

# Gaussian Processes and Bayesian Optimization

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# 1 Motivation

## 2 Gaussian Process model

## 3 GP regression

## 4 Learning Gaussian Process model

## 5 Gaussian Process classification

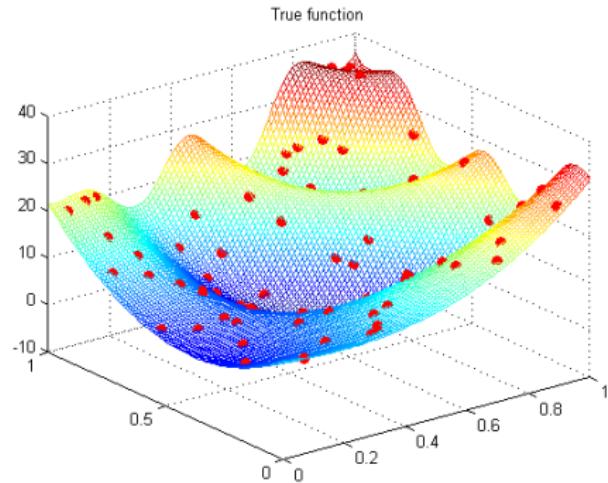
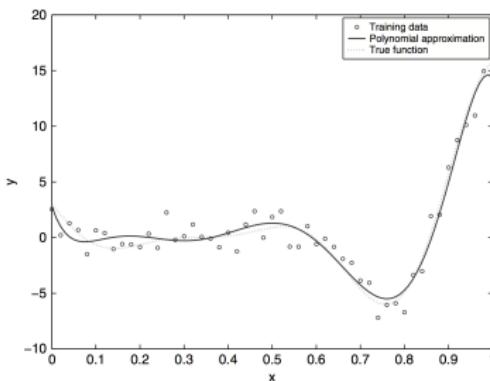
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- Learn scalar function  $f(\mathbf{x})$  of vector  $\mathbf{x}$
- We have (possibly noisy) sample  $S_m = \{\mathbf{X}, \mathbf{y}\} = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$



- **Real-valued regression:**

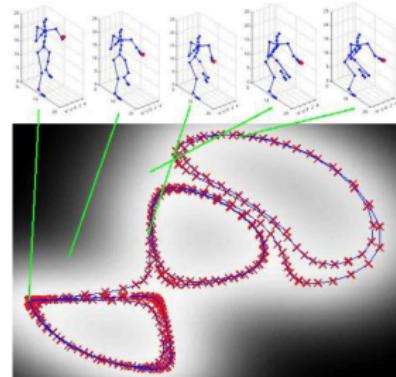
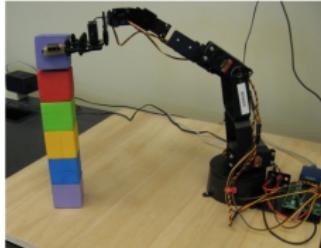
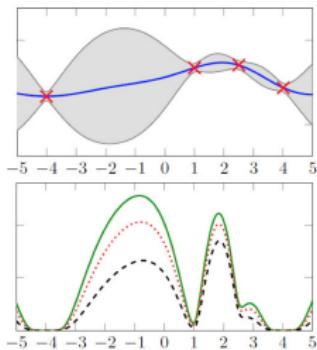
- Model-based predictive control: predict yield, quality, losses, etc.
- Surrogate surfaces for optimization or simulation
- Robotics: target state → required torques

- **Classification:**

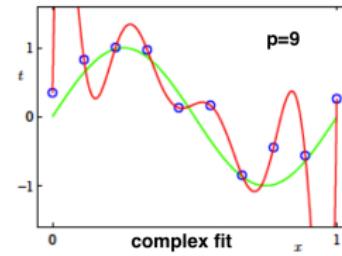
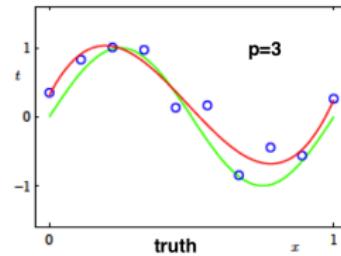
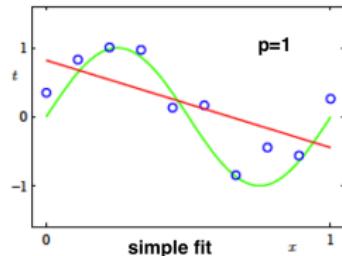
- Recognition: handwritten digits on payment docs, etc.
- Detection: fraud, screening in chemoinformatics

- **Ordinal Regression:**

- Disease harmfulness prediction
- User ratings (movies, shops, restaurants)



- Data generation process is often unknown and can be complex:



- Problems:

- Fitting complicated models can be hard
- How to find an appropriate model?
- How to avoid over-fitting?

