Foundations of Machine Learning
African Masters in Machine Intelligence

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Imperial College London

Bayesian Optimization

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Reading Material

- Brochu et al.: *A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning*, arXiv:1012.2599, 2012
- Shahriari et al.: *Taking the Human Out of the Loop: A Review of Bayesian Optimization*, Proceedings of the IEEE, 2016

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

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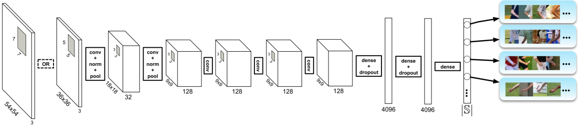
⏩ Generally hard to apply modern techniques or reproduce results

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

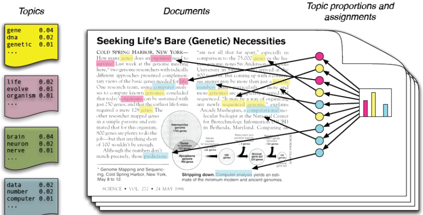
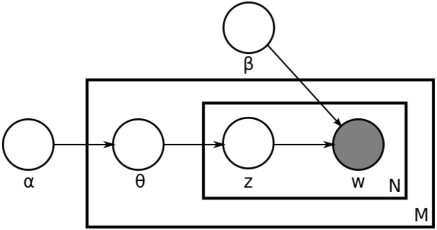
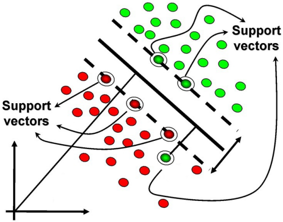


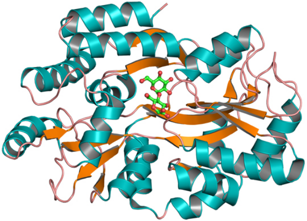
Figure by David Blei



- 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
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  - Grid search
  - Random search (very simple, works surprisingly well)
  - Manual tuning
  - Black magic

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- Standard search procedures:
  - Grid search
  - Random search (very simple, works surprisingly well)
  - 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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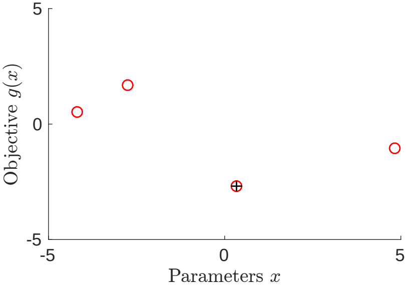
- Standard proxy: Gaussian process

Setting (2)

- Objective: Find global minimum of objective function g:

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

- 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 $\tilde{g}(\boldsymbol{x}_*)$ of proxy function $\tilde{g}$
- Evaluate true objective g at $\boldsymbol{x}_*$
- Overall: Evaluate g only once

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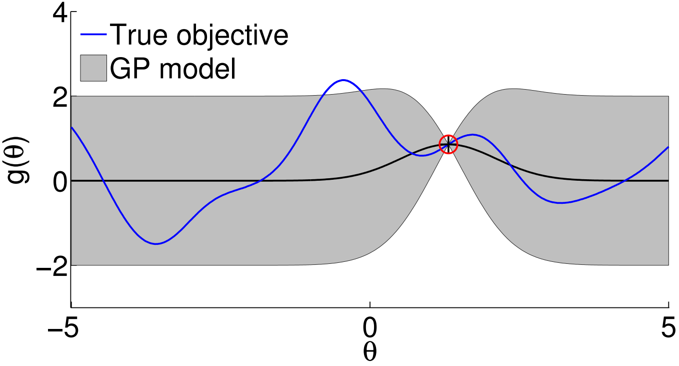
- Overall: Evaluate g only once
- Works well if $\tilde{g} \approx g$.
- Usually not the case ⏩ Repeat this cycle and keep updating $\tilde{g}$

Bayesian Optimization: Illustration



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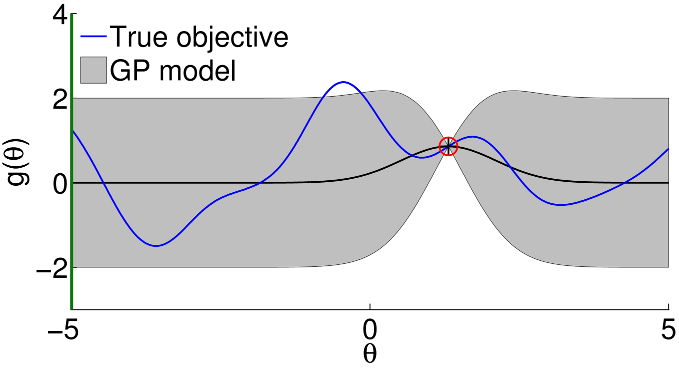

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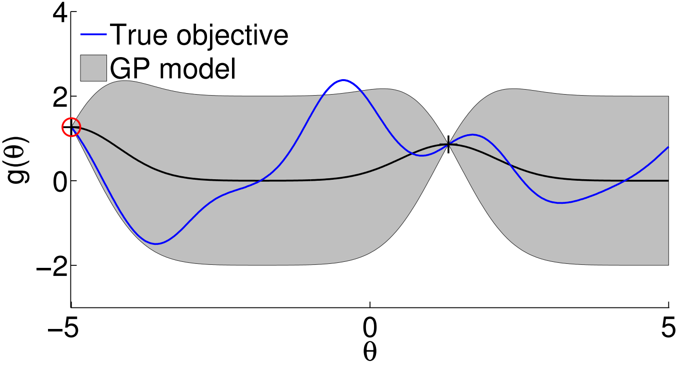

