

Bayesian Optimization

Partially based on tutorial by Ryan Adams

<http://tinyurl.com/botutorial>

Recommended reading:

Brochu et al. (2009) [1]

Shahriari et al. (2016) [18]

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Machine Learning Meta-Challenges

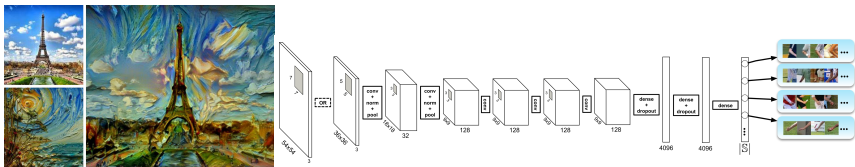
- ▶ Machine learning models are getting more and more complicated
 - ▶▶ Usually more parameters (e.g., deep neural networks)
- ▶ Non-convex optimization methods have many parameters to tune
- ▶▶ Generally hard to apply modern techniques and/or reproduce the results

Machine Learning Meta-Challenges

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Automate the selection of critical hyper-parameters (see also:
[Automated Machine Learning \(AutoML\)](#))

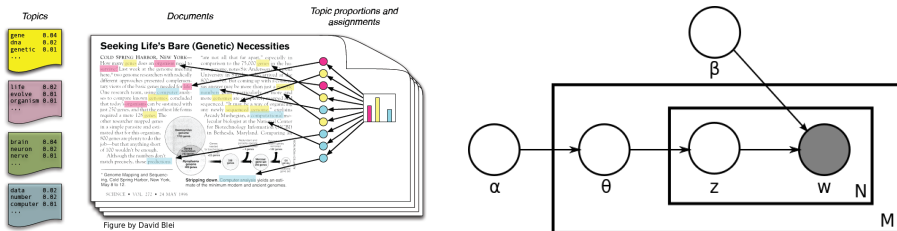
Example: Deep Neural Networks



Huge interest in large neural networks

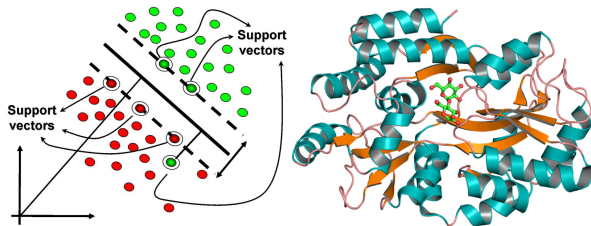
- ▶ When well-tuned, very successful for visual object identification, speech recognition, computational biology, ...
- ▶ Big investments by Google, Facebook, Microsoft, etc.
- ▶ **Many choices:** number of layers, weight regularization, layer size, which nonlinearity, batch size, learning rate schedule,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

Search for Good Hyper-parameters

- Define an objective function
 - Usually, we care about generalization performance.
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 - ▶ Usually, we care about generalization performance.
 - ▶ Cross validation to measure parameter quality
- ▶ Standard search procedures:
 - ▶ Grid search
 - ▶ Random search (very simple, works surprisingly well)
 - ▶ 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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- ▶ **Optimize cheap proxy** function to determine where to evaluate the true objective next

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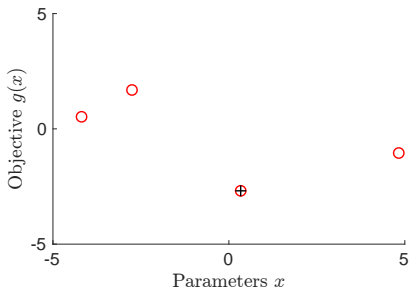
- ▶ Build a **probabilistic proxy model** for the objective using outcomes of past experiments as training data
- ▶ The proxy model is much **cheaper to evaluate** than the original objective
- ▶ **Optimize cheap proxy** function to determine where to evaluate the true objective next
- ▶ Standard proxy: **Gaussian process**

Setting (2)

- ▶ Objective: Find global minimum of objective function g :

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

- ▶ 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)



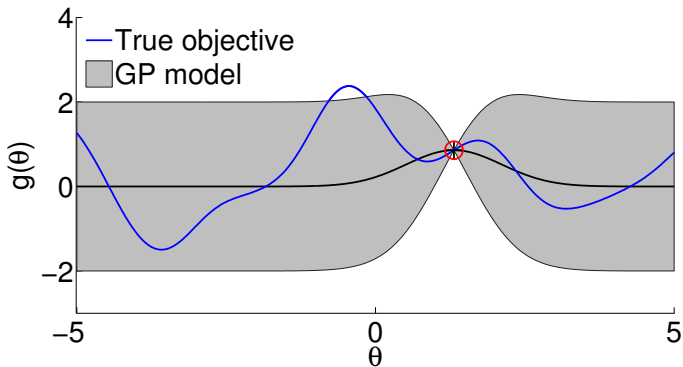
Key Steps

- ▶ 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

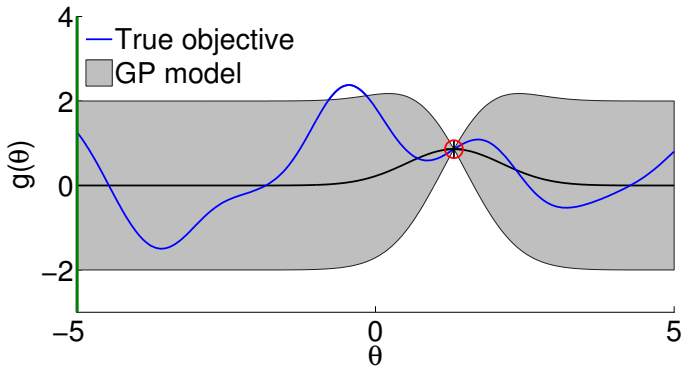
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- ▶ Overall: Evaluate g only once
- ▶ Works well if $\tilde{g} \approx g$.
- ▶ Usually not the case ►► Repeat this cycle and keep updating \tilde{g}

