


Bayesian Optimization

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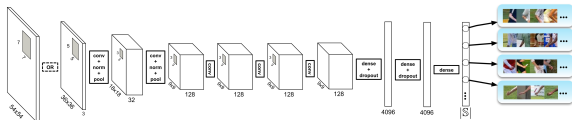
March/April 2020

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

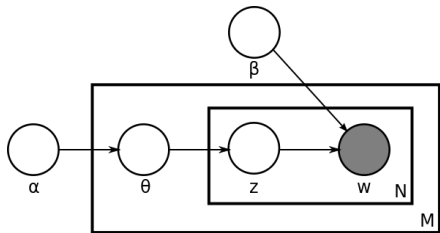
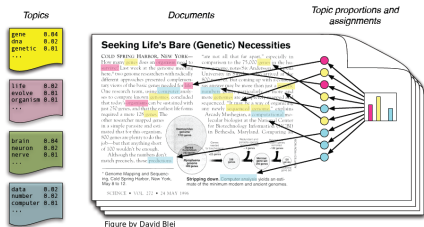
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Goal: Automate the selection of critical meta-parameters
(see also: [Automated Machine Learning \(AutoML\)](#))

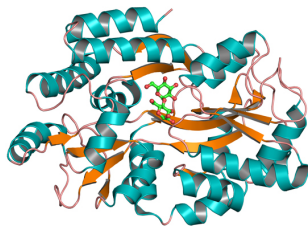
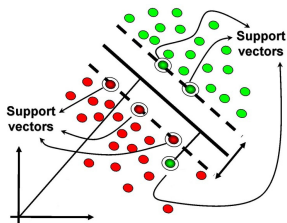


Huge interest in large neural networks

- 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



- Hoffman et al. (2010): Approximate inference for **large-scale text analysis (topic modeling) 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, ...



- 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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- Standard search procedures:
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 - Black magic
- Painful:
 - Evaluating the quality of the objective may be very expensive (e.g., time or money)
 - ▶ Imagine we would need to run a GPU/TPU cluster for 2 weeks
 - Many training cycles
 - Possibly noisy

Setting

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

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- **Optimize cheap proxy** function to determine where to evaluate the true objective next

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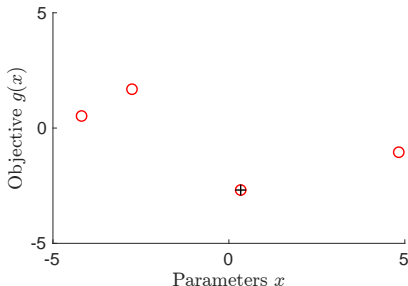
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- Standard proxy: **Gaussian process**

- Objective: Find global minimum of objective function g :

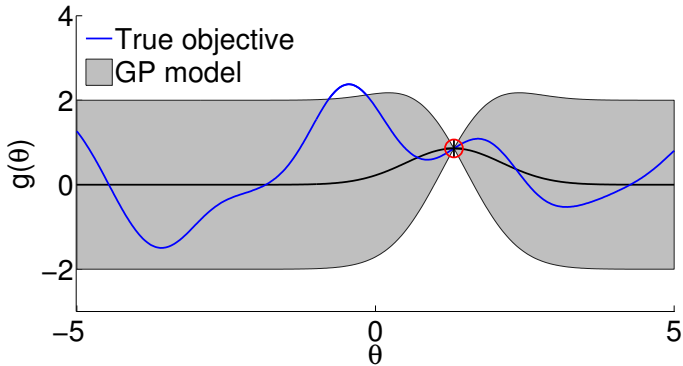
$$\mathbf{x}_* = \arg \min_{\mathbf{x}} g(\mathbf{x})$$

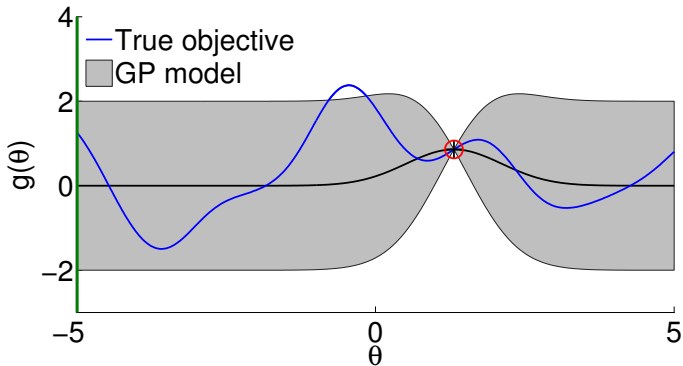
- We can evaluate the objective g pointwise, but do not have an easy functional form or gradients; observations may be noisy
- **Evaluating g is costly** (e.g., train a massive deep network)