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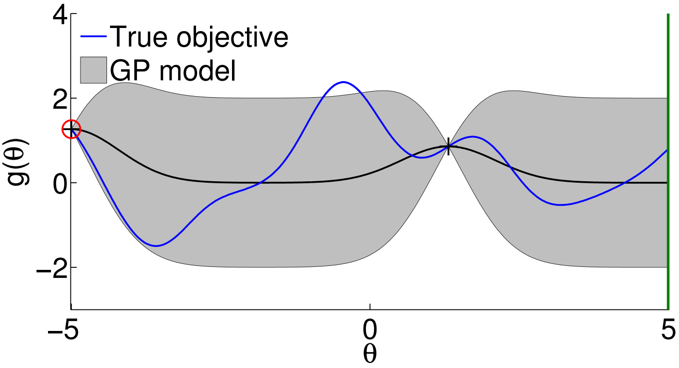

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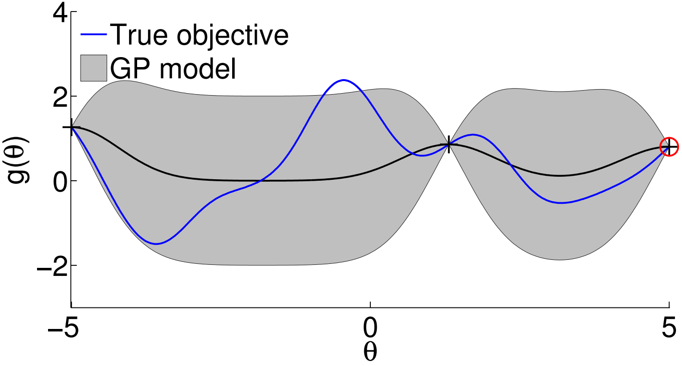

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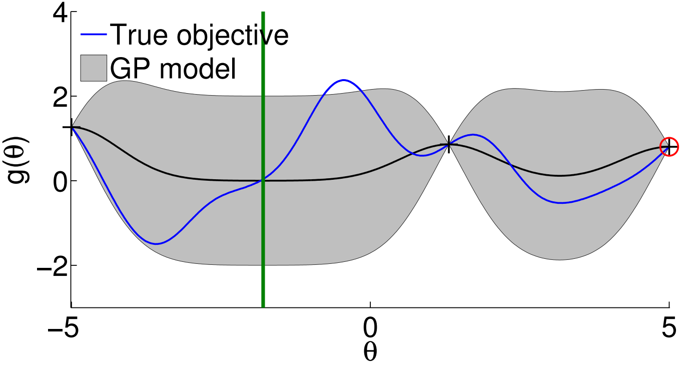

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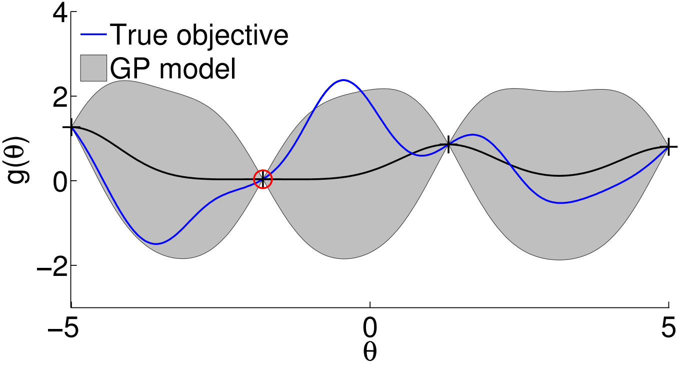

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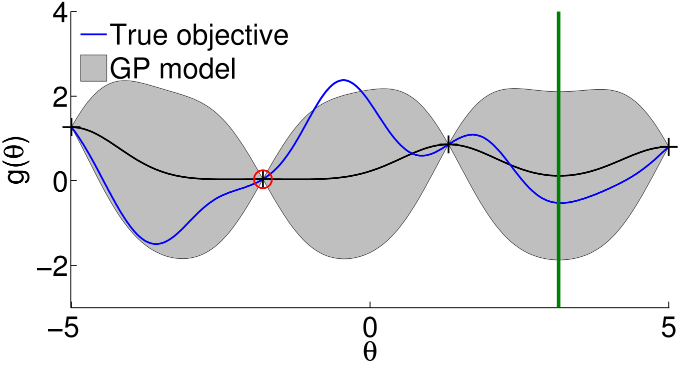

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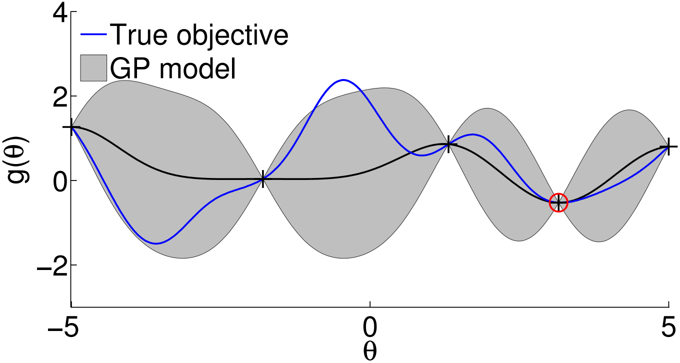

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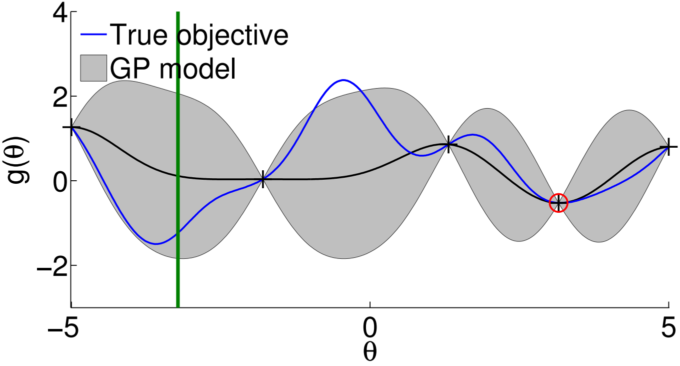