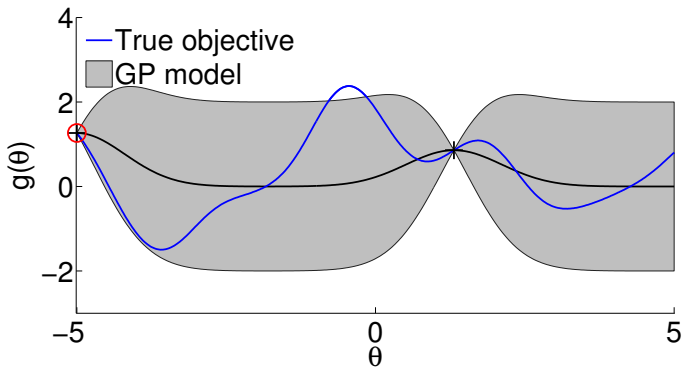
Bayesian Optimization: Illustration



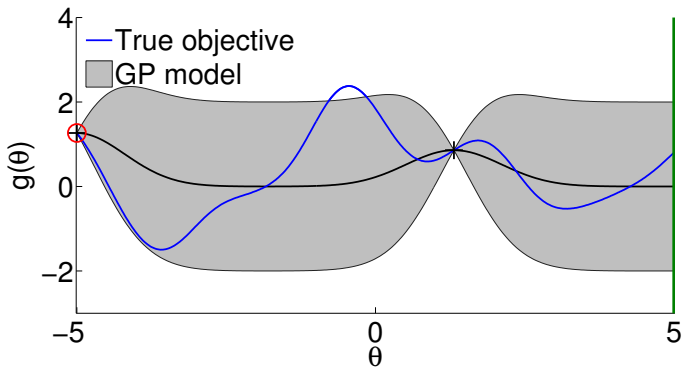
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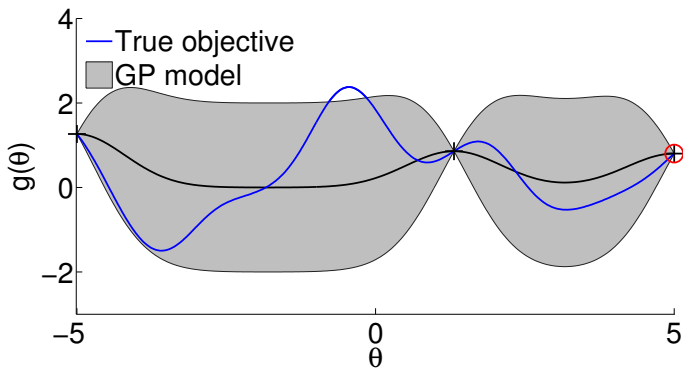
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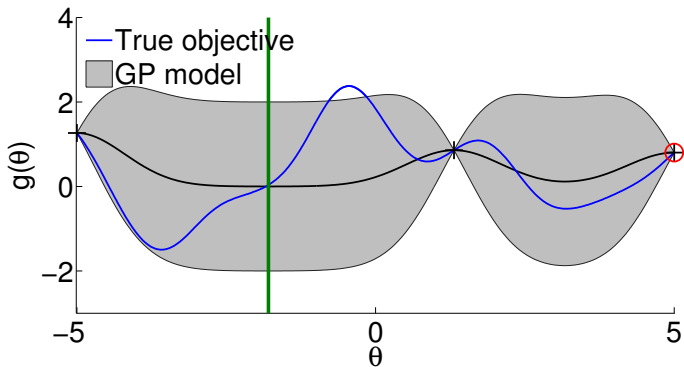
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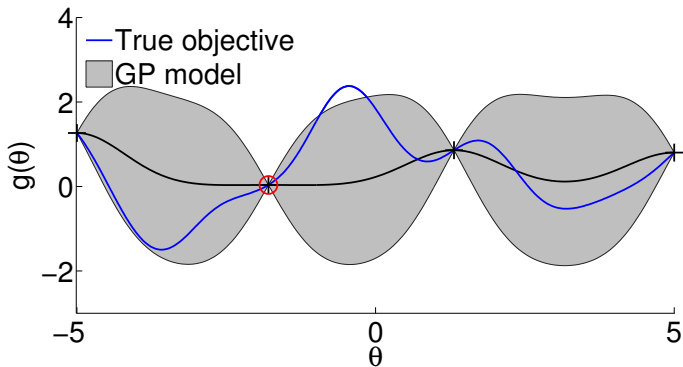
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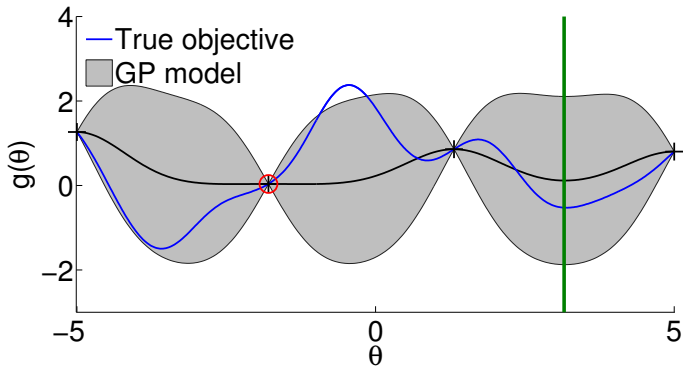
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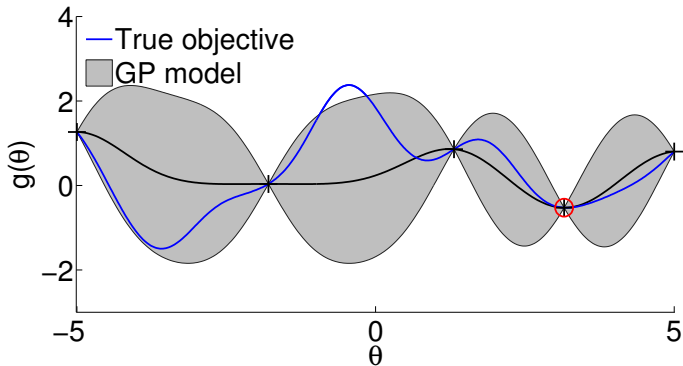
