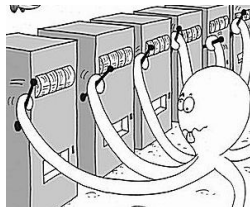# Bayesian optimization - Lecture 2

Hrvoje Stojic

May 26, 2017

The multi-armed bandit (MAB) problem

Formulation

- A tuple $\langle \mathcal{A}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a (stationary) set of K actions/arms
- $\mathcal{R}^a(r) = P[r|a]$ is an unknown probability distribution over rewards
- At each step t the agent selects an action $a_t \in \mathcal{A}$
- The environment generates a reward $r_t \sim \mathcal{R}^{a_t}$
- The goal is to maximise cumulative reward $\sum_{\tau=1}^{t} r_\tau$

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- Regret can be expressed in terms of counts and gaps:
  - The count $N_t(a)$ is expected number of selections for action a
  - The gap Δ_a is the difference in value between action a and optimal action a^*, $\Delta_a = V^* - Q(a)$
  - The cumulative regret, stated differently:

  $$L_t = \sum_{a \in \mathcal{A}} E[N_t(a)](V^* - Q(a)) = \sum_{a \in \mathcal{A}} E[N_t(a)]\Delta_a$$

Random exploration approaches

- We consider algorithms that estimate $\hat{Q}_t(a) \approx Q(a)$, by simply tracking the means

$$\hat{Q}_t(a) = \frac{1}{N_t(a)} \sum_{t=1}^{T} r_t \mathbf{1}(a_t = a)$$

or

$$\hat{Q}_t(a) = \hat{Q}_{t-1}(a) + \alpha(r_t - \hat{Q}_{t-1}(a))$$

Random exploration approaches

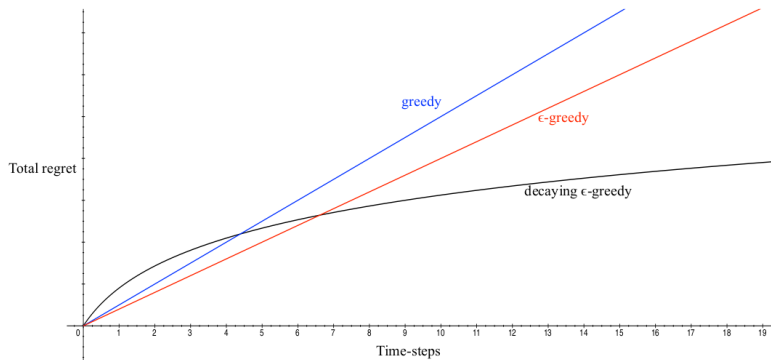- We consider algorithms that estimate $\hat{Q}_t(a) \approx Q(a)$, by simply tracking the means

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  or

$$\hat{Q}_t(a) = \hat{Q}_{t-1}(a) + \alpha(r_t - \hat{Q}_{t-1}(a))$$

- Three choice rules:
    - **greedy**: $a_t^* = \operatorname{argmax}_{a \in \mathcal{A}} \hat{Q}_t(a)$
    - ϵ-**greedy**: With probability $1 - \epsilon$ select $a_t^* = \operatorname{argmax}_{a \in \mathcal{A}} \hat{Q}_t(a)$, with probability ϵ select a random action
    - **Softmax**: $P(a_t = a) = \frac{\exp(\hat{Q}_t(a)/\tau)}{\sum_{a'=1}^{K} \exp(\hat{Q}_t(a')/\tau)}$

Linear regret
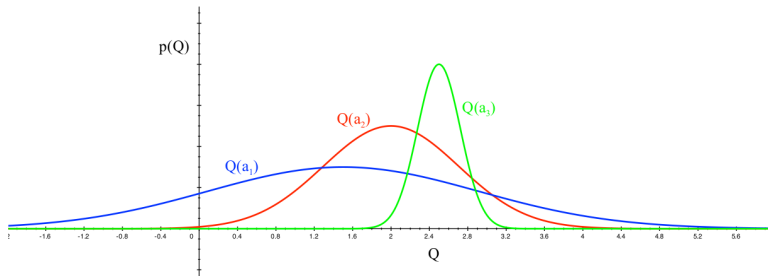

Source: David Silver lectures

Lower bound on regret

- Asymptotic total regret is at least logarithmic in number of steps (Lai & Robbins, 1985)

$$\lim_{t \to \infty} \geq \log t \sum_{a | \Delta_a > 0} \frac{\Delta_a}{KL(\mathcal{R}^a \parallel \mathcal{R}^{a^*})}$$