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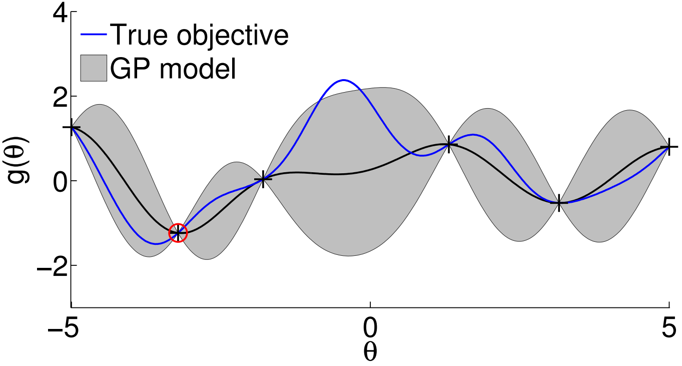

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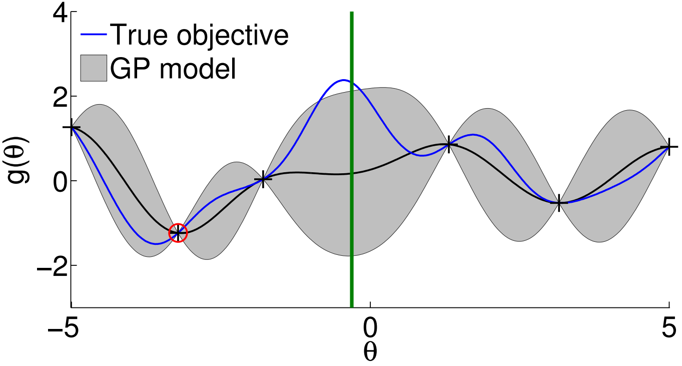

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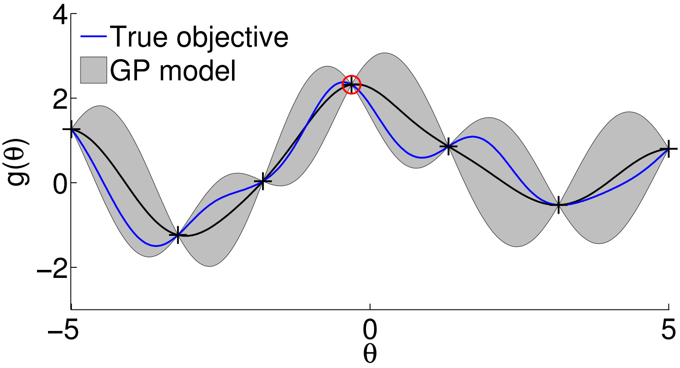

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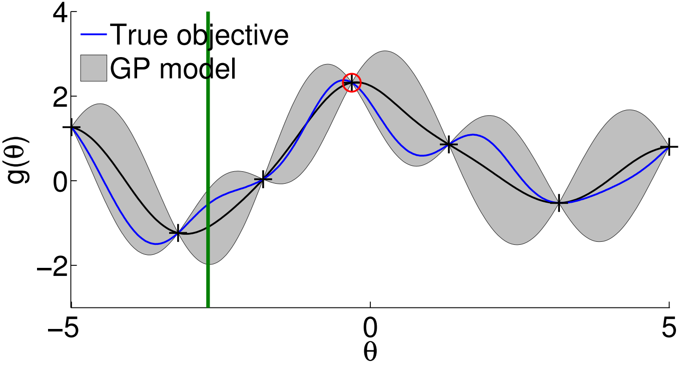

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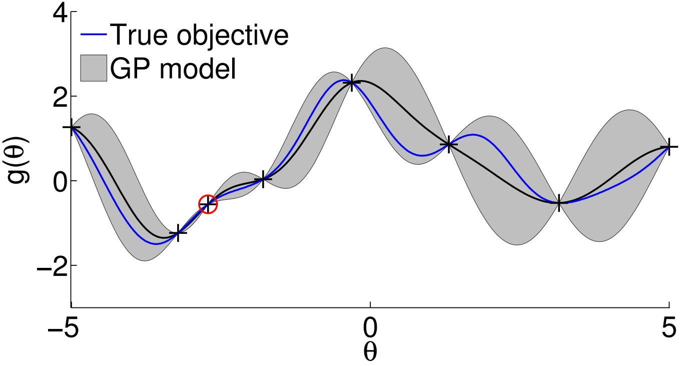

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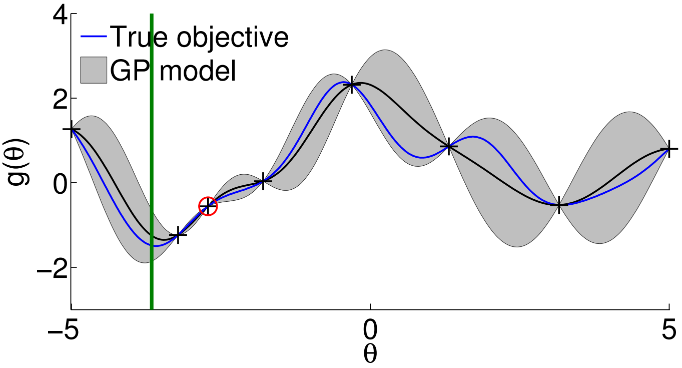