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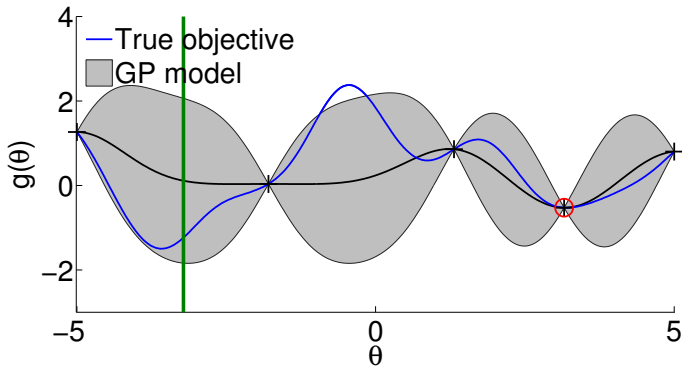
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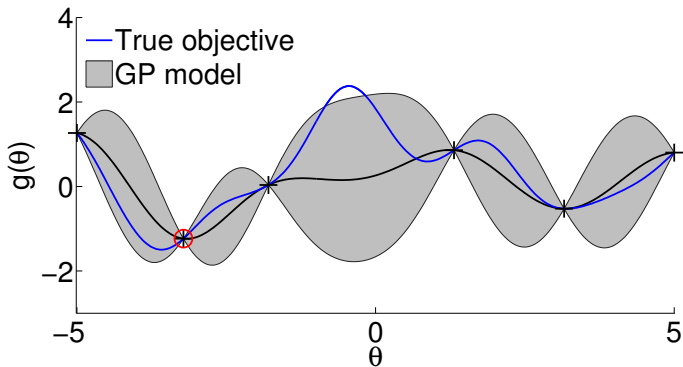
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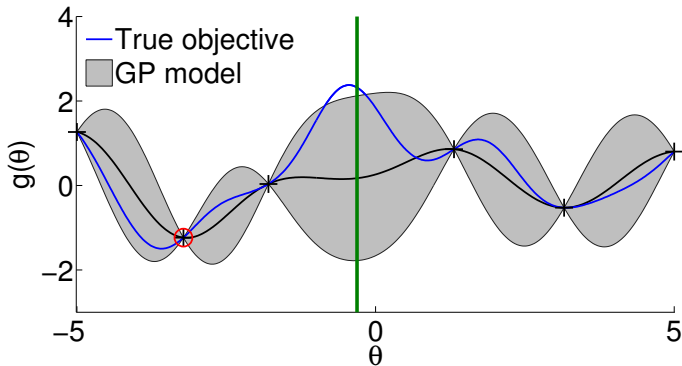
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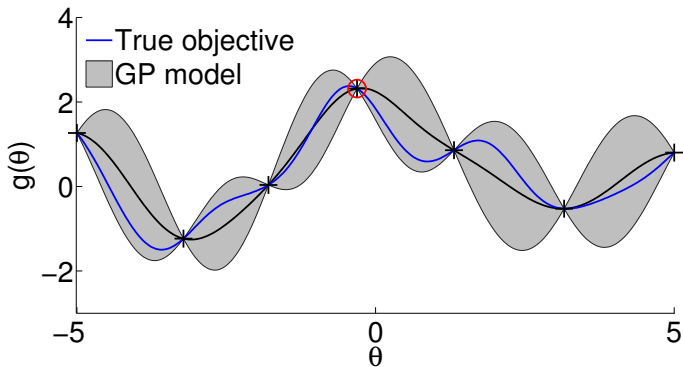
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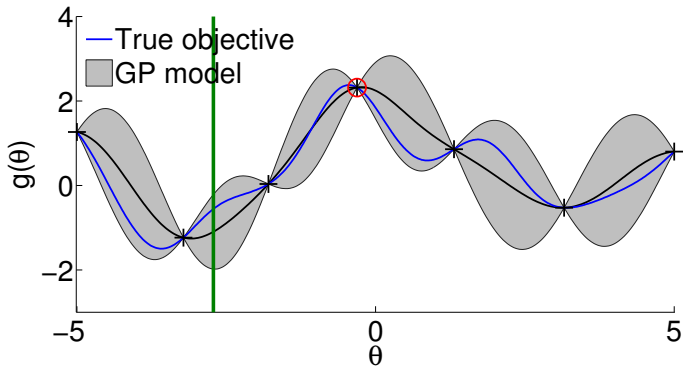
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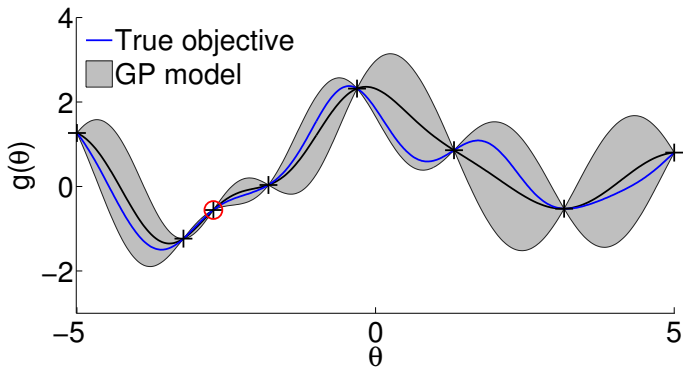
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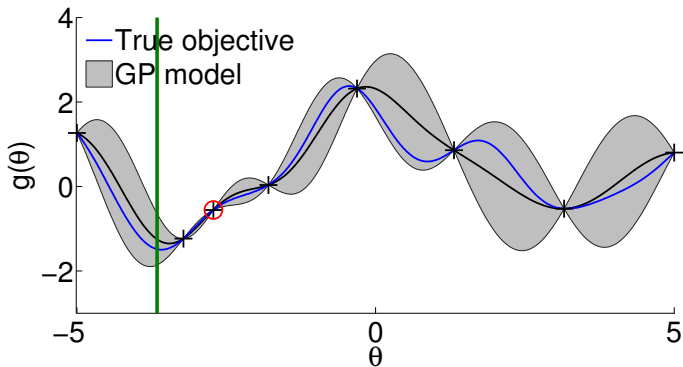
