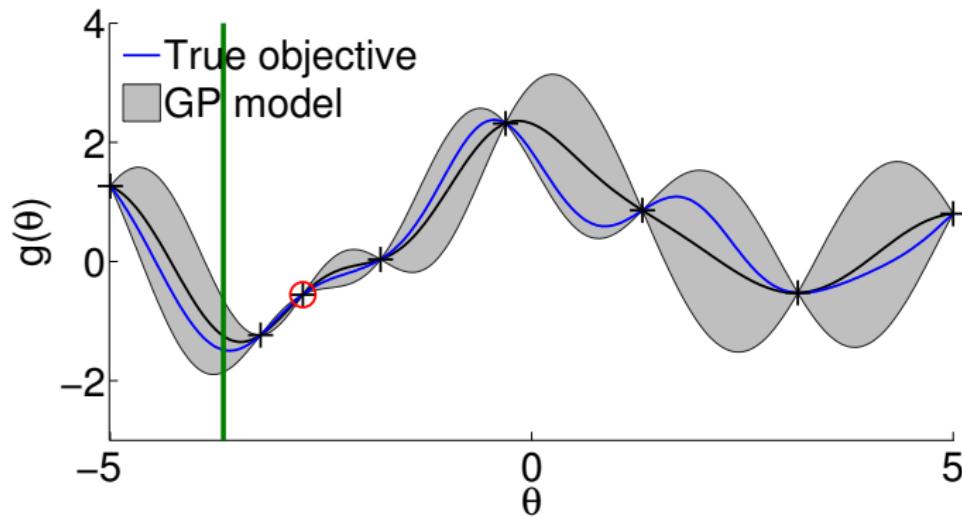
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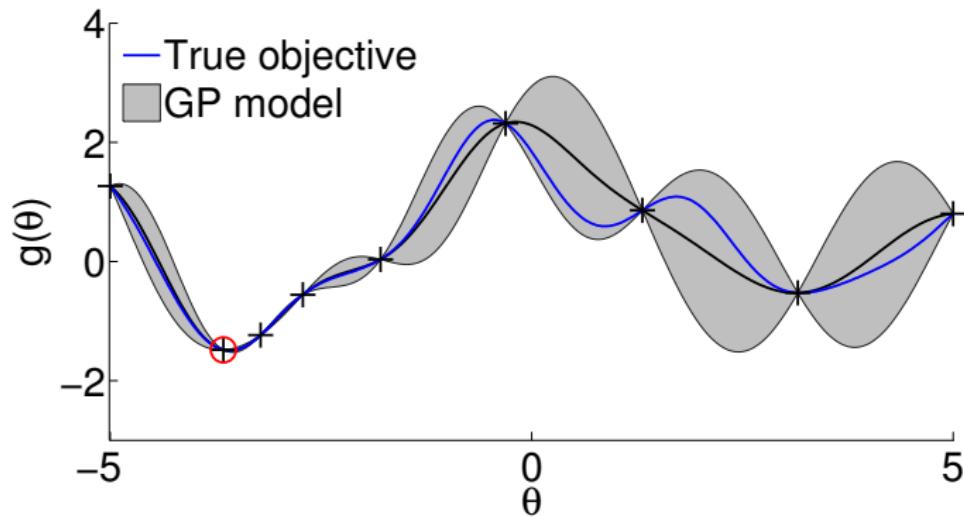
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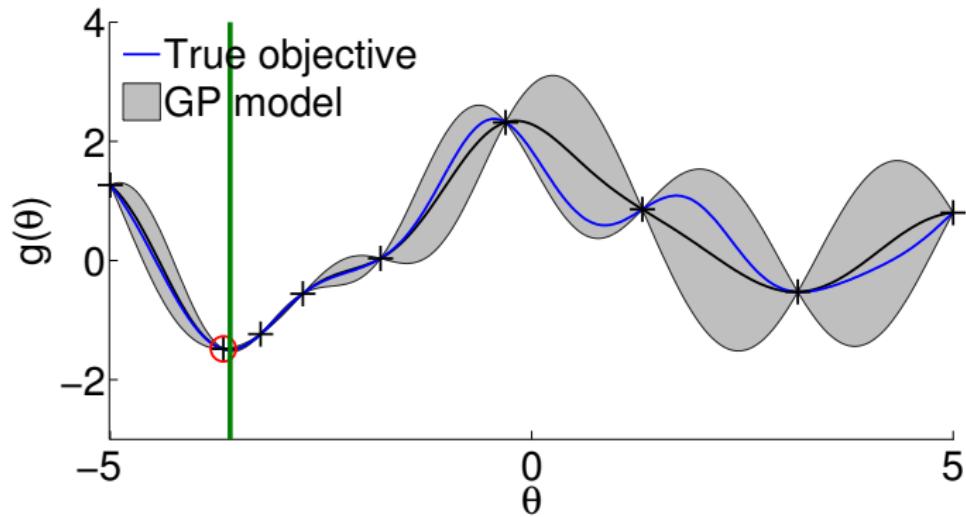
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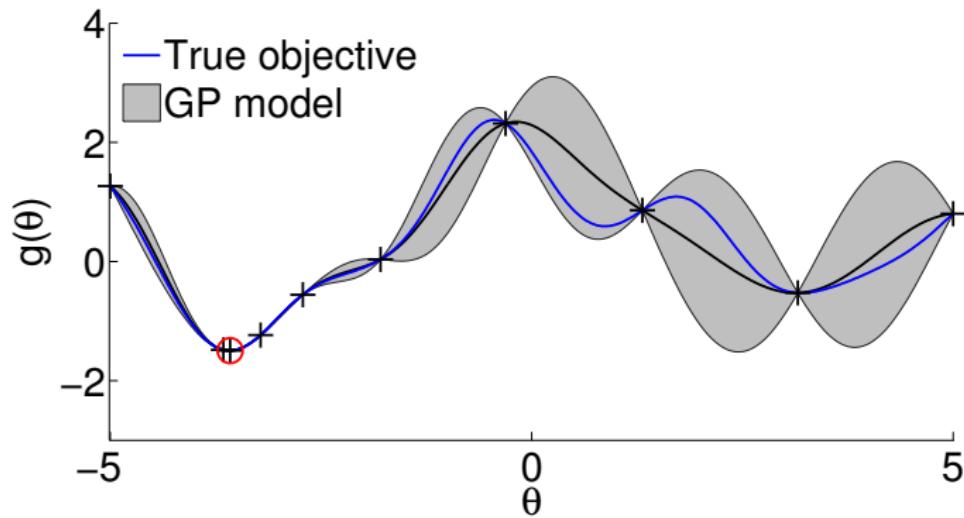