- Logarithmic regret, the second term (task difficulty) is a scalar
  - KL divergence says how similar the reward distributions of two arms are
  - The difference in expected rewards between the arms is described by the gap, Δ_a

Optimism in the face of uncertainty

Source: David Silver lectures

Optimistic initialization & ϵ_t-greedy

- ϵ-greedy with optimistic initialization
    - Simple idea: initialise $\hat{Q}(a)$ to a high value
    - Update rule:

    $$\hat{Q}_t(a_t) = \hat{Q}_{t-1}(a) + \frac{1}{N_t(a_t)}(r_t - \hat{Q}_{t-1}(a))$$

    - Everything else stays the same!

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- Decaying ϵ_t-greedy (Auer, Cesa-Bianchi, Fischer, 2002)
  - Pick a decay schedule for $\epsilon_1, \epsilon_2, \ldots$
    - e.g. $\epsilon_t = \min\{1, \frac{c|\mathcal{A}|}{\min_a \Delta_a t}\}$
  - Has logarithmic asymptotic total regret (for known gaps)
  - In practice very good performance
  - Difficult to tune the decay

Upper Confidence Bounds (UCB)

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  - Let $X_1, ..., X_t$ be IID random variables in $[0, 1]$, and let $\bar{X}_t = \frac{1}{t} \sum_{\tau=1}^{t} X_\tau$ be the sample mean. Then

  $$P[E[X] > \bar{X}_t + u] \leq e^{-2tu^2}$$

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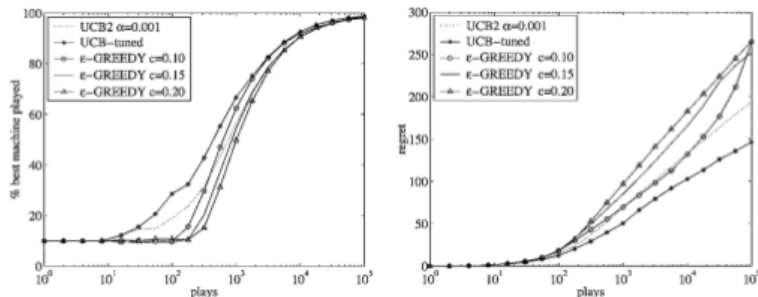 $$U_t(a) = \sqrt{\frac{2 \log t}{N_t(a)}}$$

UCB comparison

Figure 10. Comparison on distribution 12 (10 machines with parameters 0.9, 0.8, 0.8, 0.8, 0.7, 0.7, 0.7, 0.6, 0.6, 0.6).

Source: Auer, P., Cesa-Bianchi, N., & Fischer, P. (2002). Finite-time analysis of the multiarmed bandit problem. Machine Learning, 47, 235-256.

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- ▶ Wrong priors might cause issues.

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- We can fully describe f with parameter $\mathbf{w} \in (0, 1)^K$ so that $f_{\mathbf{w}}(a) = w_a$
- Observations are collected in $\mathcal{D}_t = \{(a_\tau, r_\tau)\}_\tau^t$ as a set of tuples, where a_τ identifies the arm and r_τ is the reward

Thompson Sampling for Beta-Bernoulli MAB problem

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- With such conjugate prior we can efficiently compute the posterior,

$$P[\mathbf{w}|\mathcal{D}] = \prod_{a=1}^{K} \text{Beta}(w_a|\alpha + n_{,1}, \beta + n_{a,0})$$

  - $n_{,1}$ is a count of 1 outcomes whenever for arm a
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▶ Thompson sampling (Thompson, 1933; Chapelle, Li, 2010)
  ▶ Sample $\mathbf{w}'$ from each posterior and then maximize,

  $$a_{t+1} = \mathrm{argmax}_a f_{\mathbf{w}'}(a), \text{where } \mathbf{w}' \sim P[\mathbf{w}|\mathcal{D}_t]$$

  ▶ Thompson sampling achieves Lai and Robbins lower bound!