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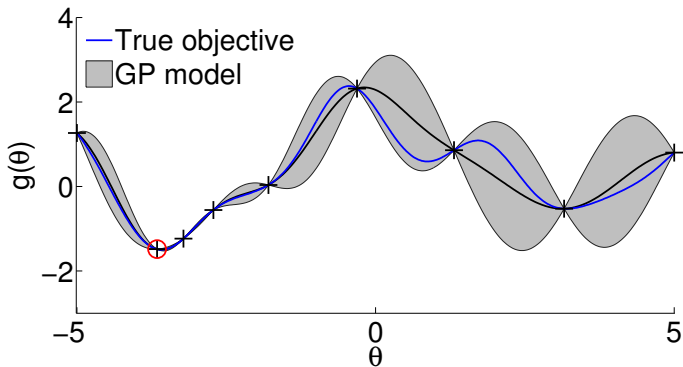
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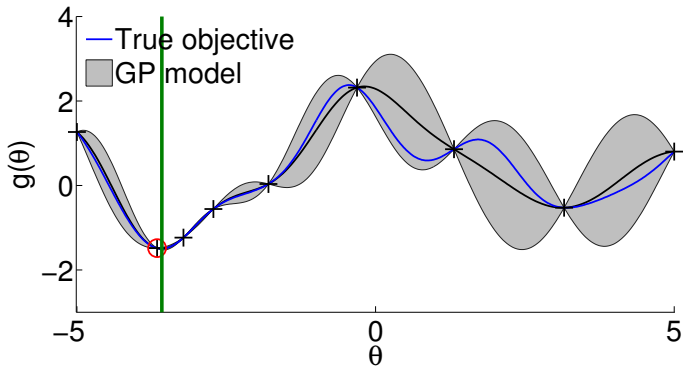
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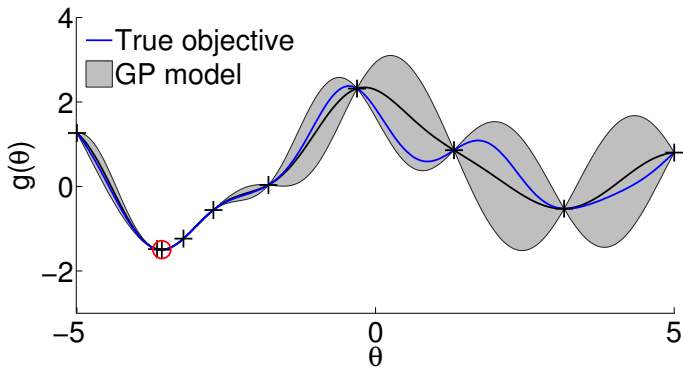
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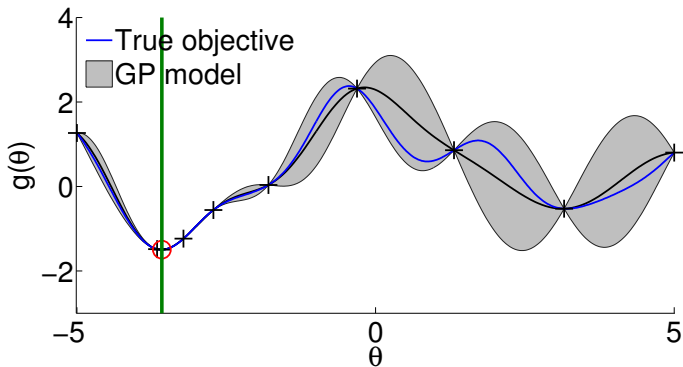
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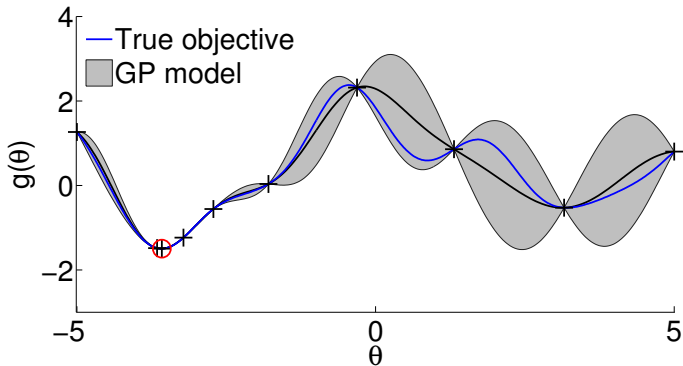
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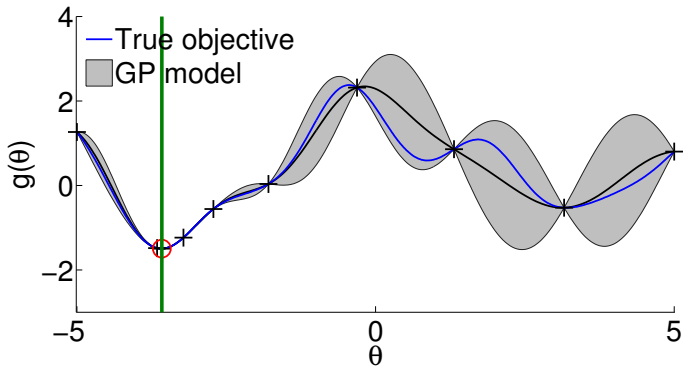
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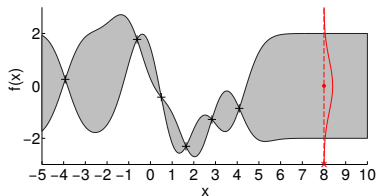