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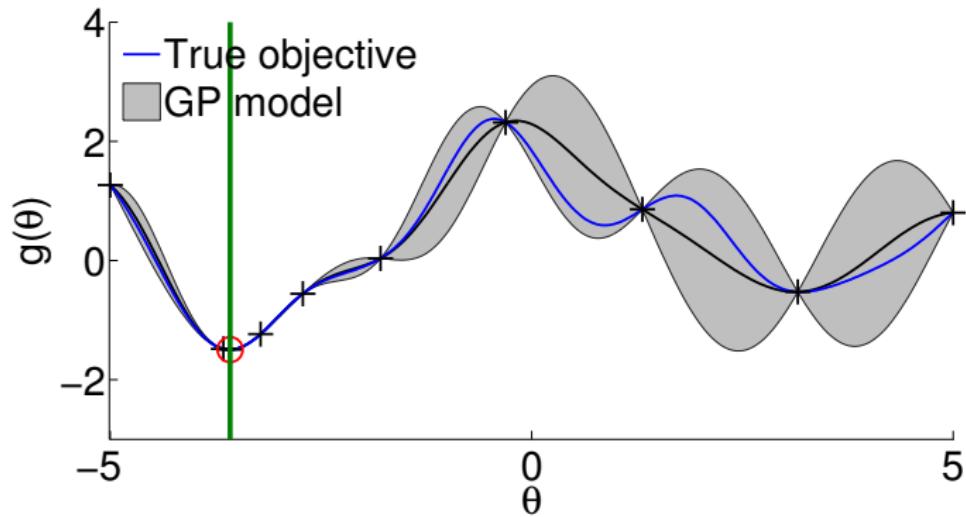
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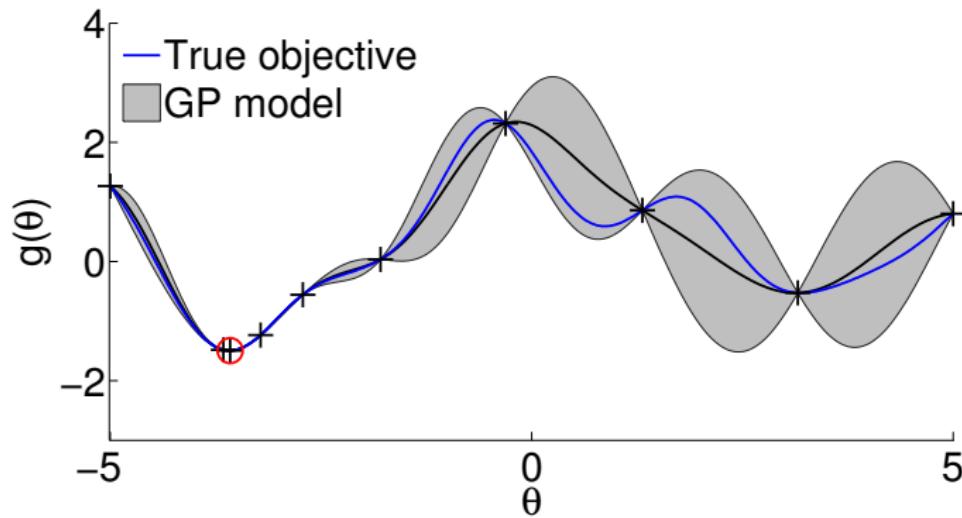
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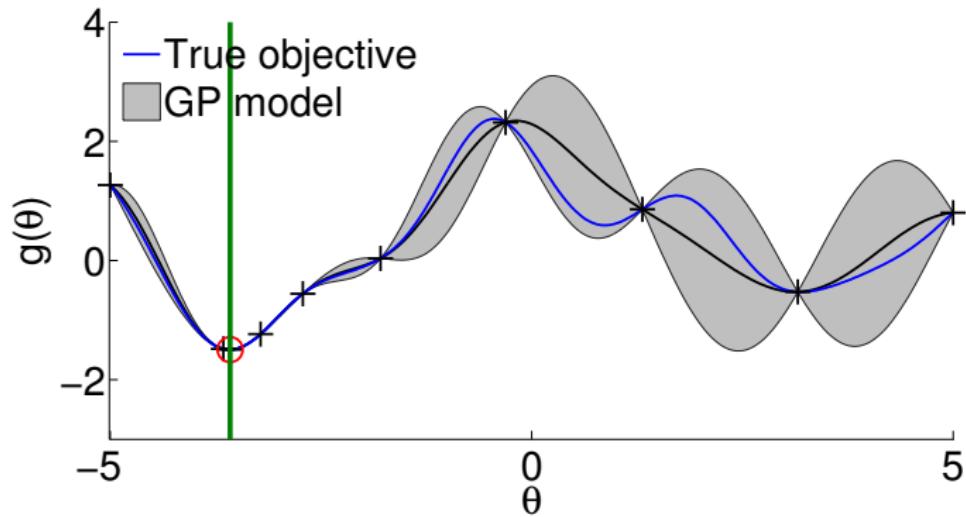
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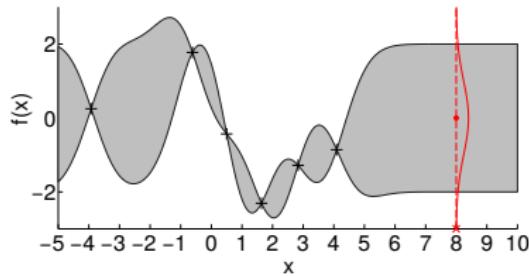