Algorithm & Example

Algorithm 2: Thompson Sampling for Beta-Bernoulli Bandit

Require: α, β: hyperparameters of the beta prior
1: Initialize $n_{a,0} = n_{a,1} = i = 0$ for all a
2: **repeat**
3:   **for** $a = 1, \ldots, K$ **do**
4:     $\bar{w}_a \sim \text{beta}(\alpha + n_{a,1}, \beta + n_{a,0})$
5:   **end for**
6:   $a_i = \arg\max_a \bar{w}_a$
7:   Observe y_i by pulling arm a_i
8:   **if** $y_i = 0$ **then**
9:     $n_{a_i,0} = n_{a_i,0} + 1$
10:   **else**
11:     $n_{a_i,1} = n_{a_i,1} + 1$
12:   **end if**
13:   $i = i + 1$
14: **until** stopping criterion reached

$p(w) = \text{Beta}(w|2,2)$

A   **Buy now!** $\text{Beta}(w_A|7,3)$

B   **Purchase** $\text{Beta}(w_B|3,5)$

C   **Check out** $\text{Beta}(w_C|5,4)$
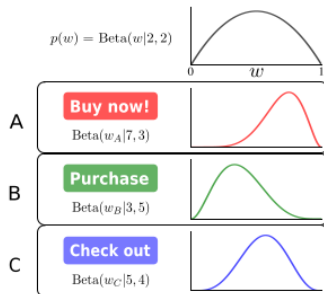
Fig. 2. *Example of the beta-Bernoulli model for A/B testing. Three different buttons are being tested with various colors and text. Each option is given two successes (click-throughs) and two failures as a prior (top). As data are observed, each option updates its posterior over w. Option A is the current best with five successes and only one observed failure.*

Source: Shahriari, B., Swersky, K., Wang, Z., Adams, R. P., & de Freitas, N. (2016). Taking the Human Out of the Loop: A Review of Bayesian Optimization. Proceedings of the IEEE, 104(1), 148-175.

Contextual Multi-armed Bandit (CMAB) problem

Formulation

- A tuple $\langle \mathcal{A}, \mathcal{S}, \mathcal{R} \rangle$
- We introduce the state representation again
- $\mathcal{A}$ is a set of actions/arms
- $\mathcal{S} = P[s]$ is an unknown distribution over states (or "contexts")
- $\mathcal{R}^a(r) = P[r|s, a]$ is an unknown probability distribution over rewards
- At each step t
  - The environment generates state $s_t \sim \int$
  - The agent selects an action $a_t \in \mathcal{A}$
  - The environment generates a reward $r_t \sim \mathcal{R}_{s_t}^{a_t}$
- The goal is to maximise cumulative reward $\sum_{\tau=1}^{t} r_\tau$
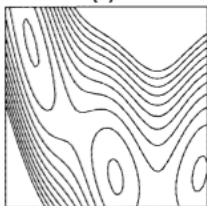
Bayesian nonparametric approach: Gaussian Processes (GP)

- Inducing a Gaussian prior over functions:

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$

- Here, $m(\mathbf{x})$ is a mean function modeling the expected output of the function and $k(\mathbf{x}, \mathbf{x}')$ is a kernel function modeling the covariance between different points.

$$m(\mathbf{x}) = E[f(\mathbf{x})]$$

and

$$k(x, x') = E[(f(\mathbf{x}) - m(x))(f(\mathbf{x}') - m(x'))]$$

- The choice of an appropriate kernel is normally based on assumptions such as smoothness and likely patterns to be expected in the data.

Gaussian Processes (GP)

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- Popular choice is the squared exponential (also called Gaussian or Radial Basis Function) kernel.

$$k(x, x') = \sigma^2 \exp\left(-\frac{(x - x')^2}{2\lambda^2}\right)$$

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- Correlation between two points decays according to a power function in dependency of the distance between the two points
- Covariance is symmetric, that is that only the distance between two points matters, but not the direction.

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- Correlation between two points decays according to a power function in dependency of the distance between the two points
- Covariance is symmetric, that is that only the distance between two points matters, but not the direction.