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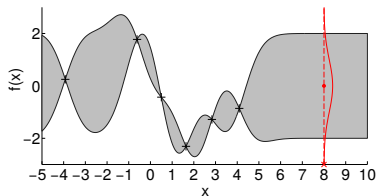
Choosing the Next Point to Evaluate the True Objective: Acquisition Functions

Using Uncertainty in Global Optimization



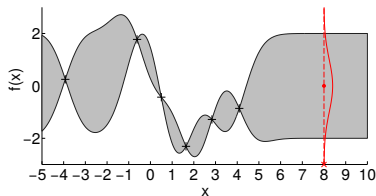
- ▶ Find a good (global) optimum
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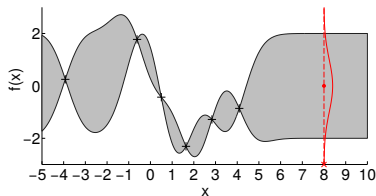
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Using Uncertainty in Global Optimization



- ▶ Find a good (global) optimum
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- ▶ 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

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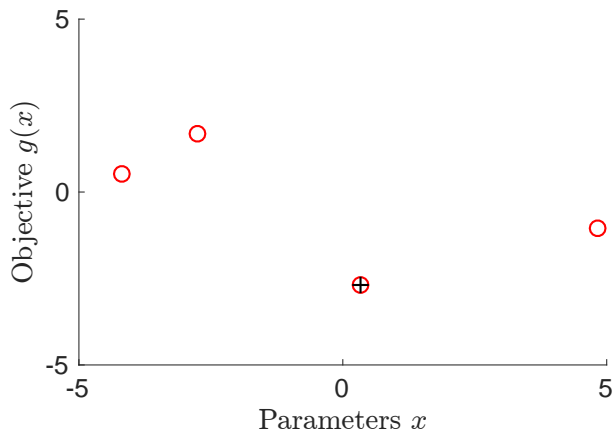


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 - ▶ **Exploration:** Seek places with high variance
 - ▶ **Exploitation:** Seek places with low mean
- ▶ **Acquisition function α trades off exploration and exploitation** for our proxy optimization

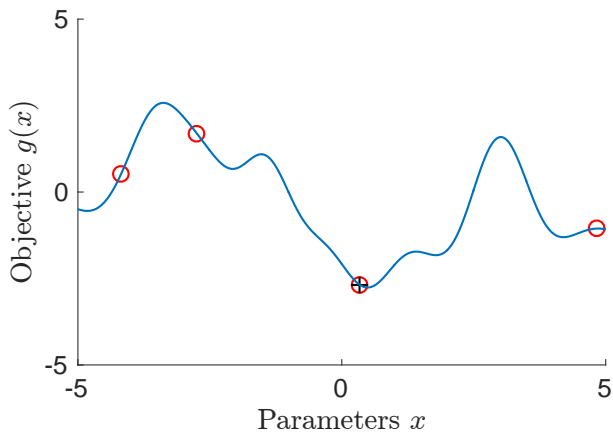
Key Steps (Pseudo-Code)

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

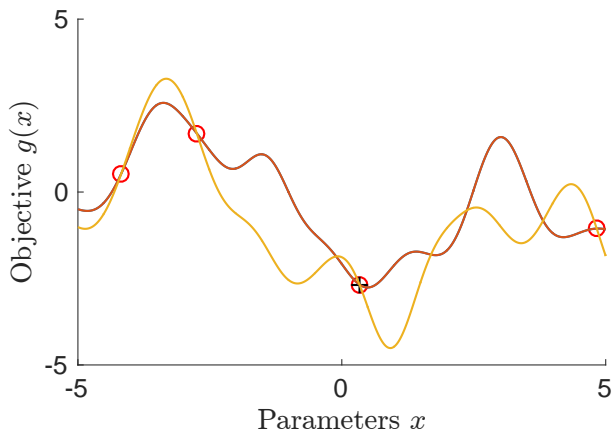
Where to Evaluate Next?