- **Problem:** Predicting Profit

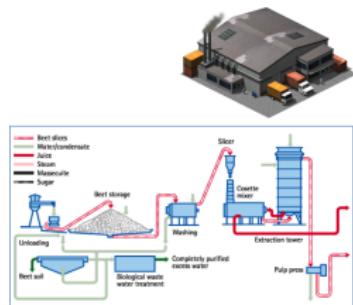
- **Object:** production of one batch of a product
- **Input  $x$ :** beet chips shape, quality, temperature, sugar content and flux; wash water temperature, pH and flux; the temperature inside the diffuser, etc.
- **Output  $y$ :** costs, losses, efficiency of sugar extraction

- **Challenges:**

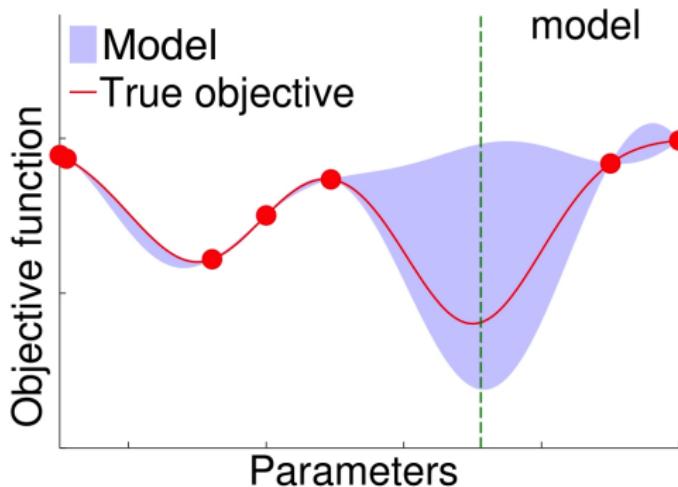
- Heterogeneous data and noise,
- Large volumes of high-dimensional stream data,
- Missing values, outliers, etc.

- **Knowing error bars is very important:**

- Setting  $x_1 \rightarrow$  profit of  $40 \pm 10$  units
- Setting  $x_2 \rightarrow$  profit of  $60 \pm 40$  units
- **Which are the best setting,  $x_1$  or  $x_2$ ?**



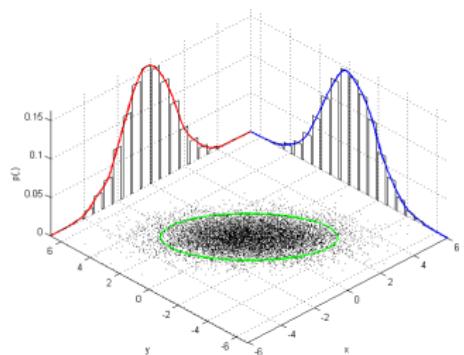
- In high-dimensional case we need many functions evaluations to be certain in results
- Often each evaluation is costly, e.g. in case of experiments



- Error bars are needed to see if a region is still promising

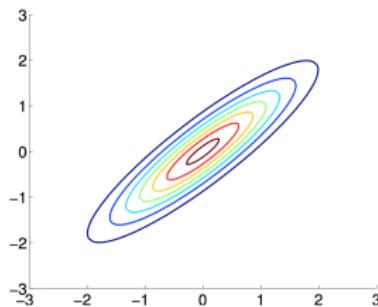
- Parametric family of functions  $f(\mathbf{x}; \boldsymbol{\theta})$
- Define a prior over  $\boldsymbol{\theta}$
- Perform predictions and estimate uncertainty
- For flexible models we a.s. get intractable integrals over  $\boldsymbol{\theta}$

**For Gaussian case usually everything is explicit**



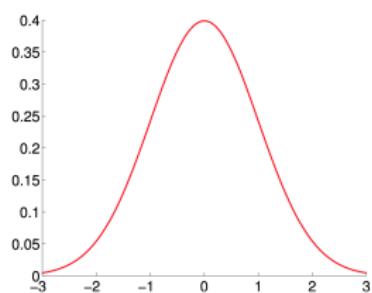
Solution of complex ML problems with simple Gaussian models?