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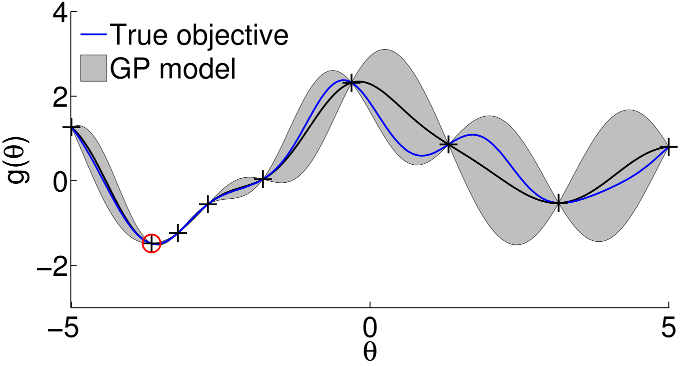

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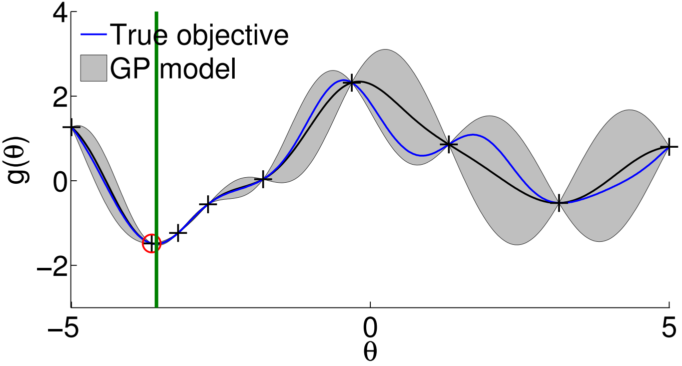

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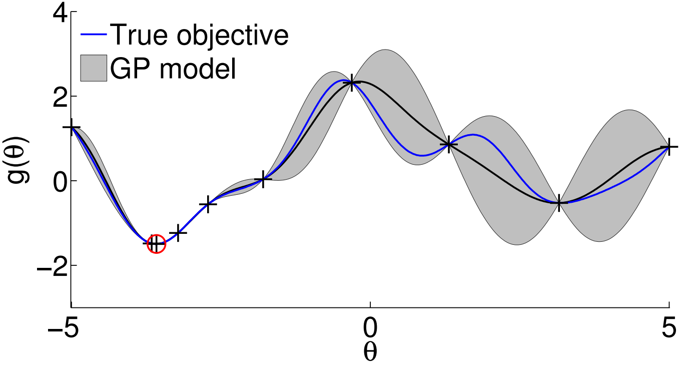

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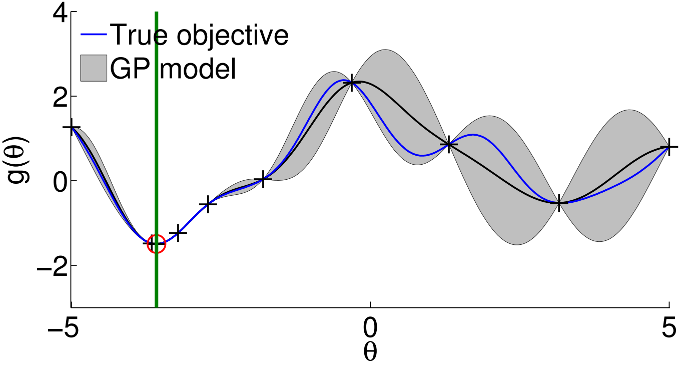

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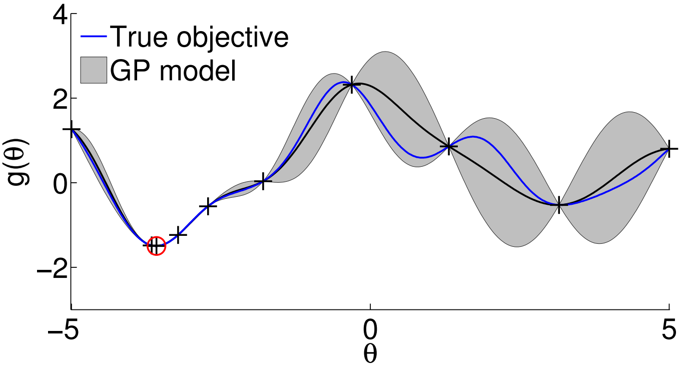

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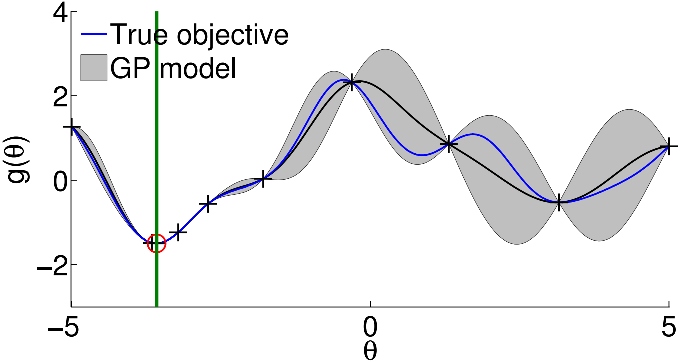
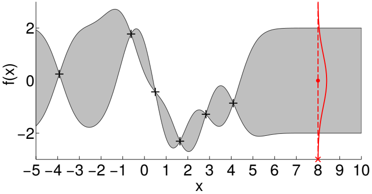


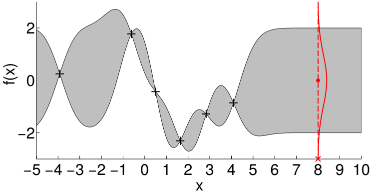
Choosing the Next Point to Evaluate the True Objective: Acquisition Functions