- Good for smooth functions, hyperparameters λ (called the length-scale) and σ^2 (the noise constant) are normally optimized by using the marginal likelihood.

Gaussian Processes (GP)

- This implies the aforementioned distribution over functions as we can easily generate samples for new input points at location $X_\star$.

$$\mathbf{f}_\star \sim \mathcal{N}(0, K(X_\star, X_\star))$$

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$$\mathbf{f}_\star \sim \mathcal{N}(0, K\left(X_\star, X_\star\right))$$

- Given observations $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ with a noise level σ, we can draw new predictions from our function $\mathbf{f}_\star$ for inputs $X_\star$ as described below.

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_\star \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X, X) + \sigma^2 I & K(X, X_\star) \\ K(X_\star, X) & K(X_\star, X_\star) \end{bmatrix} \right)$$

Gaussian Processes (GP)

- Treat a function as a vector of infinite size.
- We can simply draw outputs for finite points by using a multivariate normal distribution with a covariance matrix generated by our kernel.
- Calculating the expectation of the Gaussian Process at the new points is then

$$\mathbf{f}_\star | X, \mathbf{y}, X_\star \sim \mathcal{N}(\overline{\mathbf{f}}_\star, \text{cov}(\mathbf{f}_\star))$$

- Predictions for new points are generated based on the expected mean value and covariance function of the posterior Gaussian Process.

$$\mathbb{E}[\mathbf{f}_\star | X, \mathbf{y}, X_\star] = K(X_\star, X)[K(X, X) + \sigma^2 I]^{-1}\mathbf{y}$$

$$\text{cov}(\mathbf{f}_\star) = K(X_\star, X_\star) - K(X_\star, X)[K(X, X) + \sigma^2 I]^{-1}K(X, X_\star)$$

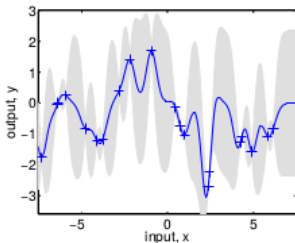# Drawing from the GP prior and posterior
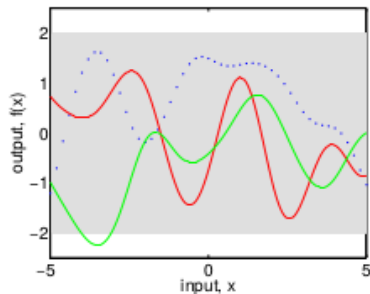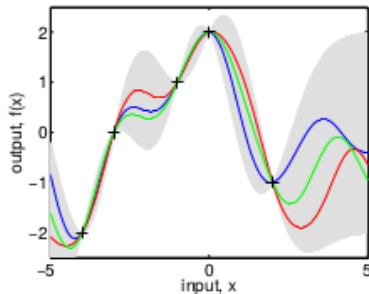
(a), prior   (b), posterior

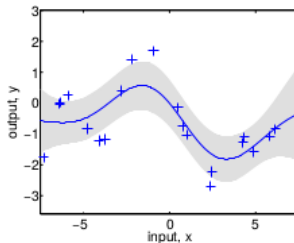Source: Rasmussen, Williams (2006)

Dependence on hyperparameters
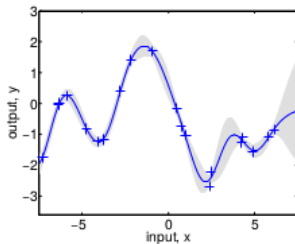
(a), $\ell = 1$

(b), $\ell = 0.3$

(c), $\ell = 3$
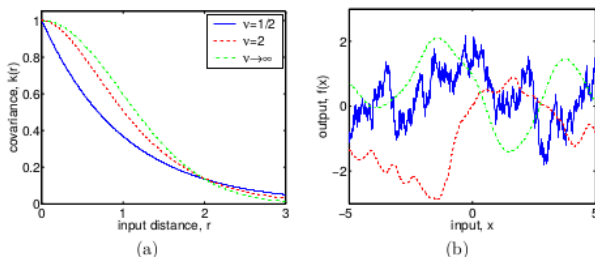
Source: Rasmussen, Williams (2006)

Matern kernel

Figure 4.1: Panel (a): covariance functions, and (b): random functions drawn from Gaussian processes with Matérn covariance functions, eq. (4.14), for different values of ν, with $\ell = 1$. The sample functions on the right were obtained using a discretization of the x-axis of 2000 equally-spaced points.