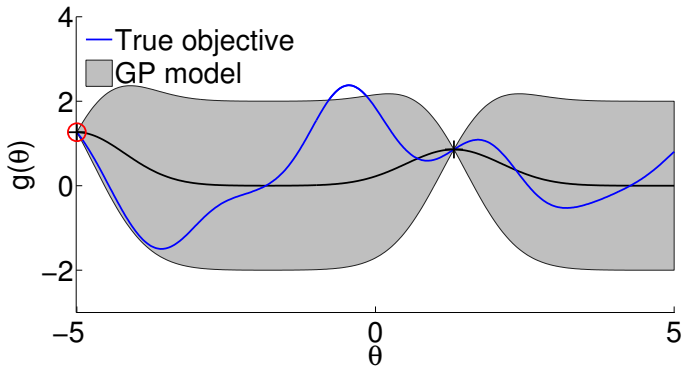


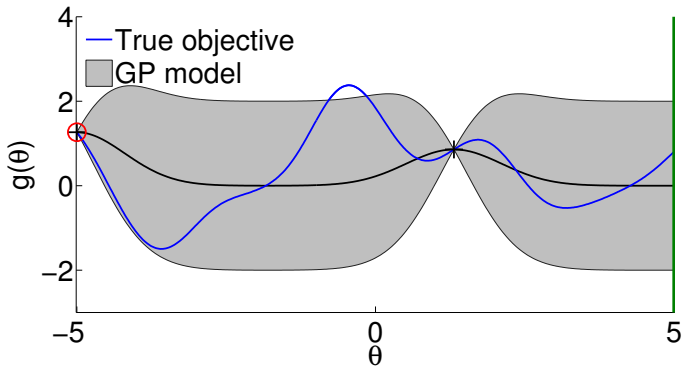
- To avoid evaluating g an excessive number of times, approximate it using a **proxy function** \tilde{g} (which is cheap to evaluate)
- Find a **global optimum** $\tilde{g}(x_*)$ of **proxy function** \tilde{g}
- Evaluate true objective g at x_*
- Overall: Evaluate g only once

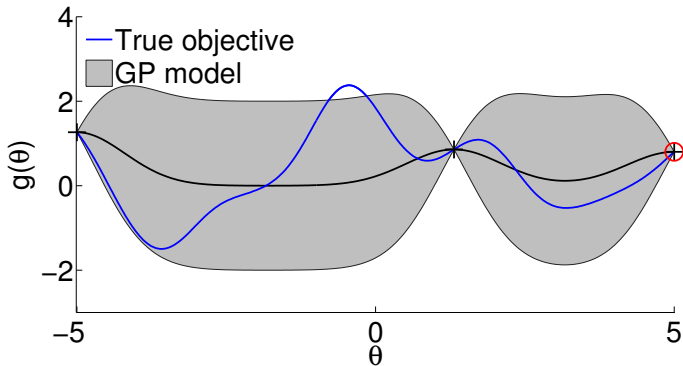
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- Overall: Evaluate g only once
- Works well if $\tilde{g} \approx g$.
- Usually not the case **▶▶** Repeat this cycle and keep updating \tilde{g}