Using Uncertainty in Global Optimization



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

Using Uncertainty in Global Optimization



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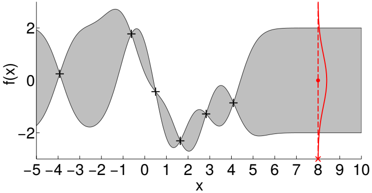

- Find a good (global) optimum
  - ⏩ Need to get out of local optima
- Extrapolate from collected knowledge
- GP gives us closed-form means and variances
  - ⏩ Trade off exploration and exploitation
    - **Exploration:** Seek places with high variance
    - **Exploitation:** Seek places with low mean

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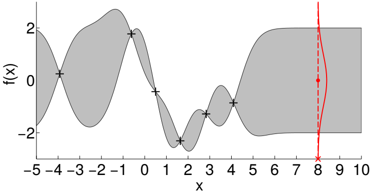

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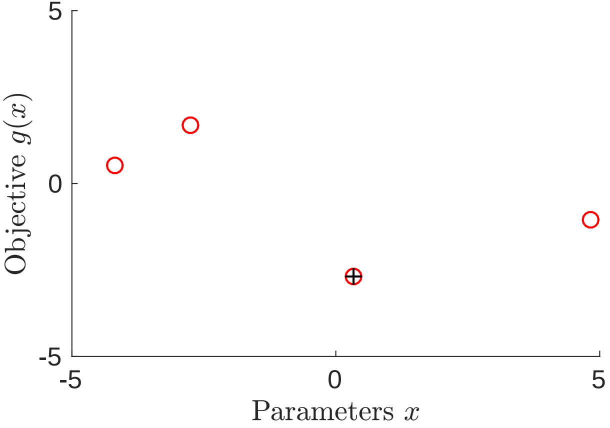
- Acquisition function α trades off exploration and exploitation for our proxy optimization

Key Steps (Pseudo-Code)

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

Where to Evaluate Next?



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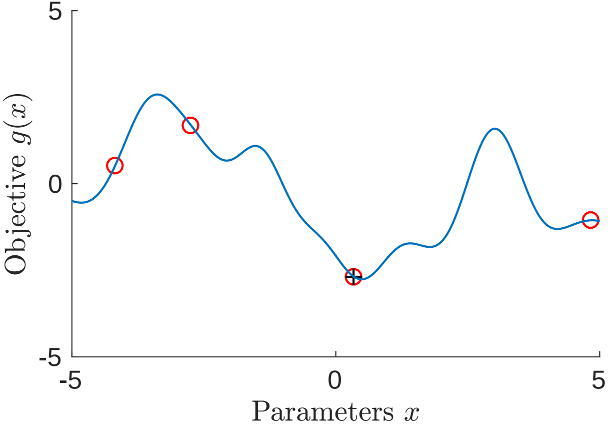

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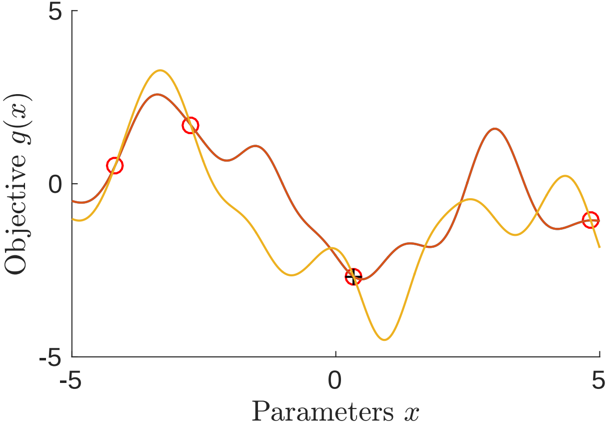

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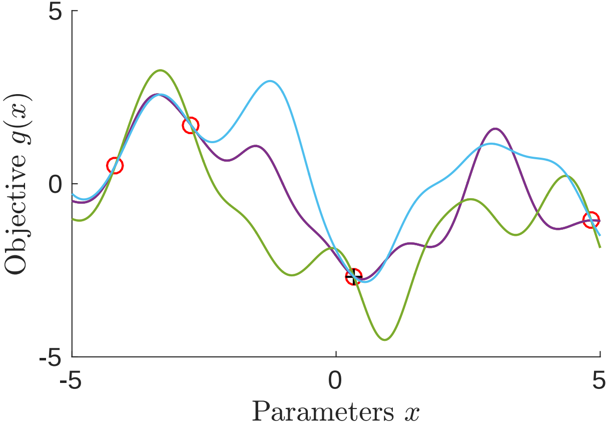

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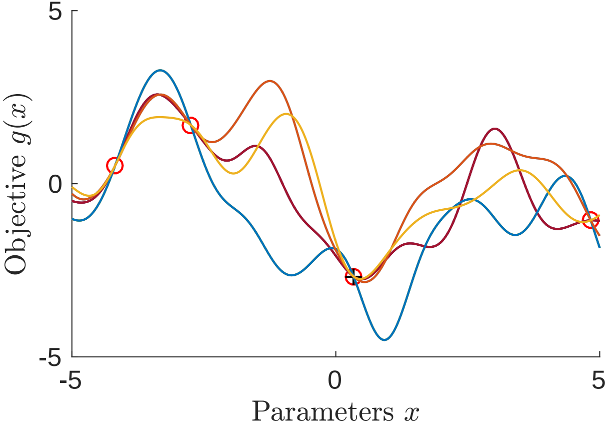