Source: Rasmussen, Williams (2006)

GP algorithm

input: X (inputs), $\mathbf{y}$ (targets), k (covariance function), σ_n^2 (noise level), $\mathbf{x}_*$ (test input)

2: $L := \text{cholesky}(K + \sigma_n^2 I)$
   $\boldsymbol{\alpha} := L^\top \backslash (L \backslash \mathbf{y})$
4: $\bar{f}_* := \mathbf{k}_*^\top \boldsymbol{\alpha}$ $\quad \} \text{ predictive mean eq. (2.25)}$
   $\mathbf{v} := L \backslash \mathbf{k}_*$
6: $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$ $\quad \} \text{ predictive variance eq. (2.26)}$
   $\log p(\mathbf{y}|X) := -\frac{1}{2}\mathbf{y}^\top \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2}\log 2\pi \quad$ eq. (2.30)
8: **return**: $\bar{f}_*$ (mean), $\mathbb{V}[f_*]$ (variance), $\log p(\mathbf{y}|X)$ (log marginal likelihood)

Algorithm 2.1: Predictions and log marginal likelihood for Gaussian process regression. The implementation addresses the matrix inversion required by eq. (2.25) and (2.26) using Cholesky factorization, see section A.4. For multiple test cases lines 4-6 are repeated. The log determinant required in eq. (2.30) is computed from the Cholesky factor (for large n it may not be possible to represent the determinant itself). The computational complexity is $n^3/6$ for the Cholesky decomposition in line 2, and $n^2/2$ for solving triangular systems in line 3 and (for each test case) in line 5.

Source: Rasmussen, Williams (2006)

Computational considerations and alternative regression models

Computational considerations and alternative regression models

- ► Although we have analytic expressions, exact inference in GP regression has a cost of $\mathcal{O}(n^3)$
- ► Due to inversion of the covariance matrix
  - ► in practice using Cholesky decomposition reduces the cost to $\mathcal{O}(n^2)$
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- ► With large budgets the cost might be prohibitive
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- ▶ Other alternative regression models?
  - ▶ Random Forests (SMAC, TPE)
  - ▶ Variance in predictions of the trees used as a proxy for uncertainty
  - ▶ Poor extrapolators
  - ▶ GPs are relatively bad as well, but they revert to prior far from the inputs, while RF is unrealistically confident

GP-UCB

Algorithm 1 The GP-UCB algorithm.

Input: Input space D; GP Prior $\mu_0 = 0$, σ_0, k
for $t = 1, 2, \ldots$ **do**
    Choose $\boldsymbol{x}_t = \underset{\boldsymbol{x} \in D}{\operatorname{argmax}} \, \mu_{t-1}(\boldsymbol{x}) + \sqrt{\beta_t} \sigma_{t-1}(\boldsymbol{x})$
    Sample $y_t = f(\boldsymbol{x}_t) + \epsilon_t$
    Perform Bayesian update to obtain μ_t and σ_t
end for

- Regret bounds, Srinivas et al (2010)
- Expected improvement, Probability of improvement, Entropy search, predictive entropy search, Portfolios of acquisition functions (Hedge, Entropy search portfolio)

Expected Improvement

- $EI(\mathbf{x}) = \mathbb{E}\left[\max\left\{0, f(\mathbf{x}) - f(\hat{\mathbf{x}})\right\}\right]$, where $\hat{\mathbf{x}}$ is the current optimal set of hyperparameters.

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- We can actually compute EI expectation under the GP model

$$EI(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\hat{\mathbf{x}}))\Phi(Z) + \sigma(\mathbf{x})\phi(Z) & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases} \tag{1}$$

$$Z = \frac{\mu(\mathbf{x}) - f(\hat{\mathbf{x}})}{\sigma(\mathbf{x})} \tag{2}$$

where $\Phi(z)$, and $\phi(z)$, are the cumulative distribution and probability density function of the (multivariate) standard normal distribution.