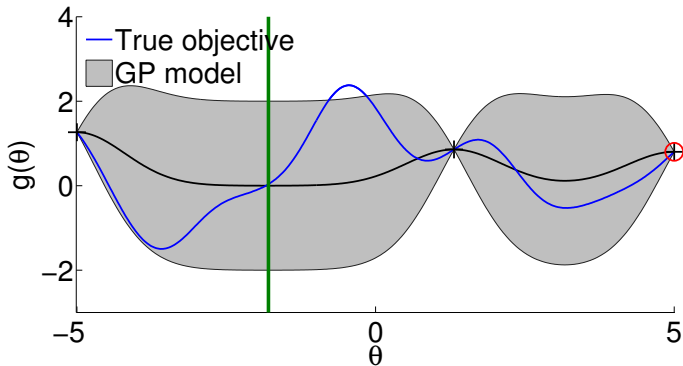


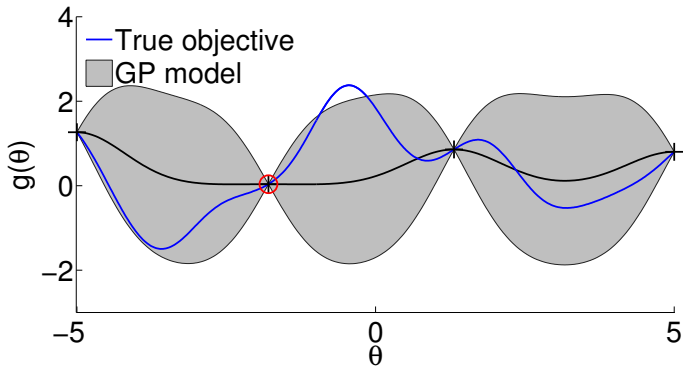


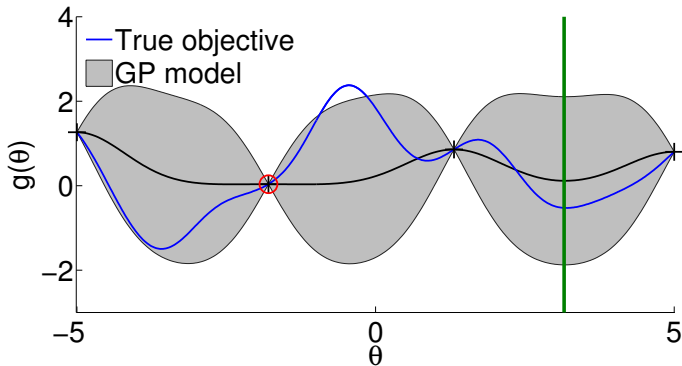


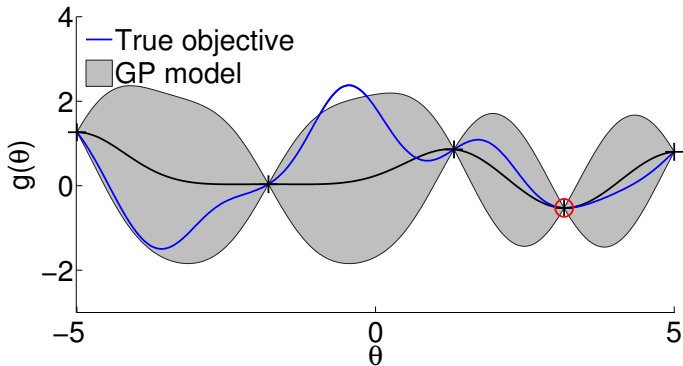


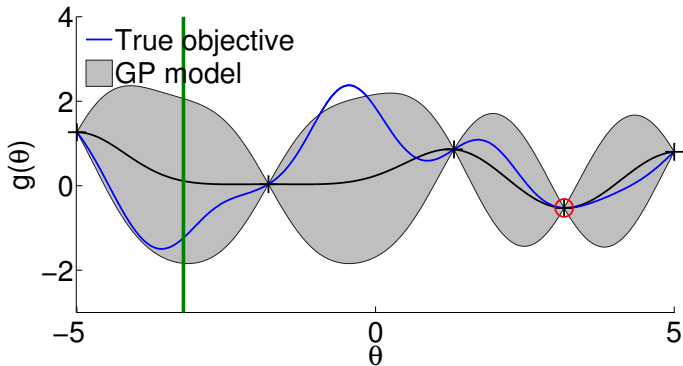


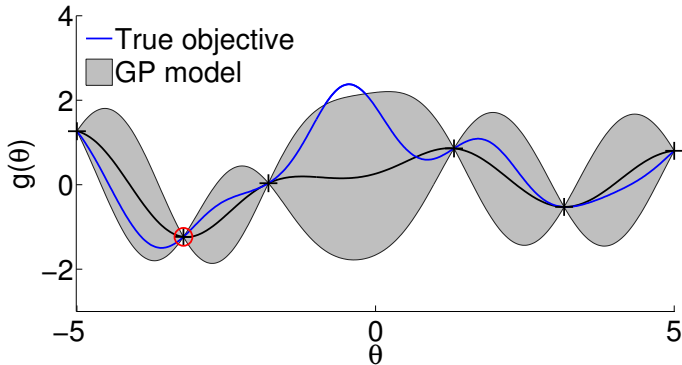


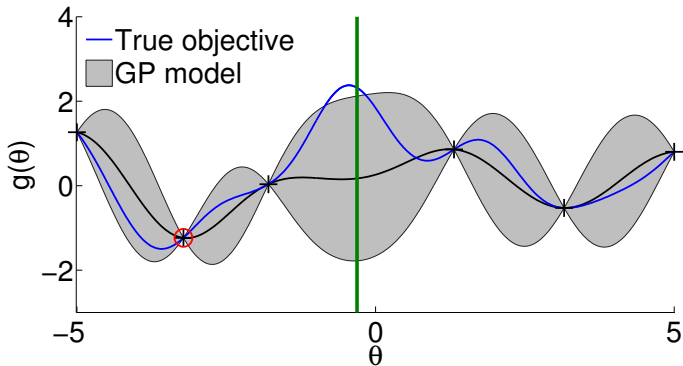


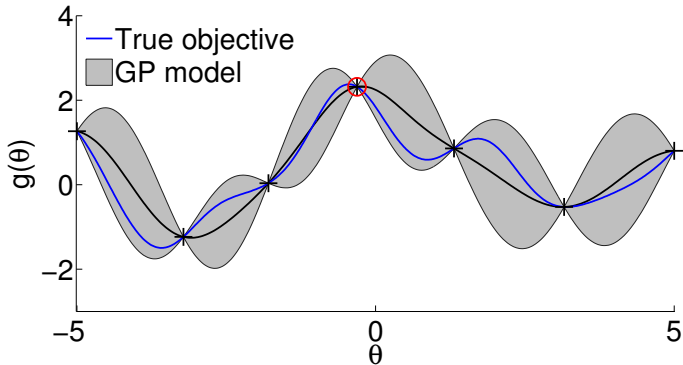


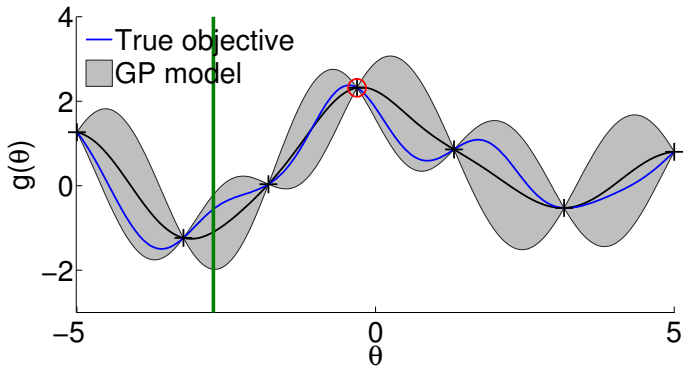


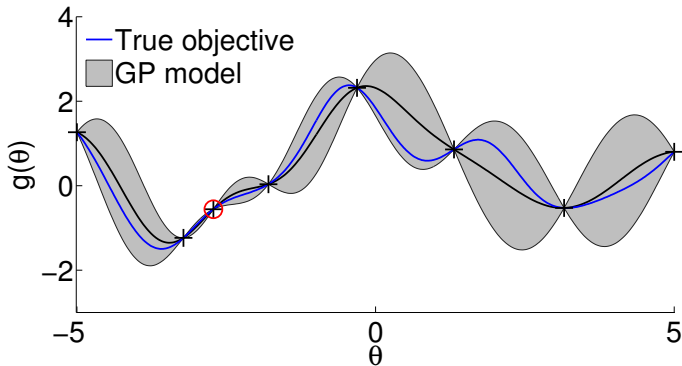


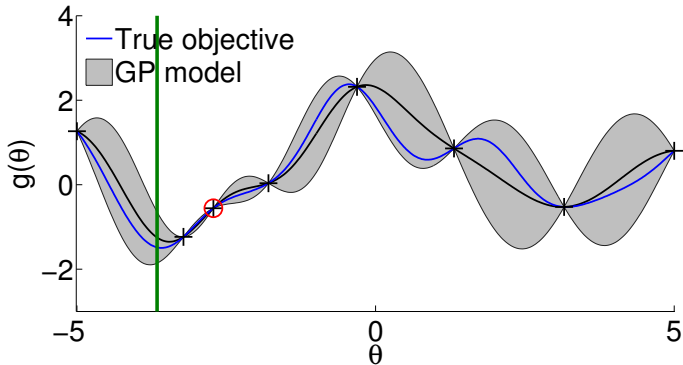