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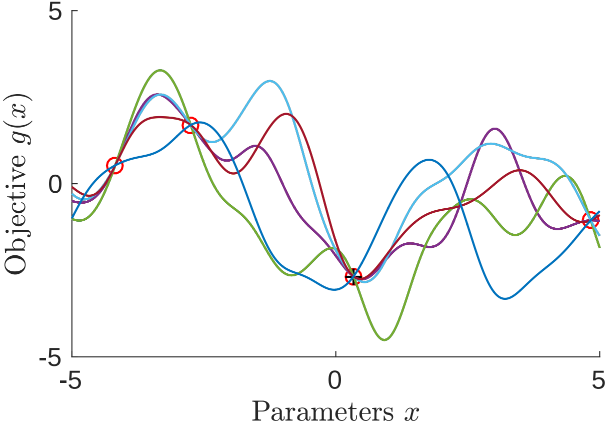
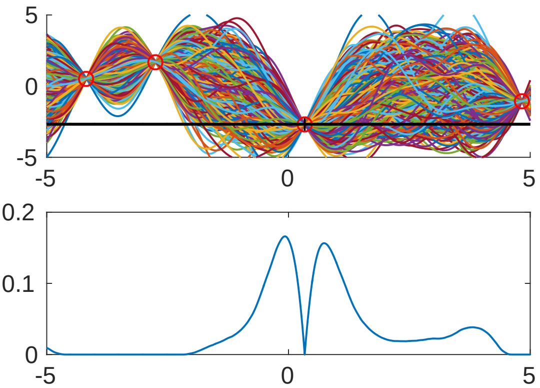


Where to Evaluate Next to Improve Most?



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

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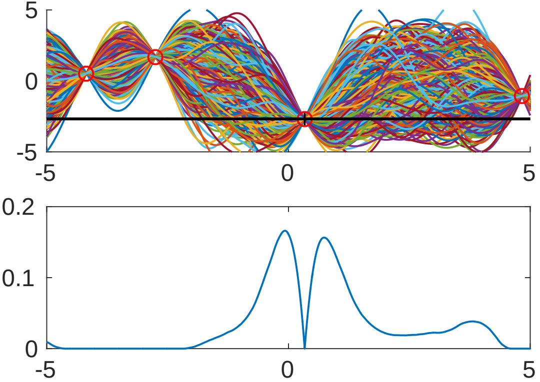

- Upper panel: Samples from a probabilistic proxy $\tilde{g}$
- Lower panel: Corresponding expected improvement over the best solution so far (black cross)

  ▶▶ Evaluate g at the maximum of the expected improvement

Closed-Form Acquisition Functions

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

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

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

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

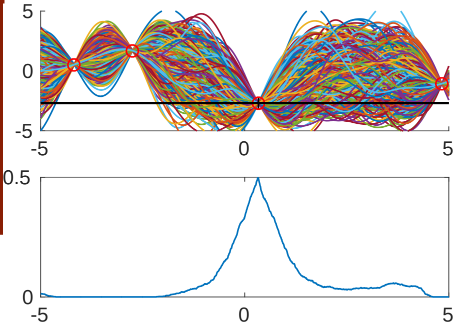
- **Expected Improvement (Mockus 1978):**

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

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

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

Probability of Improvement (1)



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

$$\alpha_{\text{PI}}(\boldsymbol{x}) = p(g(\boldsymbol{x}) < g(\boldsymbol{x}_{\text{best}})) \approx \frac{1}{N}\sum\nolimits_{i=1}^{N} \delta\big(g_i(\boldsymbol{x}) < g(\boldsymbol{x}_{\text{best}})\big)$$

▶▶ Can lead to continued exploitation in an ϵ-region around $\boldsymbol{x}_{\text{best}}$.

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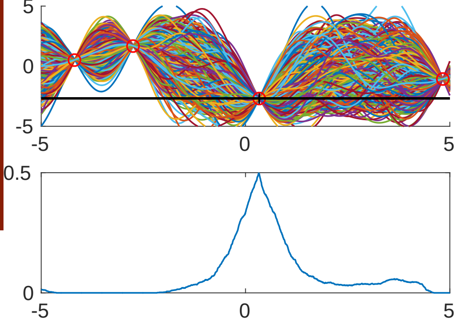

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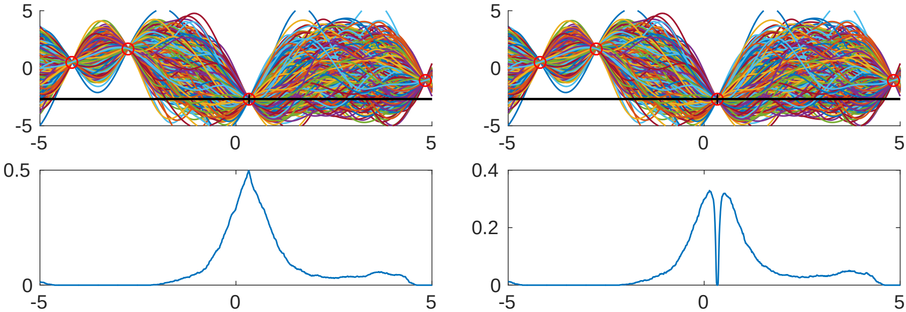
▶▶ Can lead to continued exploitation in an ϵ-region around $\boldsymbol{x}_{\text{best}}$.
▶▶ Introduce a "slack variable" ξ for more aggressive exploration

Probability of Improvement (2)