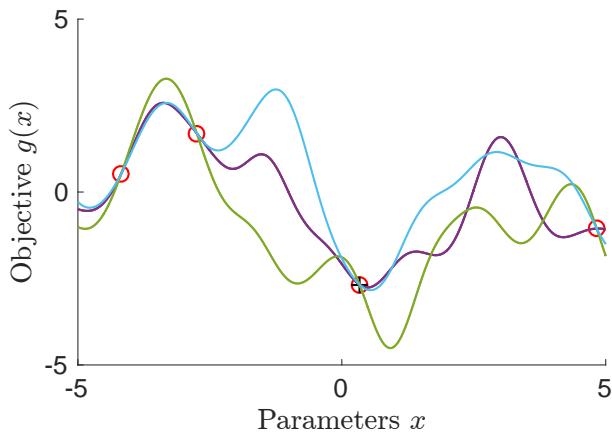
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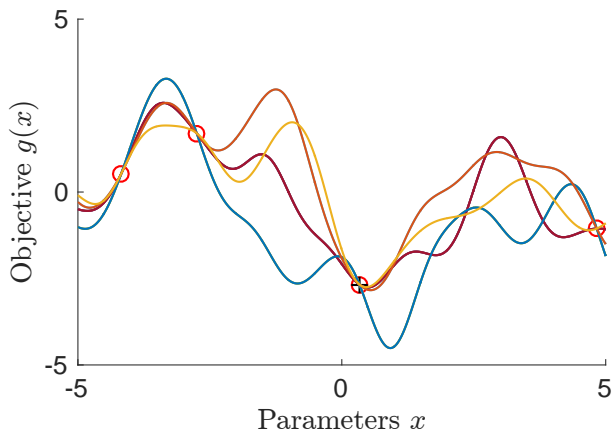
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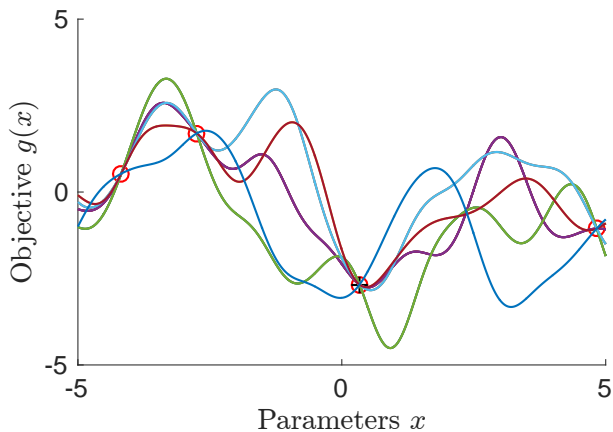
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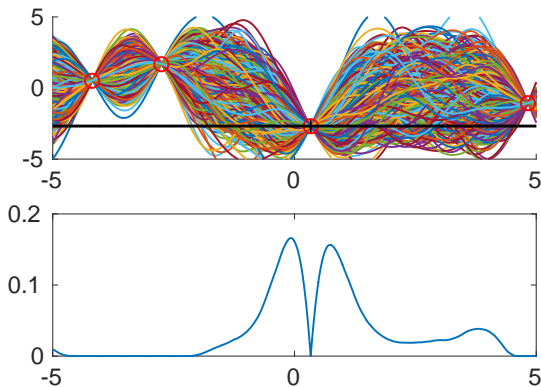
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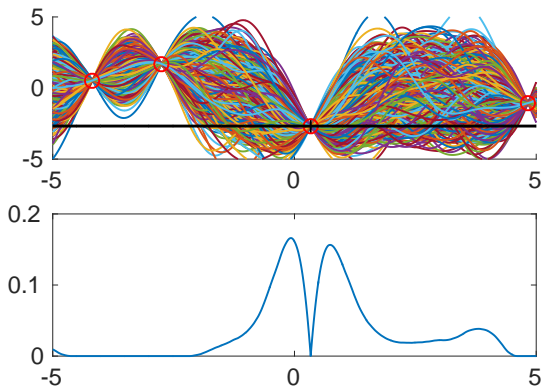


Where to Evaluate Next to Improve Most?



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

- ▶ **Probability of Improvement (Kushner 1964):**

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

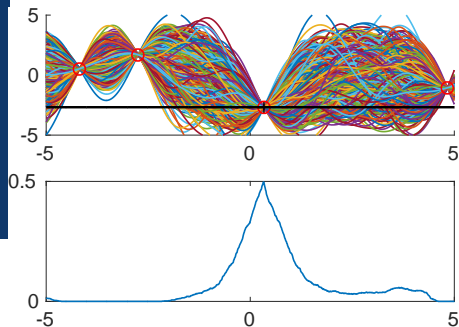
- ▶ **Expected Improvement (Mockus 1978):**

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

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

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

Probability of Improvement (1)

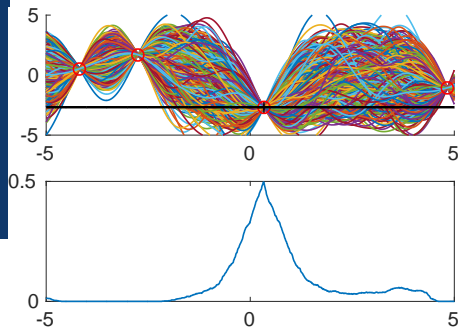


- ▶ **Idea:** Determine the probability that \mathbf{x}_* leads to a better function value than the currently best one $f(\mathbf{x}_{\text{best}})$
- ▶ **Sampling-based setting:** Sample N functions f_i , at every input \mathbf{x} and compute a Monte-Carlo estimate

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

▶ Can lead to heavy exploitation in an ϵ region around \mathbf{x}_{best} .