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where $\Phi(z)$, and $\phi(z)$, are the cumulative distribution and probability density function of the (multivariate) standard normal distribution.

1. EI is high when the (posterior) expected value $\mu(\mathbf{x})$ is higher than the current best value $f(\hat{\mathbf{x}})$; or
2. EI is high when the uncertainty $\sigma(\mathbf{x})$ around the point $\mathbf{x}$ is high.

Acquisition functions illustration
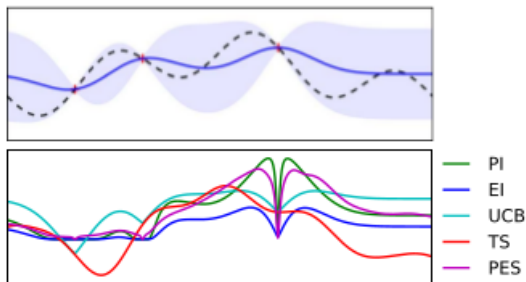
Fig. 5. *Visualization of the surrogate regression model and various acquisition functions. (Top) The true objective function is shown as a dashed line and the probabilistic regression model is shown as a blue line with a shaded region delimiting the $2\sigma_n$ credible intervals. Finally, the observations are shown as red crosses. (Bottom) Four acquisition functions are shown. In the case of PI, the optimal mode is much closer to the best observation as in the alternative methods, which explains its greedy behavior. In contrast, the randomization in TS allows it to explore more aggressively.*

Source: Shahriari et al (2016)

Optimizing acquisition functions

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  - ▶ Use the same optimism in the face of uncertainty on acquisition function optimization level as well
  - ▶ E.g. Wang, SShakibi, Jin and de Freitas (2014) propose BamSOO: shrink the region that we examine in every iteration to the most promising regions

Optimizing acquisition functions: Optimistic optimization (BamSOO)
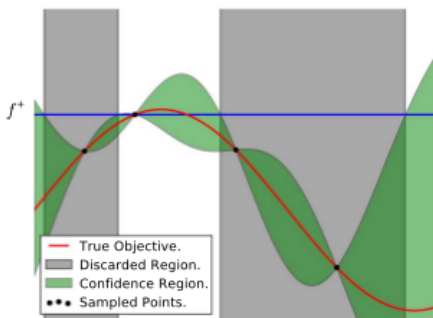
Fig. 7. *Conditioned on the unknown objective function (red) lying between the surrogate confidence bounds (green region) with high probability, we can discard regions of the space where the upper bound is lower than the best lower bound encountered thus far. Figure from [43].*

Source: Shahriari et al (2016)

Acquisition functions comparison
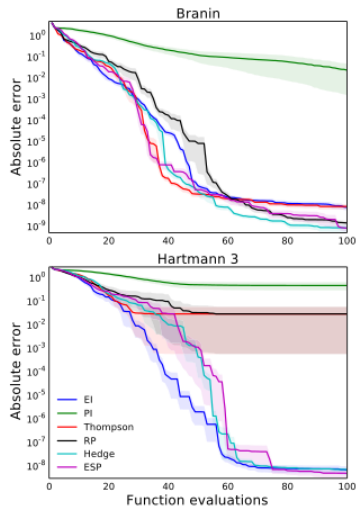
- Shahriari et al (2016) conclude choice of acquisition function matters less than the regression model

Example: Tuning the SVM hyperparameters

- 20 dimensional problem, where the predictors are independent Gaussian random variables with mean zero and a variance of 9 (Sapp et al. 2014)