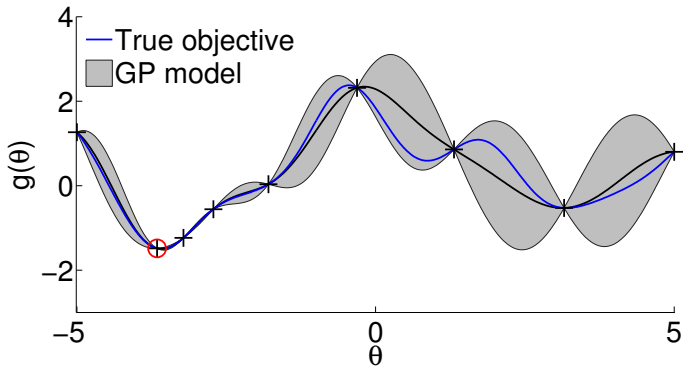


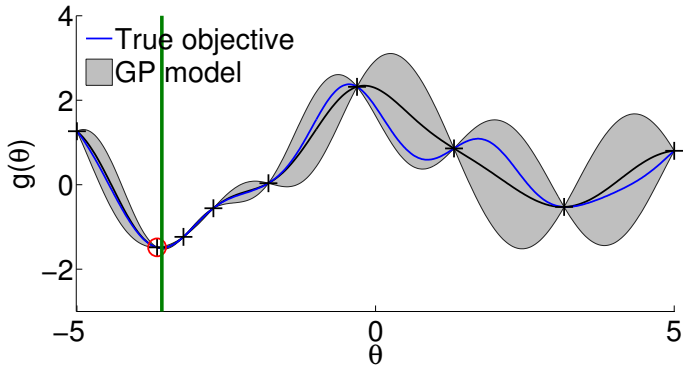


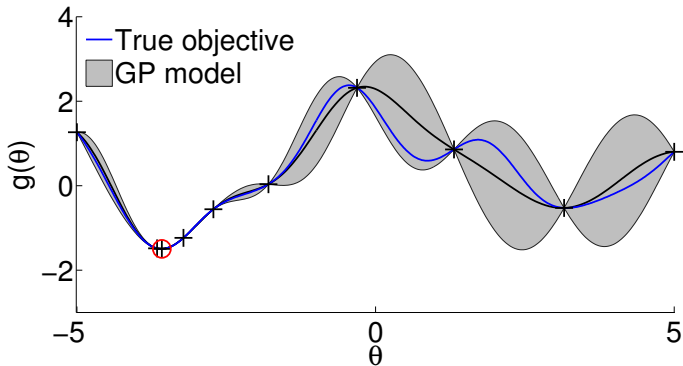


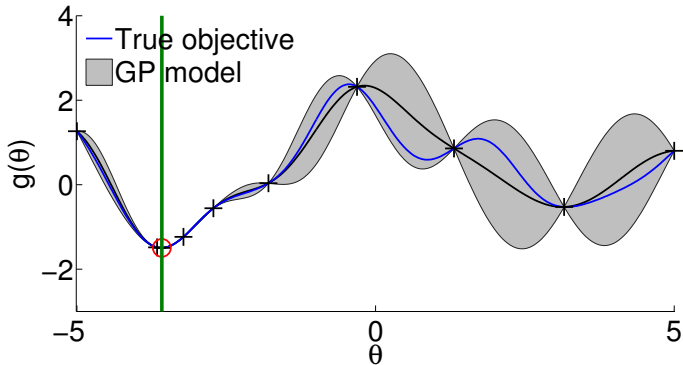


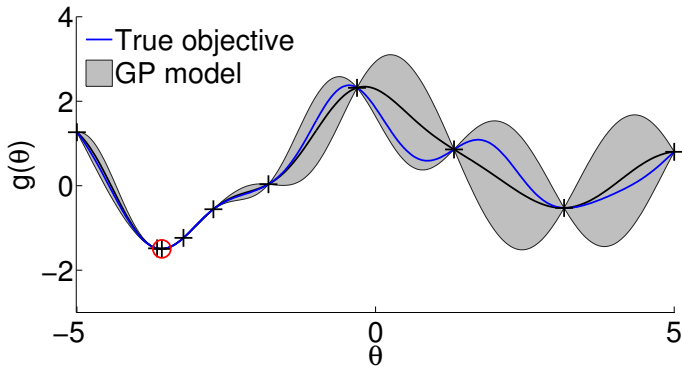


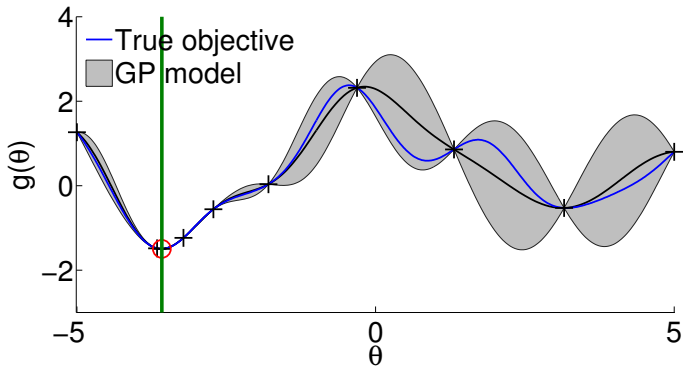




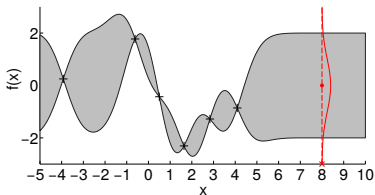




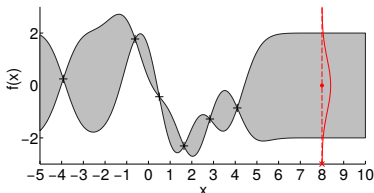




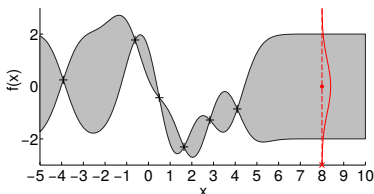
Choosing the Next Point to Evaluate the True Objective: Acquisition Functions