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

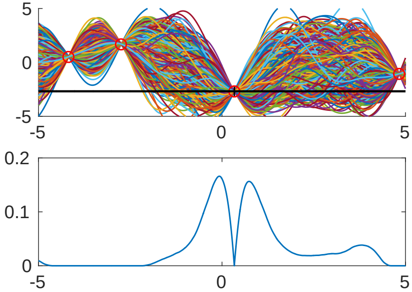
$$\alpha_{\mathrm{PI}}(\boldsymbol{x}) = p(g(\boldsymbol{x}) < g(\boldsymbol{x}_{\mathrm{best}}) - \xi) \approx \frac{1}{N}\sum_{i=1}^{N} \delta\big(g_i(\boldsymbol{x}) < g(\boldsymbol{x}_{\mathrm{best}}) - \xi\big)$$

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

$$\alpha_{\mathrm{PI}}(\boldsymbol{x}) = \Phi(\gamma(\boldsymbol{x}, \xi)), \qquad \gamma(\boldsymbol{x}, \xi) = \frac{g(\boldsymbol{x}_{\mathrm{best}}) - \xi - \mu(\boldsymbol{x})}{\sigma(\boldsymbol{x})}$$

Expected Improvement

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



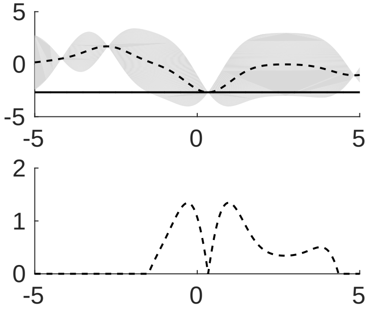
$$\alpha_{\mathrm{EI}}(\boldsymbol{x}) = \mathbb{E}[\max\{0, g(\boldsymbol{x}_{\mathrm{best}}) - g(\boldsymbol{x})\}]$$
$$\approx \frac{1}{N}\sum_{i=1}^{N} \max\{0, g(\boldsymbol{x}_{\mathrm{best}}) - g_i(\boldsymbol{x})\}$$

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

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

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

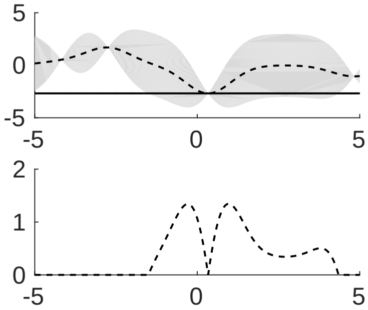
GP-Lower Confidence Bound (1)



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

$$\alpha_{\text{LCB}}(\boldsymbol{x}_t) = -\big(\mu(\boldsymbol{x}_t) - \sqrt{\kappa}\sigma(\boldsymbol{x}_t)\big)$$

GP-Lower Confidence Bound (2)



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

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

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

▶▶ Continue exploration

Optimizing the Acquisition Function

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- What have we gained?

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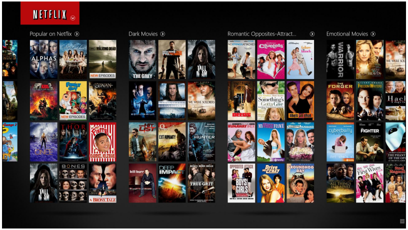
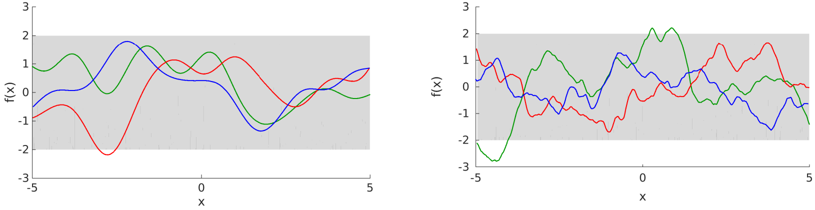
- What have we gained?
- Evaluating the acquisition function is cheap compared to evaluating the true objective
  - ▶▶ We can afford evaluating it many times



Limitations

- Getting the function model (e.g., covariance function) 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 (Gaussian))

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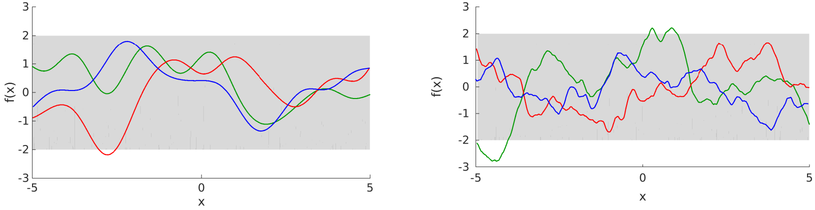

- Covariance function selection is crucial for good performance
  ⏩ Choose a sufficiently flexible and adaptive kernel, e.g., Matérn (but not the squared exponential (Gaussian))
- Nice side-effect of Matérn: Exploration is more encouraged than with the Gaussian kernel

Choosing Covariance Functions

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

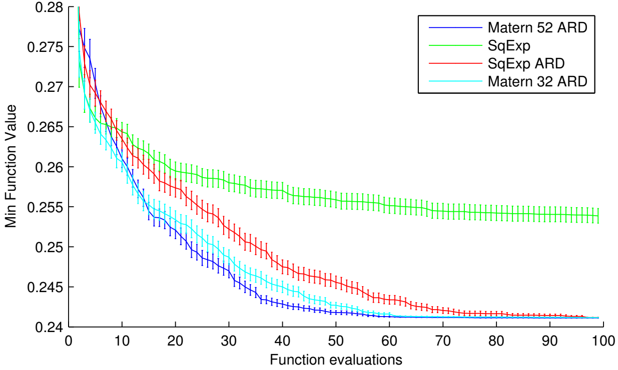

Figure: Figure from Snoek et al. (2012)