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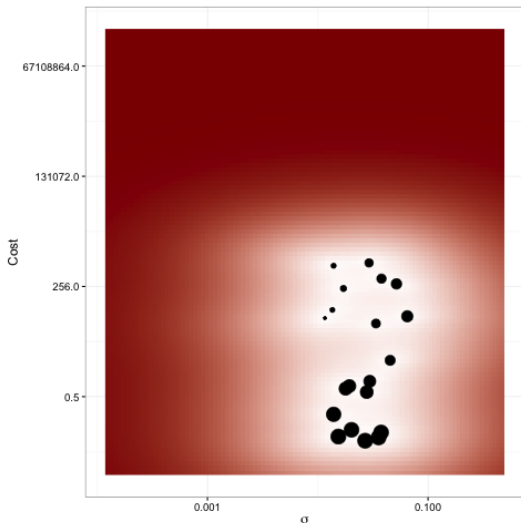 - using kernlab and rBayesianOptimization
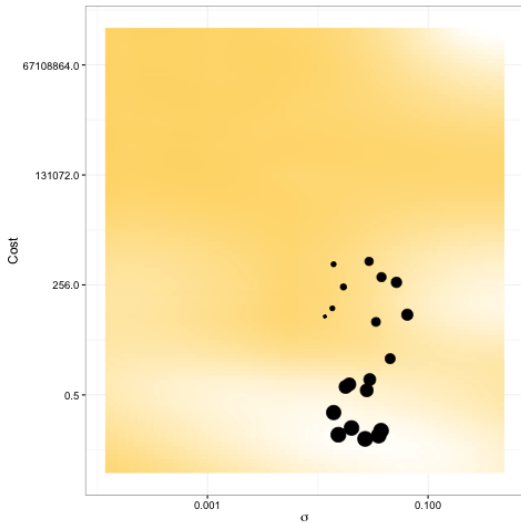
Example: RMSE surface
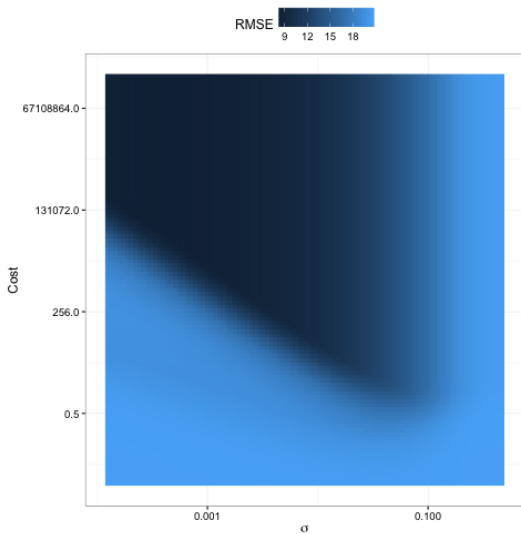
Example: Random search
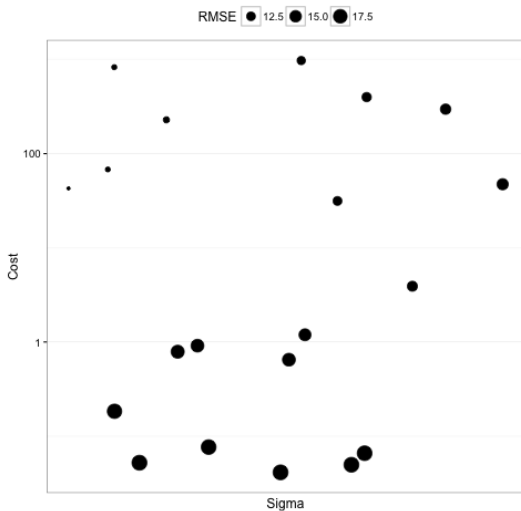
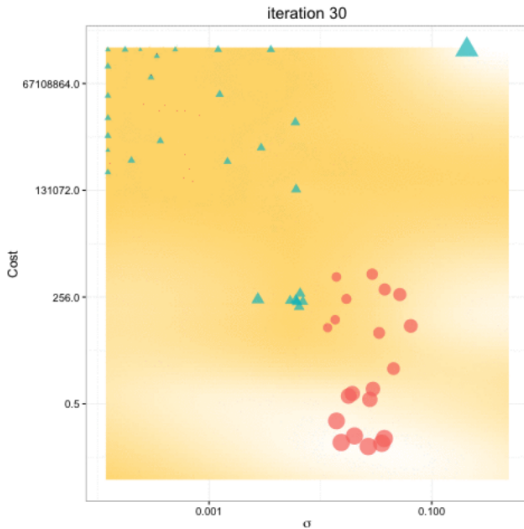# Example: GP predictive mean (based on initial random search)
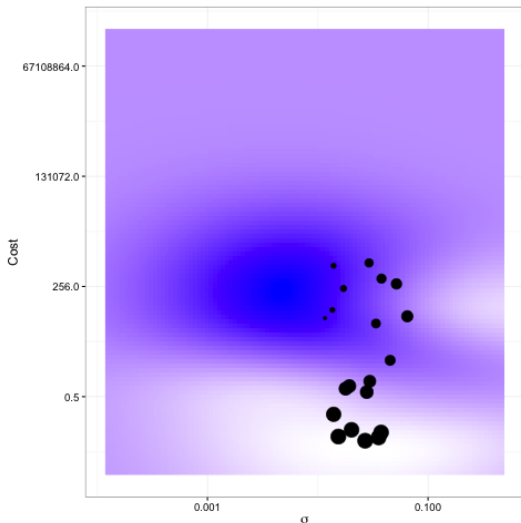
Example: GP predictive variance (based on initial random search)