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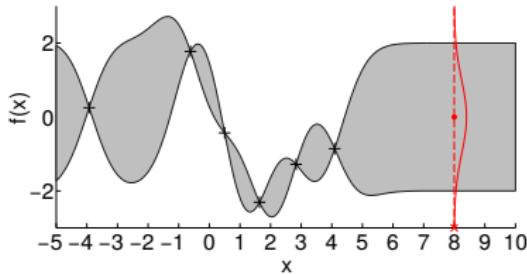
Choosing the Next Point to Evaluate the True Objective: Acquisition Functions

Using Uncertainty in Global Optimization



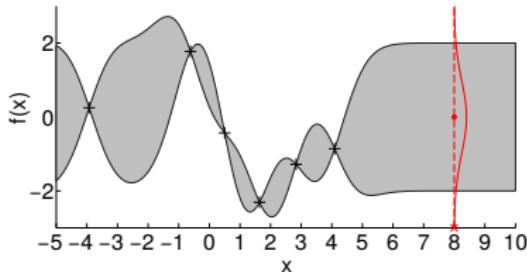
- ▶ Find a good (global) optimum
 - ▶ Need to get out of local optima

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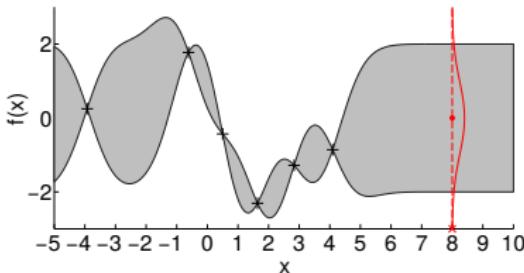
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- ▶ Extrapolate from collected knowledge

Using Uncertainty in Global Optimization



- Find a good (global) optimum
 - ▶ Need to get out of local optima
- Extrapolate from collected knowledge
- GP gives us closed-form means and variances
 - ▶ Trade off exploration and exploitation
 - **Exploration:** Seek places with high variance
 - **Exploitation:** Seek places with low mean

Using Uncertainty in Global Optimization

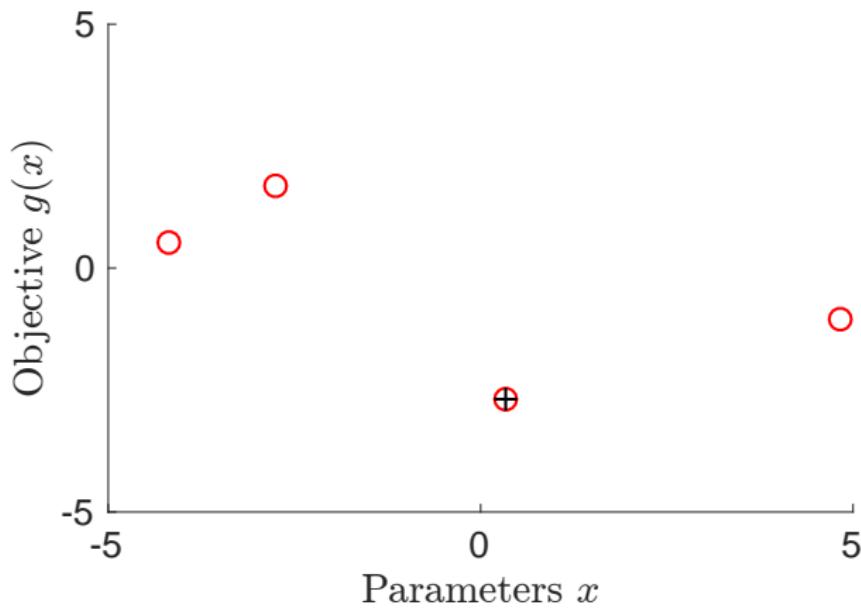


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 - **Exploration:** Seek places with high variance
 - **Exploitation:** Seek places with low mean
- **Acquisition function α** trades off exploration and exploitation for our proxy optimization

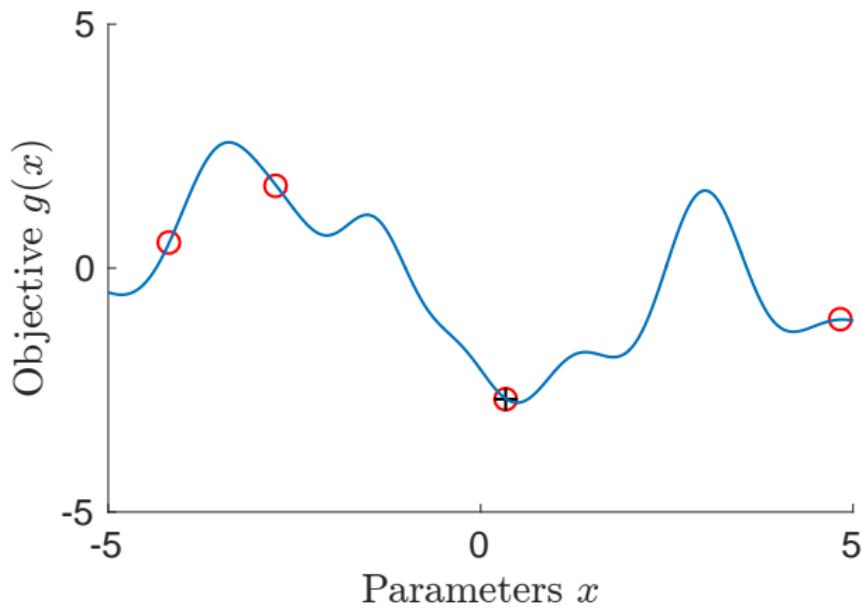
Key Steps (Pseudo-Code)

- 1: **Init:** Data set $\mathcal{D}_0 = \{X_0, y_0\}$
- 2: **for** iterations $t = 1, 2, \dots$ **do**
- 3: Update GP using data \mathcal{D}_{t-1}
- 4: Select $x_t = \arg \max_x \alpha(x)$ by optimizing acquisition function
- 5: Query true objective g at x_t
- 6: Augment data set $\mathcal{D}_t = \mathcal{D}_{t-1} \cup \{(x_t, y_t)\}$
- 7: **end for**
- 8: **Return** best input in data set: $x^* = \arg \min_x y(x)$

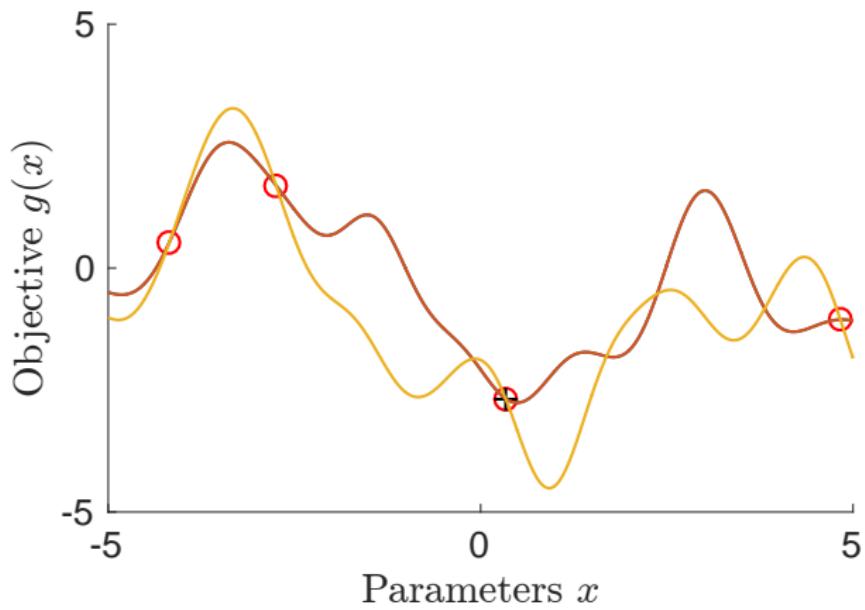
Where to Evaluate Next?