# The Gaussian Distribution



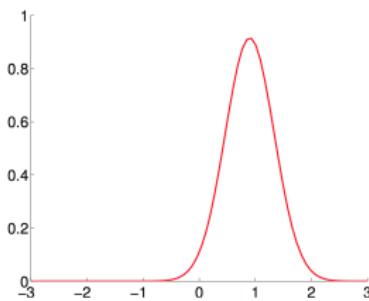
$$p(\mathbf{f}_1, \mathbf{f}_2) \sim \mathcal{N}(\mathbf{f}_1, \mathbf{f}_2 | \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Joint



$$p(\mathbf{f}_1)$$

Marginal



$$p(\mathbf{f}_1 | \mathbf{f}_2)$$

Conditional

The **marginal** and **conditional** distributions are also Gaussians:

$$\begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix} \sim \mathcal{N} \left( \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{bmatrix} \right)$$

$$p(\mathbf{f}_1) = \int p(\mathbf{f}_1, \mathbf{f}_2) d\mathbf{f}_2 = \mathcal{N}(\mathbf{f}_1 | \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$$

$$p(\mathbf{f}_1 | \mathbf{f}_2) = \mathcal{N}(\mathbf{f}_1 | \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{f}_2 - \boldsymbol{\mu}_2), \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{12}^T)$$

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- **Hypothesis set**  $\mathcal{F} \subset Y^X$  is a subset of functions out of which the learner selects his/her hypothesis
  - represents a prior knowledge about the task at hand
  - depends on available features
- Typical examples (from statistics)
  - Sobolev-type classes:

$$\mathcal{F}_L^k = \left\{ f : \int \left\| \frac{\partial^k f(\mathbf{x})}{\partial \mathbf{x}^k} \right\|^2 d\mathbf{x} \leq L \right\}$$

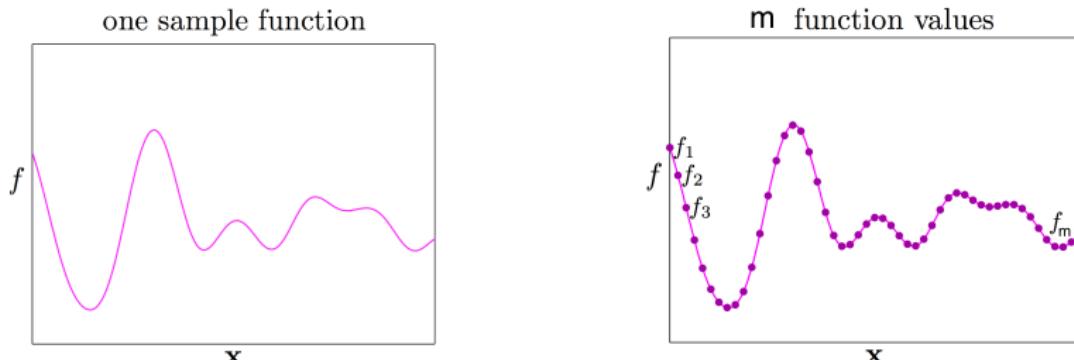
- Lipschitz classes:

$$\mathcal{F}_L = \{f : |f(\mathbf{x}) - f(\mathbf{x}')| \leq L\rho(\mathbf{x}, \mathbf{x}')\}$$

- How to impose regularity on a function in Bayesian case?

# What is a Gaussian process?

- Continuous stochastic process — random functions — a set of random variables  $f(\mathbf{x})$  indexed by a continuous variable  $\mathbf{x}$



- Let us denote by
  - $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_m\}$  a set of  $d$ -dimensional inputs,
  - $\mathbf{f} = \{f_1, \dots, f_m\}$  a set of random function values  $f_i = f(\mathbf{x}_i)$
- **GP:** Any set of function variables  $\{f_i\}_{i=1}^m$  has joint Gaussian distribution

$$p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{K})$$

- Conditional model — density of inputs is not modeled

Where do the mean value  $\mu$  and covariance matrix  $\mathbf{K}$  come from?