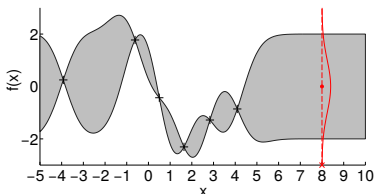
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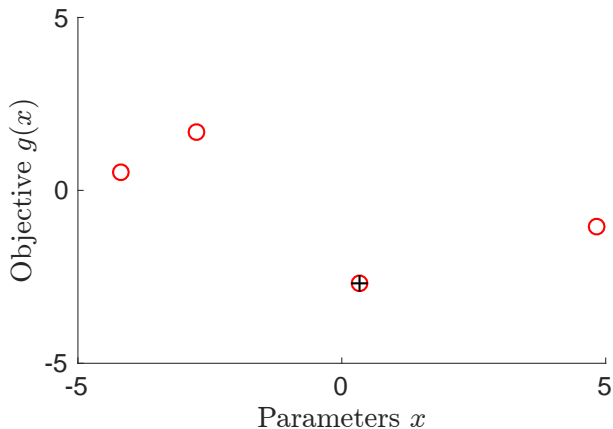


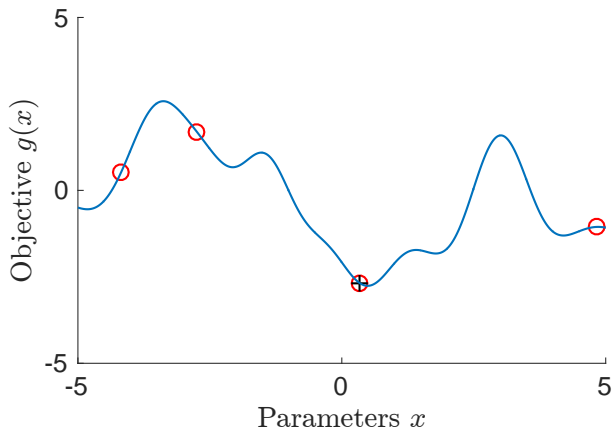
- Find a good (global) optimum
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- GP gives us closed-form means and variances
 - ▶▶ Trade off exploration and exploitation
 - **Exploration:** Seek places with high variance/uncertainty
 - **Exploitation:** Seek places with low mean