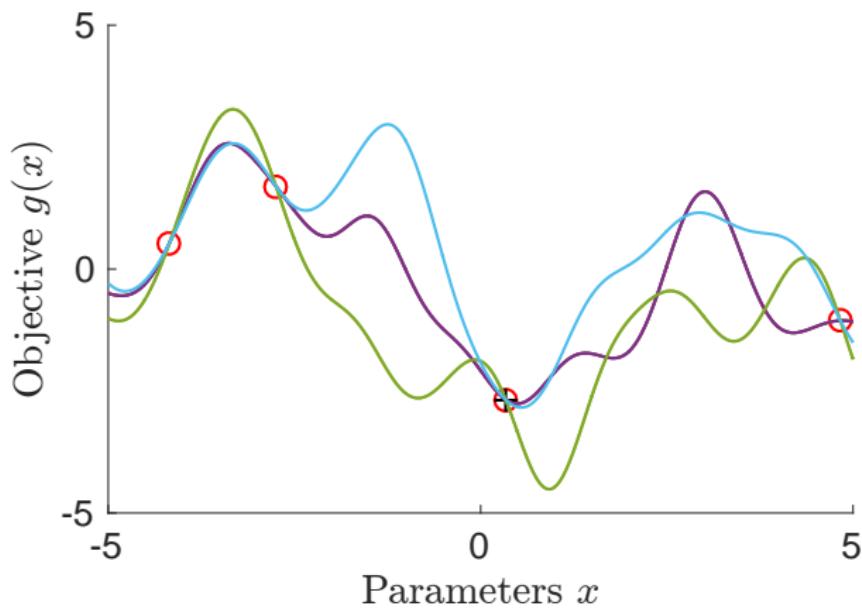
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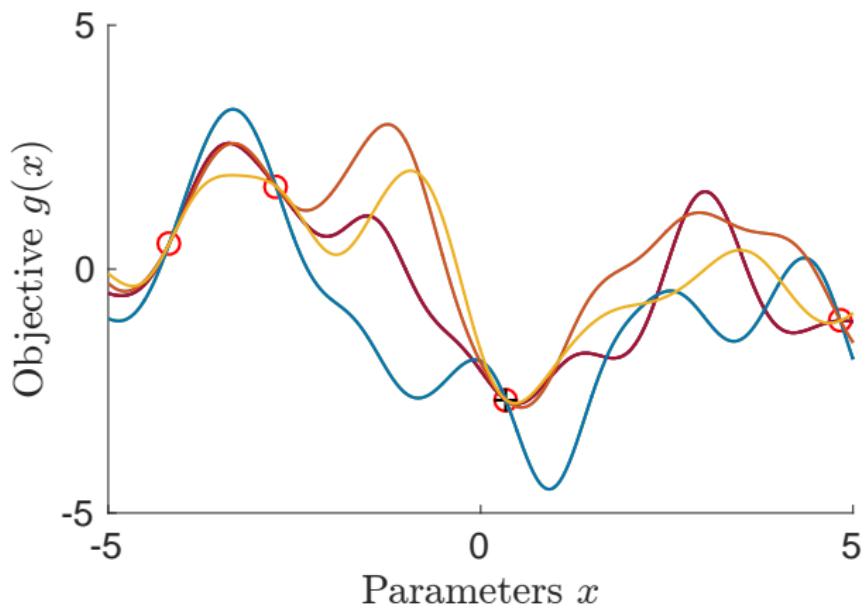
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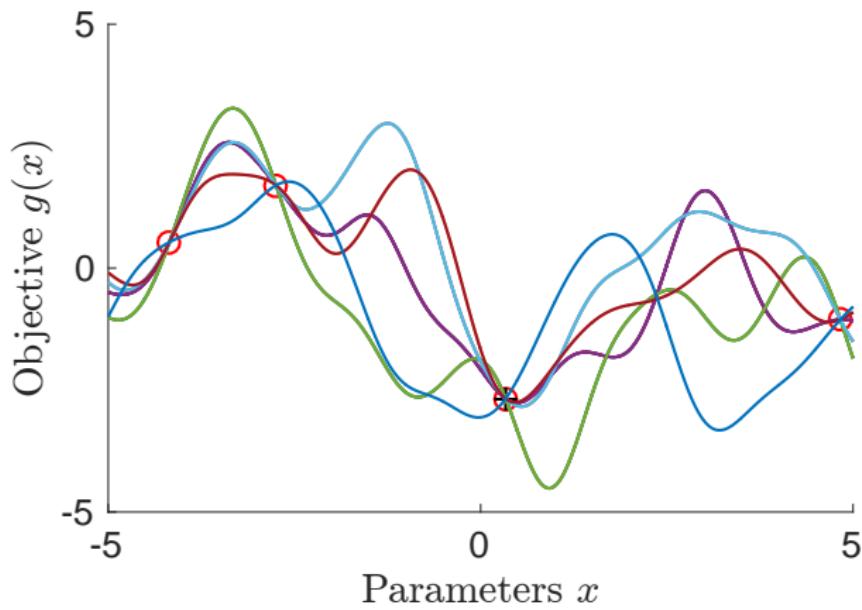
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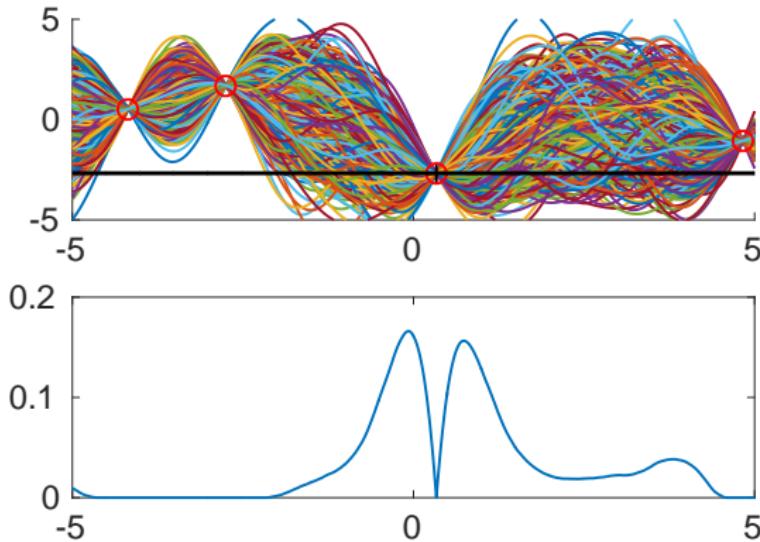
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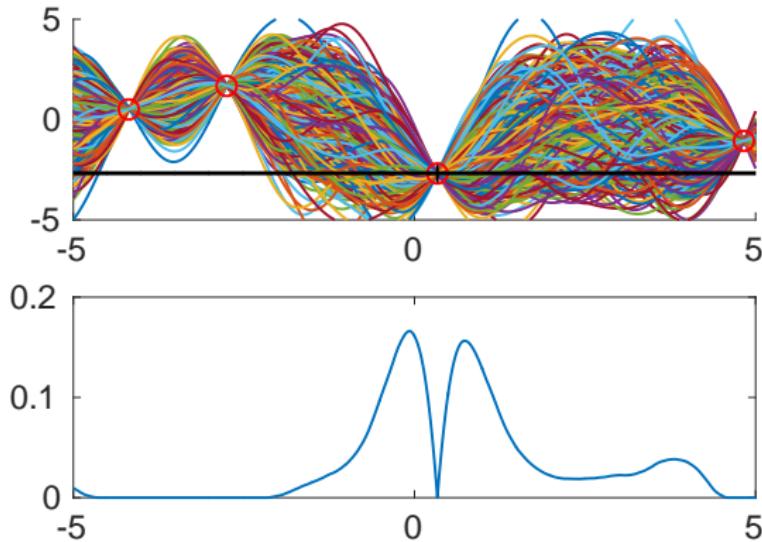