Example: GP-UCB (based on initial random search)

Example: GP-UCB solution after 30 evaluations

Some extensions

Full Bayesian treatment

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$$\hat{a}(\mathbf{x}; \mathbf{x}_t, y_t) = \int a(\mathbf{x}; \{\mathbf{x}_t, y_t\}, \theta) P[\theta | \{\mathbf{x}_t, y_t\}^t] d\theta$$

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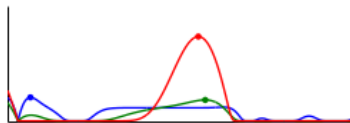$$\hat{a}(\mathbf{x}; \mathbf{x}_t, y_t) = \int a(\mathbf{x}; \{\mathbf{x}_t, y_t\}, \theta) P[\theta | \{\mathbf{x}_t, y_t\}^t] d\theta$$

- Monte Carlo estimate, can be acquired efficiently with slice sampling (see Murray & Adams, 2010)
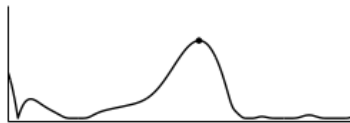
Example
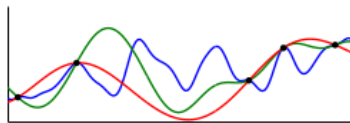
(a) Posterior samples under varying hyperparameters

(b) Expected improvement under varying hyperparameters

(c) Integrated expected improvement

Source: Snoek et al (2012). Practical Bayesian Optimization of
Machine Learning Algorithms. In Advances in Neural Information
Processing Systems (pp. 2951–2959).

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Example
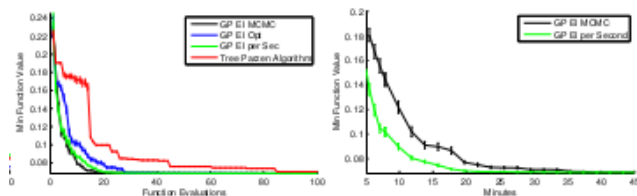
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- With function like EI we can leverage Gaussian integration property
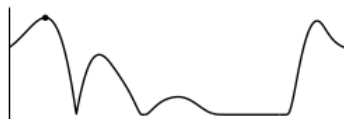
Example
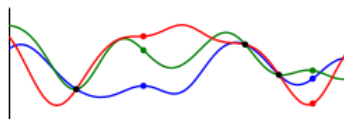
(a) Posterior samples after three data
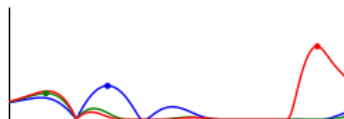
(b) Expected improvement under three fantasies

(c) Expected improvement across fantasies

Source: Snoek et al (2012). Practical Bayesian Optimization of Machine Learning Algorithms. In Advances in Neural Information Processing Systems (pp. 2951–2959).

Other applications of BO

Tackling any other (C)MAB problem

- ► Ad placement:
    - ► Placing an ad that has been shown to attract the most clicks (exploiting)
    - ► Or placing a different ad that we know less about, that might attract more clicks (exploring)
- ► Recommender system
    - ► People are interested in true exploration, not only seeing what other similar people have looked for
    - ► In some setups, like news recommendation, choice sets are changing all the time, RL approach is more suitable
- ► Learning user preferences
    - ► Market research, finding an optimal combination of features in a new product
    - ► E.g. tuning the recommender system so it is customized for each user