- Mean value is constructed from a priori given deterministic function

$$\boldsymbol{\mu} = \{\mu_i\} = \{\mu(\mathbf{x}_i)\}$$

- Covariance matrix is constructed from covariance function

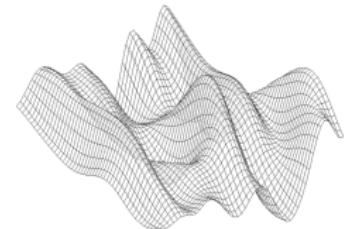
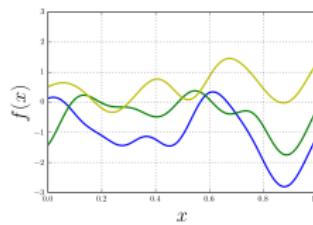
$$\mathbf{K} = \{\mathbf{K}_{ij}\} = \{K(\mathbf{x}_i, \mathbf{x}_j)\}$$

- Covariance function characterizes covariance between points in the process

$$K(\mathbf{x}, \mathbf{x}') = \text{cov}(f(\mathbf{x}), f(\mathbf{x}')) = \mathbb{E} (f(\mathbf{x}) - \mu(\mathbf{x})) (f(\mathbf{x}') - \mu(\mathbf{x}'))$$

- Must produce positive semidefinite covariance matrices  $\mathbf{v}^T \mathbf{K} \mathbf{v} \geq 0$

$$f(\mathbf{x}) \sim \mathcal{GP}(\cdot | \mu(\mathbf{x}), K(\mathbf{x}, \mathbf{x}'))$$



- In order to define  $f(\mathbf{x}) \sim \mathcal{GP}(\cdot)$  we have to define a **mean function**  $\mu(\mathbf{x})$  and a **covariance function**  $K(\mathbf{x}, \mathbf{x}')$
- Bayesian linear model

$$f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b = \sum_{i=1}^p w_i \phi_i(\mathbf{x}) + b$$

$$\mathbf{w} \sim \mathcal{N}(0, \sigma_f^2 \cdot \mathbf{I}_p)$$

$$b \sim \mathcal{N}(0, \sigma_1^2)$$

- We can easily obtain that

$$\mu(\mathbf{x}) = 0, \text{ cov}(f(\mathbf{x}), f(\mathbf{x}')) = \sigma_f^2 \phi(\mathbf{x})^T \phi(\mathbf{x}') + \sigma_1^2$$

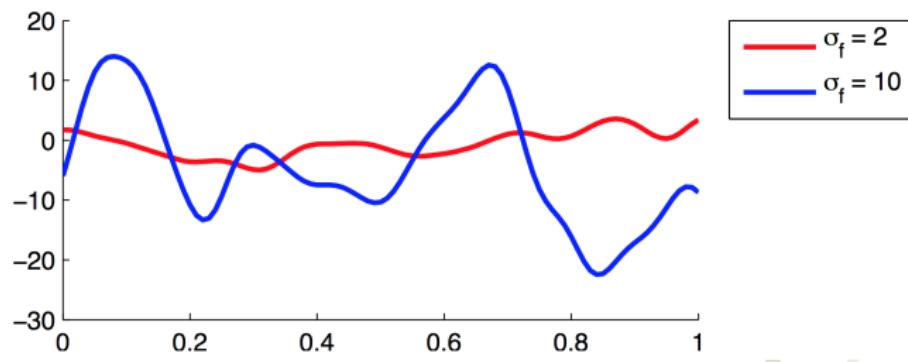
- Kernel parameters  $\sigma_f^2$  and  $\sigma_1^2$  are hyper-parameters in the Bayesian hierarchical model
- More interesting kernels come from models with a large or infinite feature space  $p \gg 1$ . Because feature weights  $\mathbf{w}$  are integrated out, this is computationally no more expensive

- An infinite number of radial-basis functions can give

$$K(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp \left\{ -\sum_{i=1}^d \frac{(x_i - x'_i)^2}{2r_i^2} \right\}$$

the most commonly-used kernel in machine learning

- A GP need not use the Gaussian kernel. There are a lot of other choices
- Consider  $\mathbf{x} = \mathbf{x}' \rightarrow$  marginal function variance is  $\sigma_f^2$