Where to Evaluate Next to Improve Most?



- Upper panel: Samples from a probabilistic proxy \tilde{g}

Where to Evaluate Next to Improve Most?



- ▶ Upper panel: Samples from a probabilistic proxy \tilde{g}
- ▶ Lower panel: Corresponding **expected improvement** over the best solution so far (black cross)
- ▶ Evaluate g at the maximum of the expected improvement

Closed-Form Acquisition Functions

- For all $\mathbf{x} \in \mathbb{R}^D$ the GP posterior gives a predictive mean $\mu(\mathbf{x})$ variance $\sigma^2(\mathbf{x})$
- Define

$$\gamma(\mathbf{x}) = \frac{f(\mathbf{x}_{\text{best}}) - \mu(\mathbf{x})}{\sigma(\mathbf{x})}$$

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- Probability of Improvement (Kushner 1964):**

$$\alpha_{\text{PI}}(x) = \Phi(\gamma(x))$$

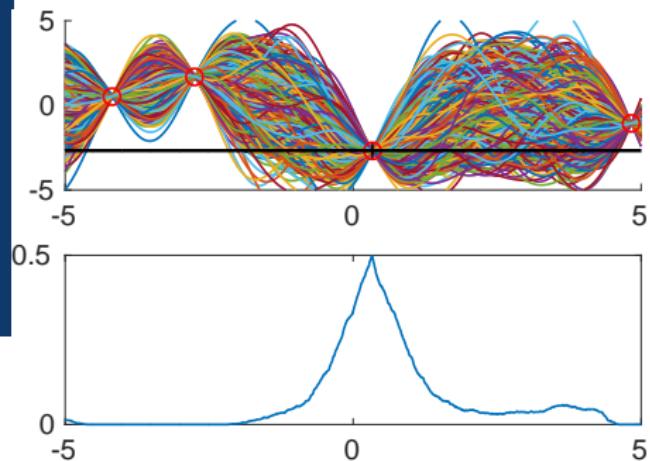
- Expected Improvement (Mockus 1978):**

$$\alpha_{\text{EI}}(x) = \sigma(x)(\gamma(x)\Phi(\gamma(x)) + \mathcal{N}(\gamma(x) | 0, 1))$$

- GP Lower Confidence Bound (Srinivas et al., 2010):**

$$\alpha_{\text{LCB}}(x) = -(\mu(x) - \kappa\sigma(x)), \quad \kappa > 0$$

Probability of Improvement (1)

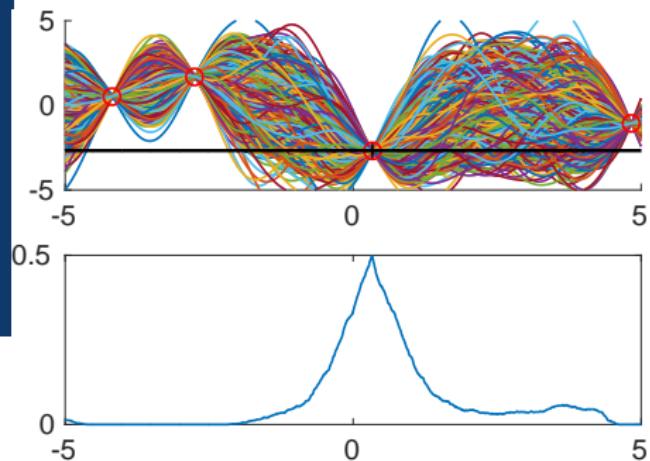


- Idea: Determine the probability that x_* leads to a better function value than the currently best one $f(x_{\text{best}})$
- Sampling-based setting:
Sample N functions f_i ; at every input x compute a Monte-Carlo estimate

$$\alpha_{\text{PI}}(x) = p(f(x) < f(x_{\text{best}})) \approx \frac{1}{N} \sum_{i=1}^N \delta(f_i(x) < f(x_{\text{best}}))$$

- Can lead to continued exploitation in an ϵ -region around x_{best} .