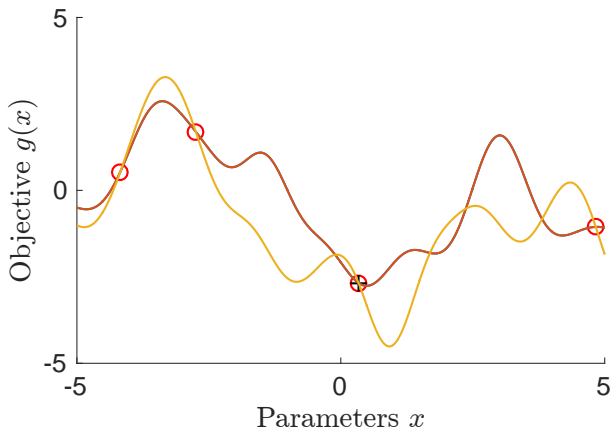


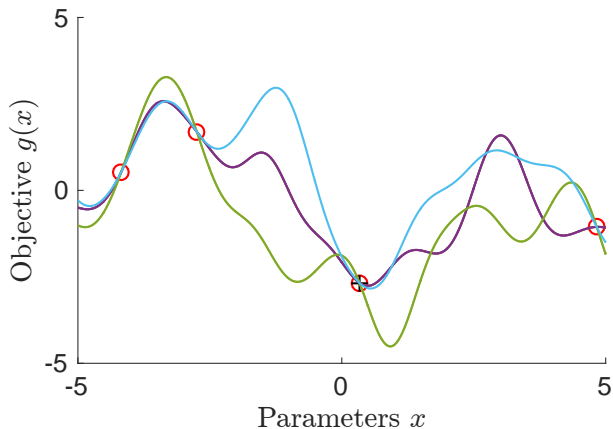
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 - **Exploration:** Seek places with high variance/uncertainty
 - **Exploitation:** Seek places with low mean
- Acquisition function α trades off exploration and exploitation for our proxy optimization

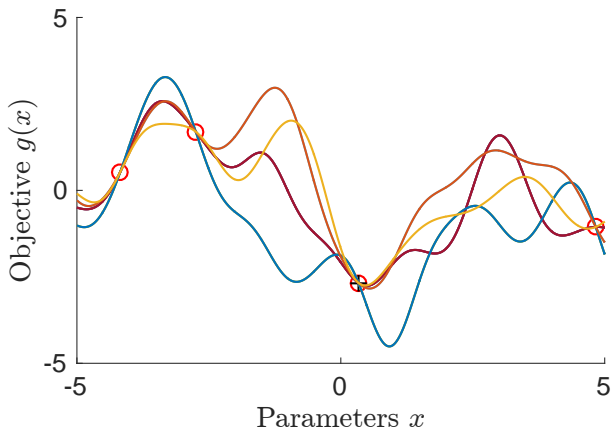
- 1: **Init:** Data set $\mathcal{D}_0 = \{\mathbf{X}_0, \mathbf{y}_0\}$
- 2: **for** iterations $t = 1, 2, \dots$ **do**
- 3: **Update GP** using data \mathcal{D}_{t-1}
- 4: Select $\mathbf{x}_t = \arg \max_{\mathbf{x}} \alpha(\mathbf{x})$ by **optimizing acquisition function**
- 5: Query true objective 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: $\mathbf{x}^* = \arg \min_{\mathbf{x}} y(\mathbf{x})$

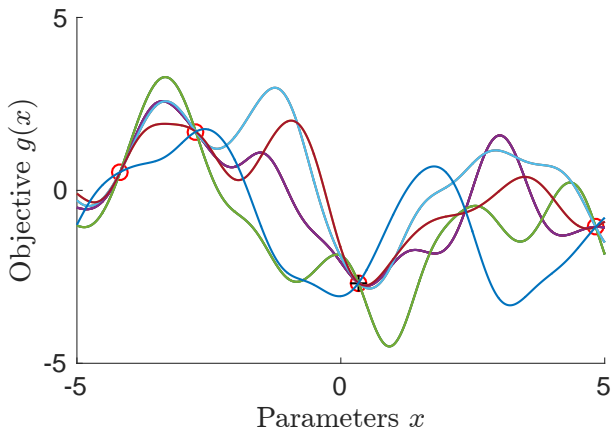


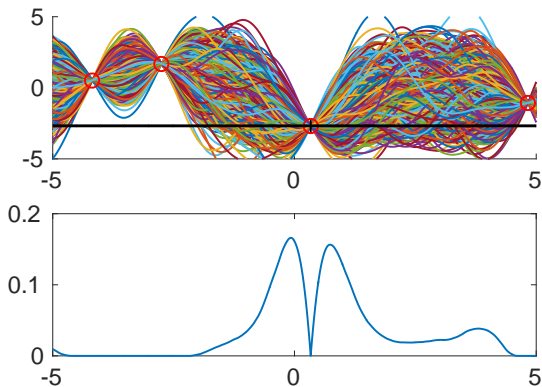




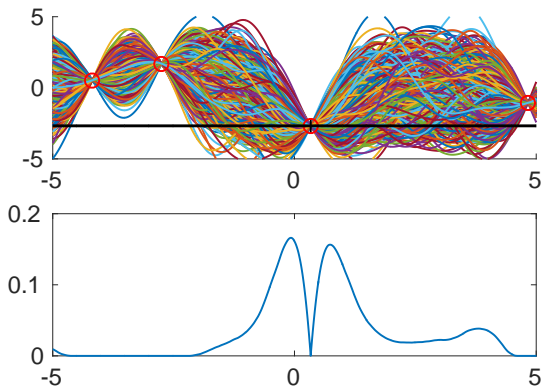








- Upper panel: Samples from a probabilistic proxy \tilde{g}



- 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

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

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

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

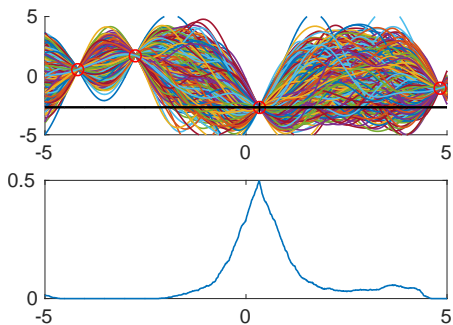
$$\alpha_{\text{PI}}(\mathbf{x}) = \Phi(\gamma(\mathbf{x}))$$