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 $\boldsymbol{\theta}$ by Markov Chain Monte Carlo (MCMC) sampling (e.g., slice sampling)
- Look at integrated acquisition function

$$\alpha(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{\theta}}[\alpha(\boldsymbol{x}, \boldsymbol{\theta})] = \int \alpha(\boldsymbol{x}, \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

$$\approx \frac{1}{K} \sum_{k=1}^{K} \alpha(\boldsymbol{x}, \boldsymbol{\theta}^{(k)}), \quad \boldsymbol{\theta}^{(k)} \sim \underbrace{p(\boldsymbol{\theta} | \boldsymbol{X}_n, \boldsymbol{y}_n)}_{\text{hyper-parameter posterior}}$$

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)

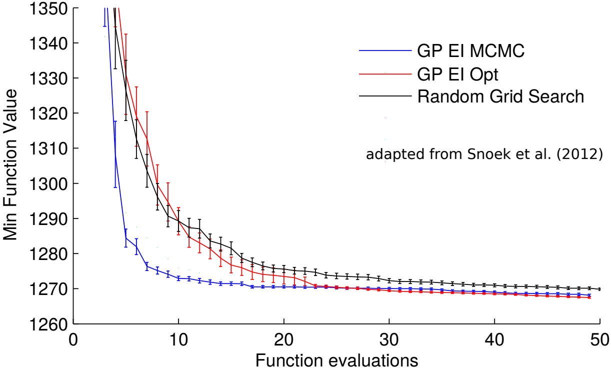
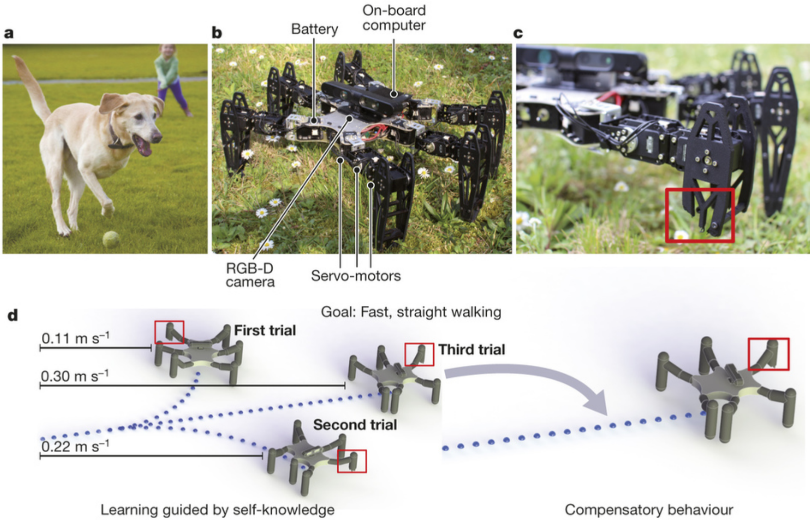


Figure: Figure from Snoek et al. (2012)

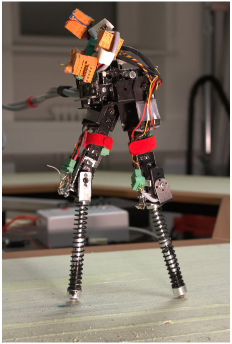
Robots That Learn to Recover from Damage



Cully et al. (2015)

Application Example: Controller Learning in Robotics (Calandra et al., 2015)

- 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)



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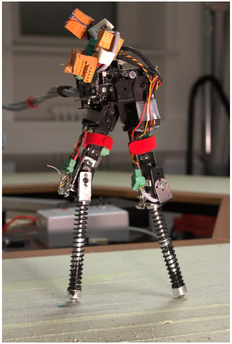
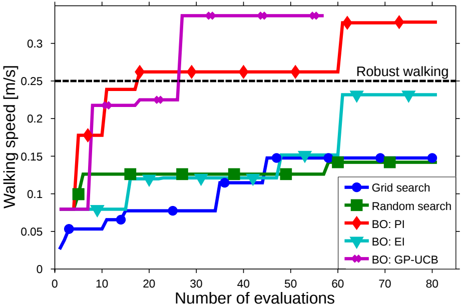
- Fragile bipedal robot
  ⏩ Only few experiments feasible
- Maximize robustness and walking speed
- 4 motors:
  2 actuated hips + 2 actuated knees
- Controller implemented as a finite-state-machine (8 parameters)
- Good parameters found after 80–100 experiments
- Substantial speed-up compared to manual parameter search



Calandra et al. (2015)

Comparison



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

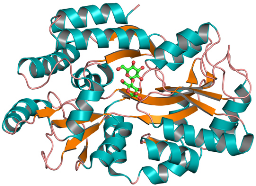
Further Topics in BO

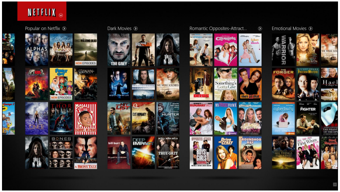
- Entropy-based acquisition functions: Directly describe the distribution over the best input location (Hennig & Schuler, 2012; Hernández-Lobato et al., 2014)
- Non-myopic Bayesian optimization (e.g., Osborne et al., 2009)
- High-dimensional optimization (e.g., Wang et al., 2016)
- Large-scale Bayesian optimization (Hutter et al., 2014)
- Efficient optimization of acquisition functions (Wilson et al., 2018)
- 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; Wilson et al., 2018)

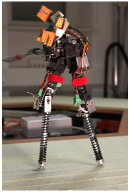
Software

- 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)

Summary







- Global optimization of black-box functions, which are expensive to evaluate ⏩ Meta-challenges in machine learning, Auto-ML
- Use a probabilistic proxy model that is cheap to evaluate and use this to suggest next experiments
- Acquisition function trades of exploration and exploitation

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