Probability of Improvement (1)

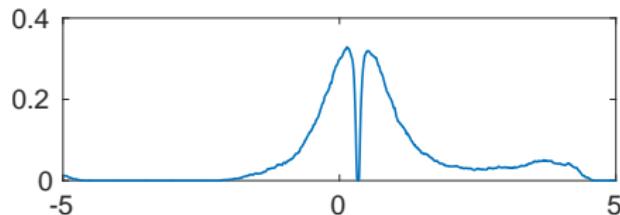
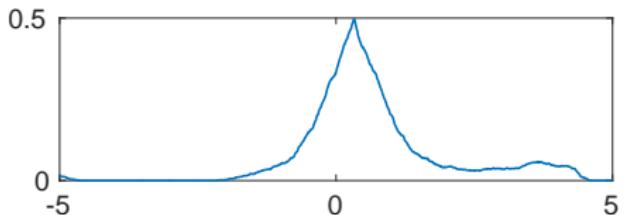
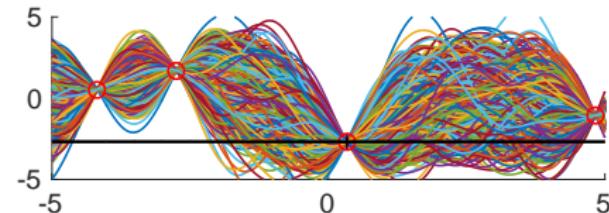
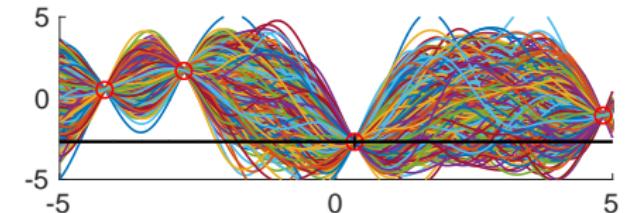


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- ▶ Can lead to continued exploitation in an ϵ -region around x_{best} .
- ▶ Introduce a “slack variable” ξ for more aggressive exploration

Probability of Improvement (2)



- ▶ Look at a minimum improvement of $\xi > 0$:

$$\alpha_{\text{PI}}(\mathbf{x}) = p(f(\mathbf{x}) < f(\mathbf{x}_{\text{best}}) - \xi) \approx \frac{1}{N} \sum_{i=1}^N \delta(f_i(\mathbf{x}) < f(\mathbf{x}_{\text{best}}) - \xi)$$

- ▶ If $f \sim GP$ and $p(f(\mathbf{x})) = \mathcal{N}(\mu(\mathbf{x}), \sigma(\mathbf{x}))$:

$$\alpha_{\text{PI}}(\mathbf{x}) = \Phi(\gamma(\mathbf{x}, \xi)), \quad \gamma(\mathbf{x}, \xi) = \frac{f(\mathbf{x}_{\text{best}}) - \xi - \mu(\mathbf{x})}{\sigma(\mathbf{x})}$$

Expected Improvement

- Idea: Quantify the amount of improvement

- Sampling-based scenario,
where $f_i \sim p(f)$:

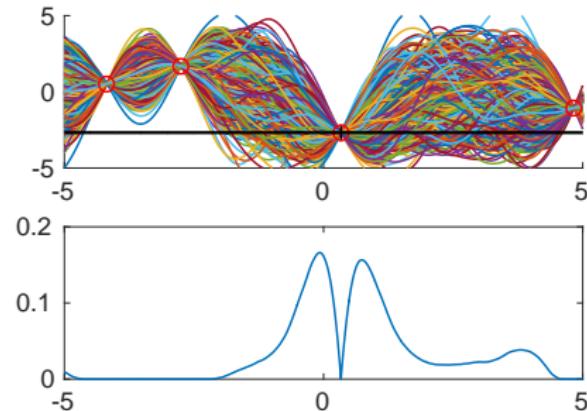
$$\alpha_{\text{EI}}(\mathbf{x}) = \mathbb{E}[\max\{0, f(\mathbf{x}_{\text{best}}) - f(\mathbf{x})\}]$$

$$\approx \frac{1}{N} \sum_{i=1}^N \max\{0, f(\mathbf{x}_{\text{best}}) - f_i(\mathbf{x})\}$$

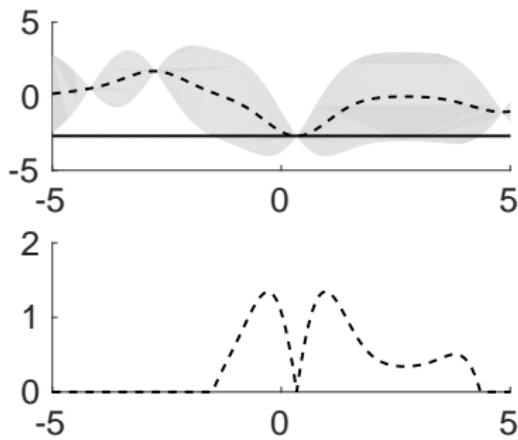
- If $f \sim GP$, we have a closed-form expression:

$$\alpha_{\text{EI}}(\mathbf{x}) = \sigma(\mathbf{x})(\gamma(\mathbf{x})\Phi(\gamma(\mathbf{x})) + \mathcal{N}(\gamma(\mathbf{x}) | 0, 1))$$

- Slack-variable approach also possible (similar to PI)



GP-Lower Confidence Bound (1)

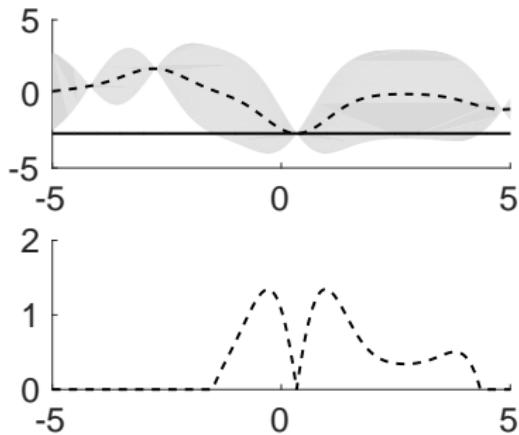


- Use the predictive mean $\mu(x)$ and variance $\sigma^2(x)$ of the GP prediction directly for targeted exploration by means of the acquisition function

$$\alpha_{LCB}(x_t) = -(\mu(x_t) - \sqrt{\kappa}\sigma(x_t))$$

In practice: Use $\max\{0, f(x_{\text{best}}) - \alpha_{LCB}(x_t)\}$

GP-Lower Confidence Bound (2)



- More generally, we can get regret bounds for iteration-dependent κ (Srinivas et al., 2010)

$$\alpha_{\text{LCB}}(\mathbf{x}_t) = -(\mu(\mathbf{x}_t) - \sqrt{\kappa_t} \sigma(\mathbf{x}_t))$$

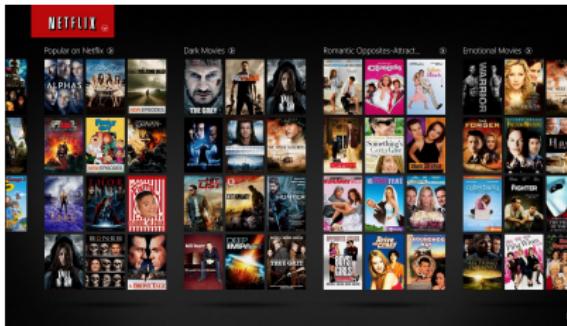
where $\kappa_t \in \mathcal{O}(\log t)$ grows with the iteration t

Optimizing the Acquisition Function

- ▶ Optimizing the acquisition function **requires us to run a global optimizer inside Bayesian optimization**
- ▶ What have we gained?