- **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):**

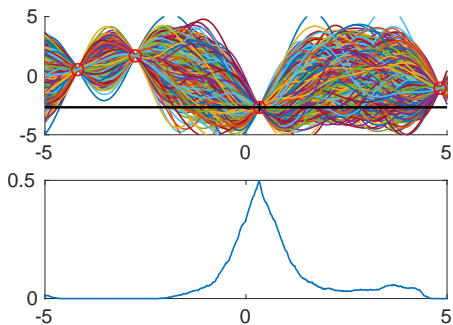
$$\alpha_{\text{LCB}}(\mathbf{x}) = -(\mu(\mathbf{x}) - \kappa\sigma(\mathbf{x})), \quad \kappa > 0$$



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

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

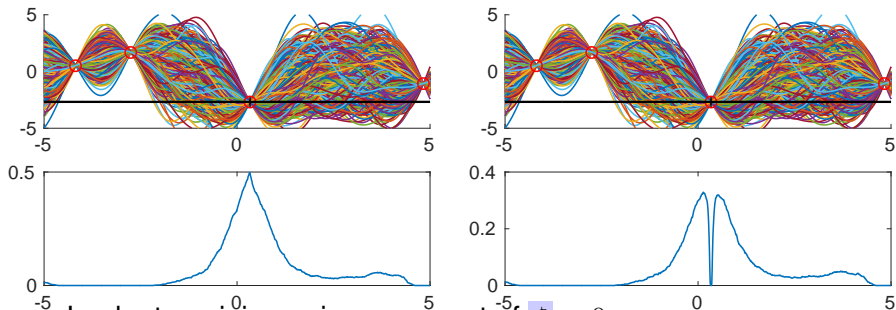
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- ▶▶ Can lead to continued exploitation in an ϵ -region around x_{best} .
- ▶▶ Introduce a “slack variable” ξ for more aggressive exploration



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

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

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

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

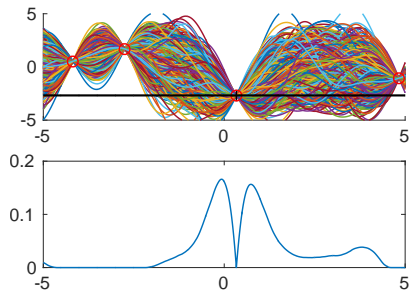
- **Idea:** Quantify the **amount of improvement**
- Sampling-based scenario, where $g_i \sim p(f)$:

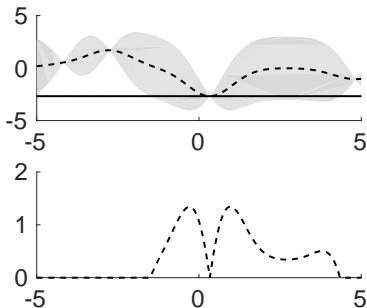
$$\alpha_{\text{EI}}(\mathbf{x}) = \mathbb{E}[\max\{0, g(\mathbf{x}_{\text{best}}) - g(\mathbf{x})\}]$$
$$\approx \frac{1}{N} \sum_{i=1}^N \max\{0, g(\mathbf{x}_{\text{best}}) - g_i(\mathbf{x})\}$$

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

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

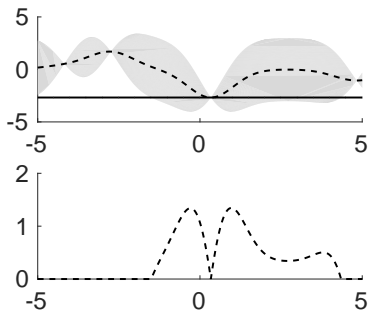
- Slack-variable approach also possible (similar to PI)





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

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



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

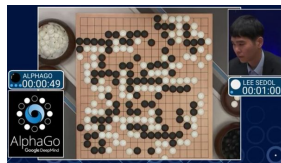
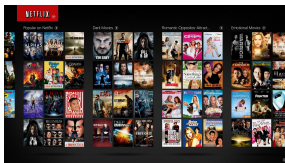
$$\alpha_{\text{LCB}}(\mathbf{x}_t) = -(\mu(\mathbf{x}_t) - \sqrt{\kappa_t}\sigma(\mathbf{x}_t))$$

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

▶▶ Continue exploration

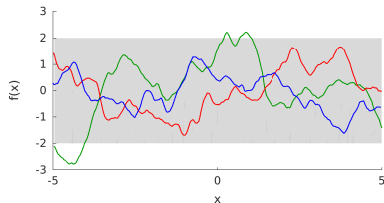
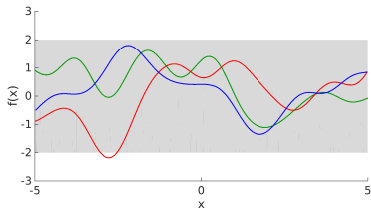
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- What have we gained?