Probability of Improvement (1)

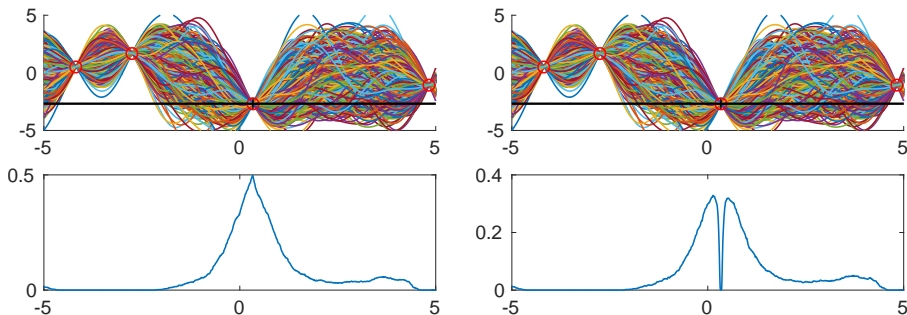


- ▶ **Idea:** Determine the probability that x_* leads to a better function value than the currently best one $f(x_{\text{best}})$
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- ▶▶ Can lead to heavy exploitation in an ϵ region around x_{best} .
- ▶▶ Introduce a “slack variable” ζ for more aggressive 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

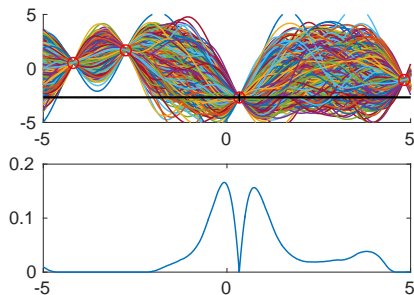
- ▶ **Idea:** Quantify the **amount of improvement**
- ▶ Sampling-based scenario, where $f_i \sim p(f)$:

$$\begin{aligned}\alpha_{\text{EI}}(\mathbf{x}) &= \mathbb{E}[\max\{0, f(\mathbf{x}_{\text{best}}) - f(\mathbf{x})\}] \\ &\approx \frac{1}{N} \sum_{i=1}^N \max\{0, f(\mathbf{x}_{\text{best}}) - f_i(\mathbf{x})\}\end{aligned}$$

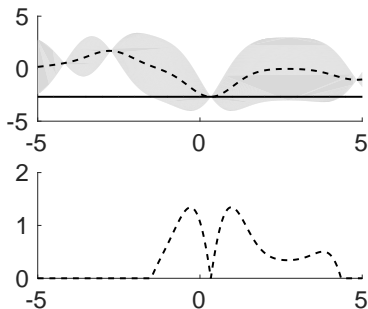
- ▶ If $f \sim GP$, we have a closed-form expression:

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

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



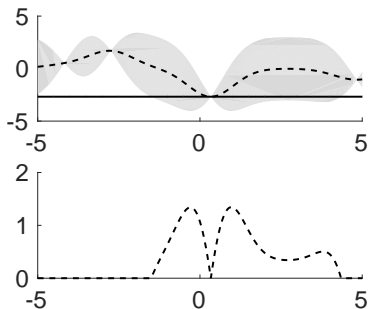
GP-Lower Confidence Bound (1)



- 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

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

GP-Lower Confidence Bound (2)



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

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

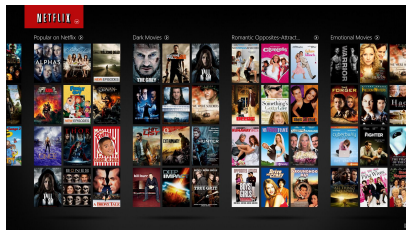
where $\kappa_t \in \mathcal{O}(\log t)$ grows with the iteration t

Optimizing the Acquisition Function

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

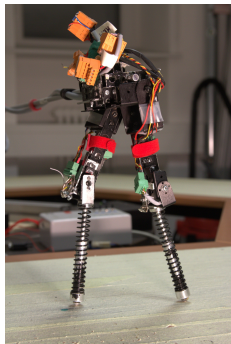
Optimizing the Acquisition Function

- ▶ 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

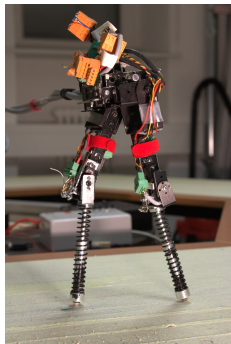
- ▶ Fragile bipedal robot
 - ▶▶ Only few experiments feasible
- ▶ Maximize robustness and walking speed
- ▶ 4 motors:
 - 2 actuated hips + 2 actuated knees
- ▶ Controller implemented as a finite-state-machine (8 parameters)