Optimizing the Acquisition Function

- Optimizing the acquisition function **requires us to run a global optimizer inside Bayesian optimization**
- What have we gained?
- Evaluating the acquisition function is cheap compared to evaluating the true objective
- We can afford evaluating it many times



Application Example: Controller Learning in Robotics (Calandra et al., 2016)

- Fragile bipedal robot
 - ▶ Only few experiments feasible
- Maximize robustness and walking speed
- 4 motors:
 - 2 actuated hips + 2 actuated knees
- Controller implemented as a finite-state-machine (8 parameters)



Calandra et al. (2015)

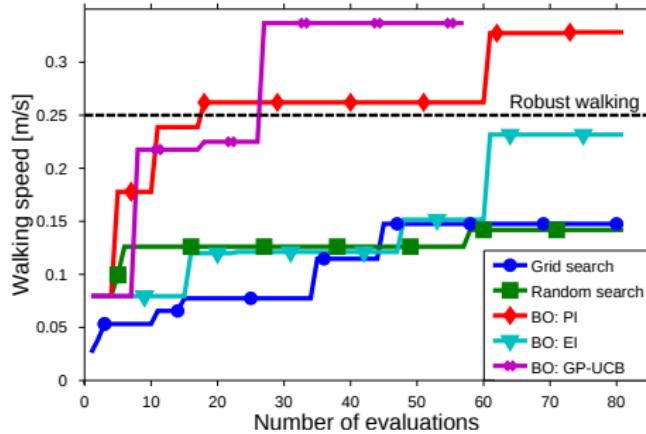
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- ▶ 4 motors:
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- ▶ Controller implemented as a finite-state-machine (8 parameters)
- ▶ Good parameters found after 80–100 experiments
- ▶ **Substantial speed-up** compared to manual parameter search



Calandra et al. (2015)

Comparison



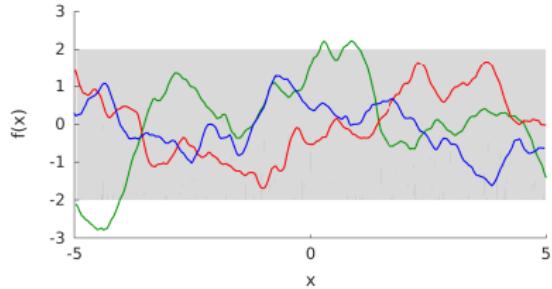
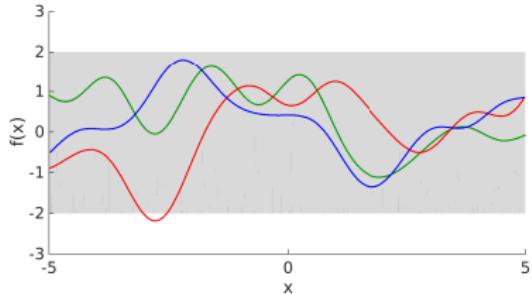
- Squared exponential covariance function
- Learned GP hyper-parameters (no MCMC for integrating them out)

Limitations

- Getting the function model wrong can be catastrophic
- Limited scalability in the number of dimensions and/or evaluations of the true objective function

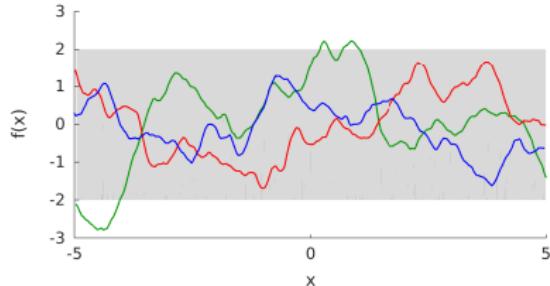
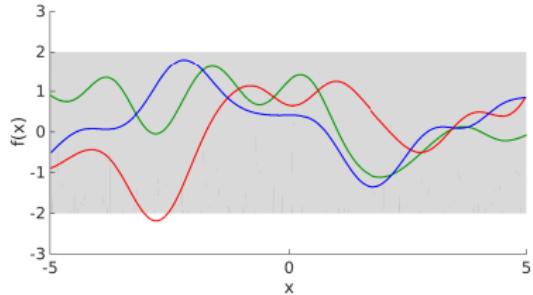
Why?

Poor Model Choice



- Covariance function selection is crucial for good performance
 - Choose a sufficiently flexible and adaptive kernel, e.g., Matérn (but not the squared exponential)

Poor Model Choice



- Covariance function selection is crucial for good performance
 - ▶ Choose a sufficiently flexible and adaptive kernel, e.g., Matérn (but not the squared exponential)
- Nice side-effect of Matérn: Exploration is more encouraged than with the squared exponential kernel

Choosing Covariance Functions

- Structured SVM for Protein Motif Finding (Miller et al., 2012)
- Optimize hyper-parameters of SSVM using BO (Snoek et al., 2012)

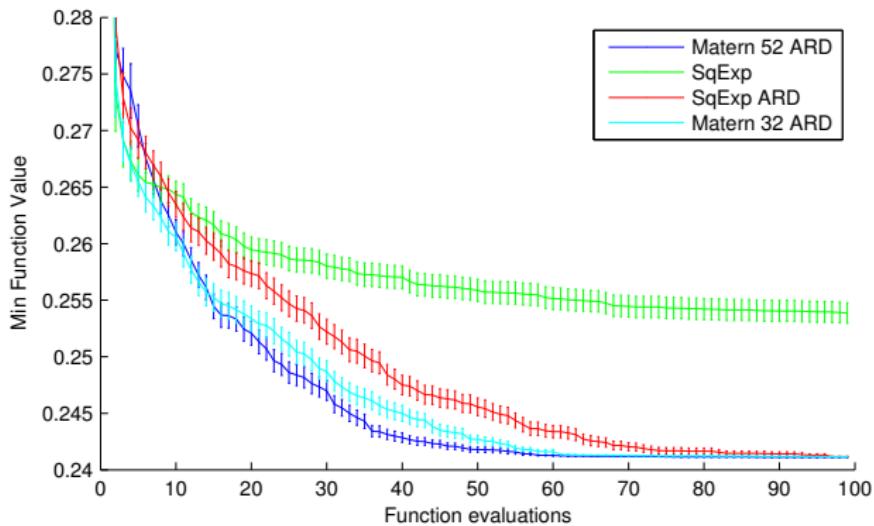


Figure: Figure from Snoek et al. (2012)