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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

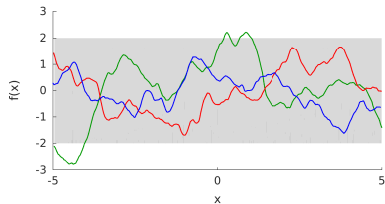
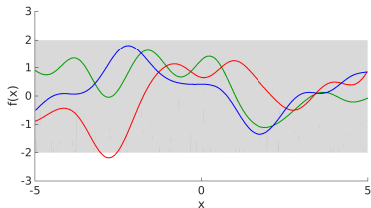


- Getting the function model (e.g., covariance function) wrong can be catastrophic
- Limited scalability in the number of dimensions and/or evaluations of the true objective function

Why?



- 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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 - ▶ 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

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

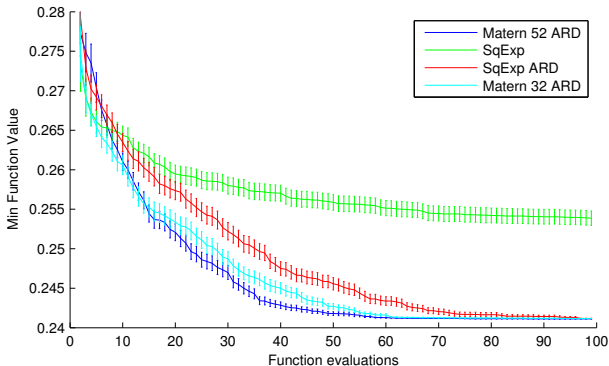


Figure: Figure from Snoek et al. (2012)

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- Solution: Integrate out the GP hyper-parameters θ by Markov Chain Monte Carlo (MCMC) sampling (e.g., slice sampling)

- 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

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

- 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)

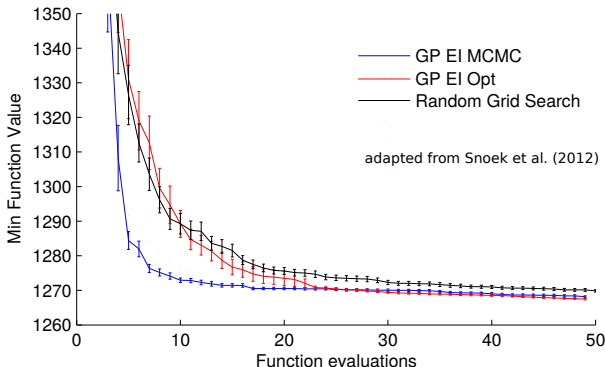
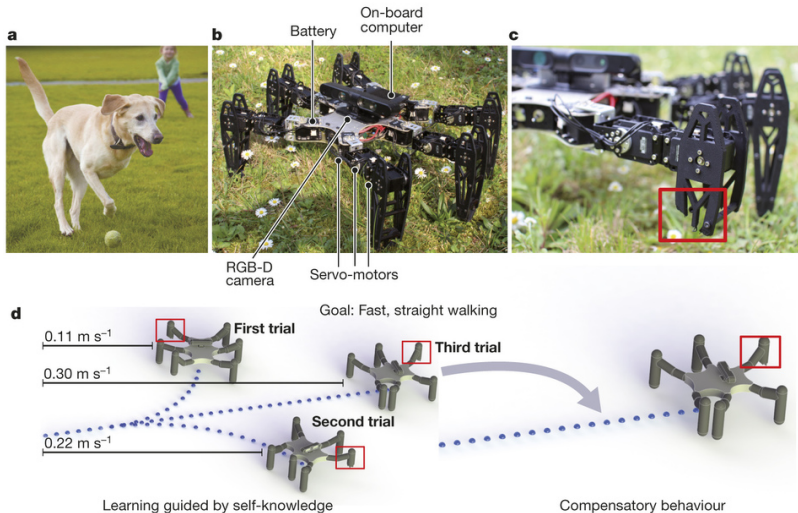
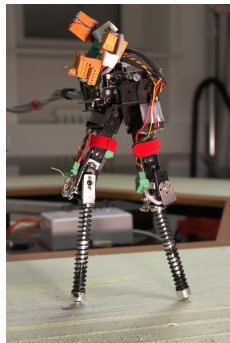


Figure: Figure from Snoek et al. (2012)



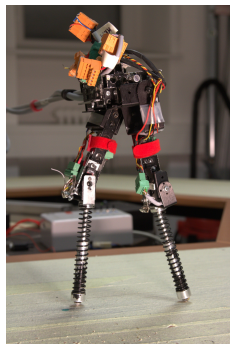
Cully et al. (2015)

- 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)

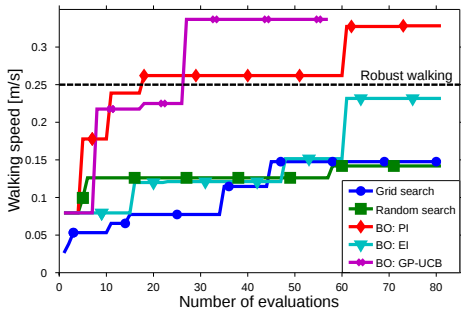


Calandra et al. (2015)

- 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)
- Good parameters found after 80–100 experiments
- **Substantial speed-up** compared to manual parameter search



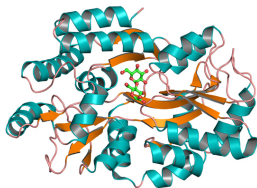
Calandra et al. (2015)



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

- **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)

- **BoTorch** <https://github.com/pytorch/botorch>
(Balandat et al., 2019)
- **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)



- 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 off exploration and exploitation

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