Calandra et al. (2015)

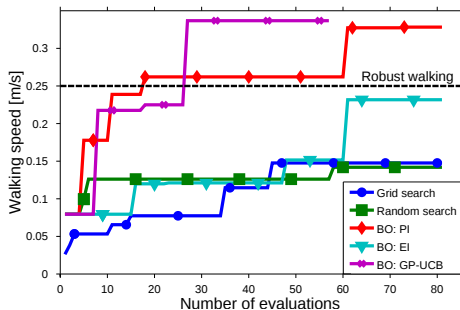
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 - 2 actuated hips + 2 actuated knees
- ▶ Controller implemented as a finite-state-machine (8 parameters)
- ▶ Good parameters found after 80–100 experiments
- ▶ **Substantial speed-up** compared to manual parameter search



Calandra et al. (2015)

Comparison



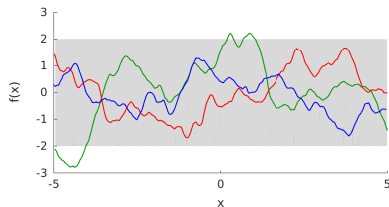
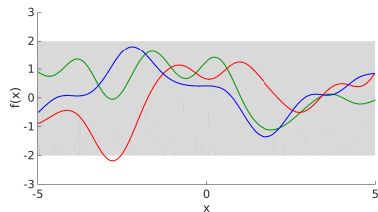
- ▶ Squared exponential covariance function
- ▶ Learned GP hyper-parameters (no MCMC for integrating them out)

Limitations

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

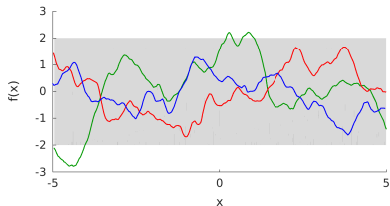
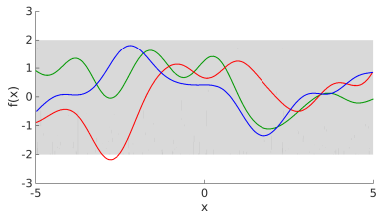
Why?

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)

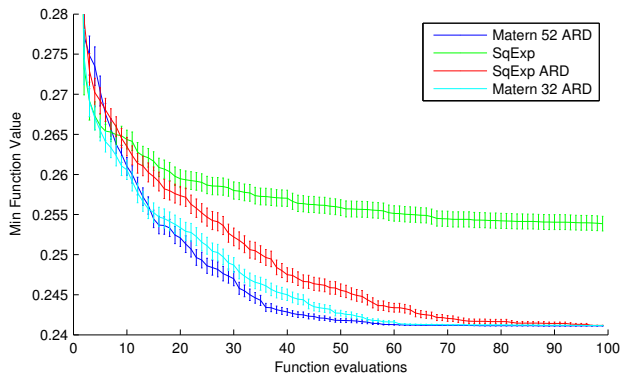


Figure: Figure from Snoek et al. (2012)

Gaussian Process Hyper-Parameters

- ▶ 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

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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**

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

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)

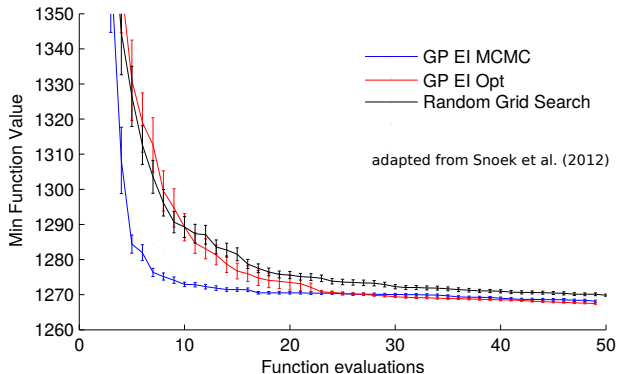
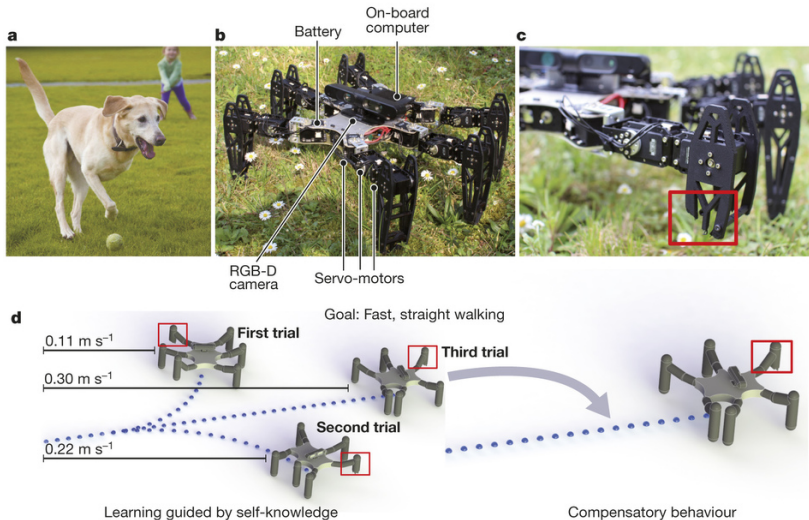


Figure: Figure from Snoek et al. (2012)

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 (Hening & 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, 2014; Snoek, 2012)

Software

- ▶ **BayesOpt** <https://bitbucket.org/rmcantini/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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