Gaussian Process Hyper-Parameters

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Gaussian Process Hyper-Parameters

- Empirical Bayes (maximize the marginal likelihood) can fail horribly, especially in the early stages of Bayesian optimization when we have only a few data points
- Solution: Integrate out the GP hyper-parameters θ by Markov Chain Monte Carlo (MCMC) sampling (e.g., slice sampling)
- Look at integrated acquisition function

$$\begin{aligned}\alpha(x) &= \mathbb{E}_\theta[\alpha(x, \theta)] = \int \alpha(x, \theta) p(\theta) d\theta \\ &\approx \frac{1}{K} \sum_{k=1}^K \alpha(x, \theta^{(k)}), \quad \theta^{(k)} \sim \underbrace{p(\theta | X_n, y_n)}_{\text{hyper-parameter posterior}}\end{aligned}$$

Integrating out GP Hyper-parameters

- ▶ Online LDA (Hoffman et al., 2010) for topic modeling
- ▶ Two critical hyper-parameters that control the learning rate learned by BO (Snoek et al., 2012)

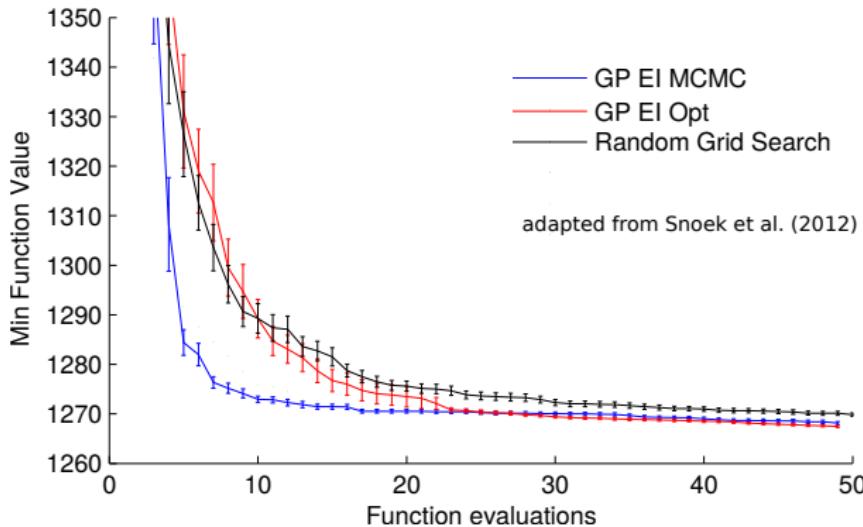
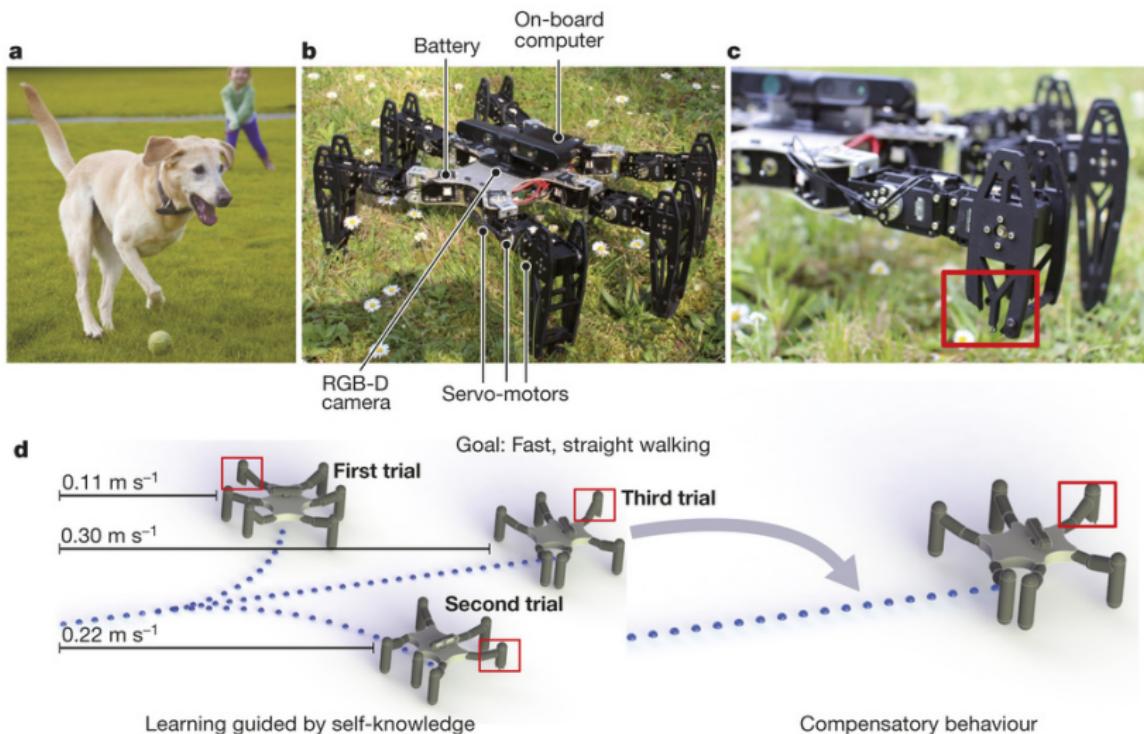


Figure: Figure from Snoek et al. (2012)

Robots That Learn to Recover from Damage



Cully et al. (2015)

Further Topics in BO

- **Entropy-based acquisition functions:** Directly describe the distribution over the best input location (Hennig & Schuler, 2012; Hernández-Lobato et al., 2014)
- **Non-myopic** Bayesian optimization (Osborne et al., 2009)
- **High-dimensional** optimization (Wang et al., 2016)
- **Large-scale** Bayesian optimization (Hutter et al., 2014)
- **Non-GP** Bayesian optimization (Hutter et al., 2014; Snoek et al., 2015)
- **Constraints** (e.g., Gelbart et al., 2014)
- **Automated machine learning** (e.g., Feurer et al., 2015)
- **Multi-tasking, parallelizing, resource allocation, ...** (e.g., Swersky et al., 2014; Snoek et al., 2012)

Software

- **BayesOpt** <https://bitbucket.org/rmcantin/bayesopt/> (Martinez-Cantin, 2014)
- **Spearmint** <https://github.com/HIPS/Spearmint>
- **Pybo** <https://github.com/mwhoffman/pybo> (Hoffman & Shariari)
- **GPyOpt** <https://github.com/SheffieldML/GPyOpt> (Gonzalez et al.)
- Matlab toolbox (bayesopt)

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