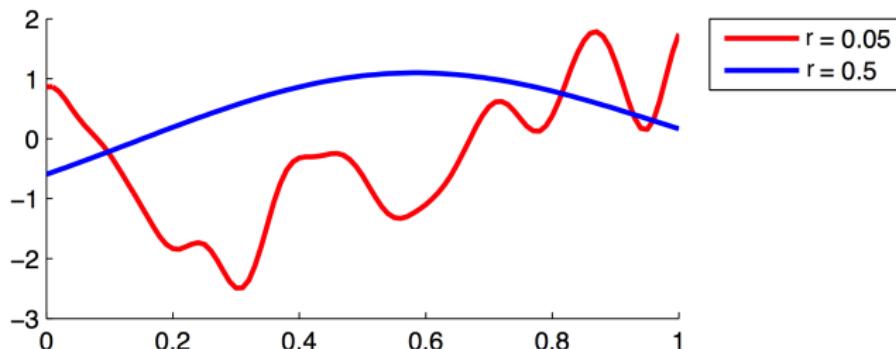


## Example: squared-exponential kernel

- The  $r_i$  parameters give the overall lengthscale in dimension  $i$

$$K(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp \left\{ - \sum_{i=1}^d \frac{(x_i - x'_i)^2}{2r_i^2} \right\}$$

- Typical distance between peaks  $\approx r$

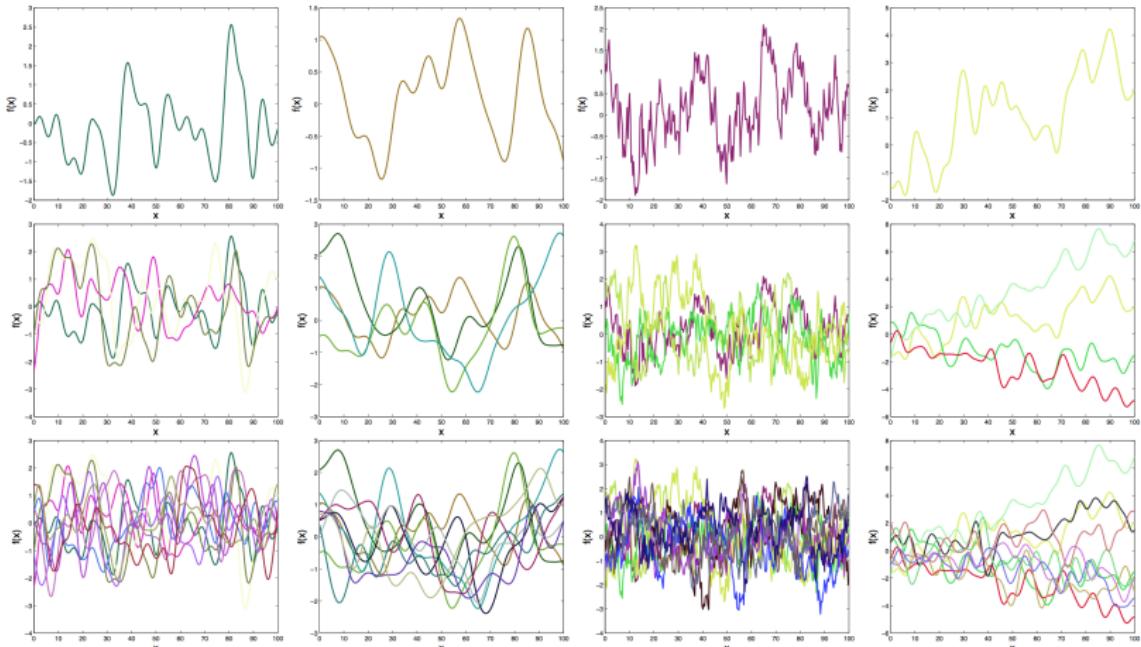


- More general example of covariance function

$$K(x, x') = \sigma_f^2 \exp \left\{ - \left( \frac{|x - x'|}{r} \right)^\alpha \right\} + \sigma_1^2 + \sigma_2^2 \delta(x - x')$$

- As usual covariance function parameters are **interpretable**
  - $\sigma_f^2$  — marginal function variance
  - $\sigma_1^2$  — variance of bias
  - $\sigma_2^2$  — noise variance
  - $r$  — lengthscale
  - $\alpha \geq 1$  — roughness
- Once the mean and covariance functions are defined, everything else about GPs follows from the basic rules of probability applied to multivariate Gaussians

# Samples from GPs with different $K(x, x')$



$$K(x, x') = \frac{\sigma_f^2 2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu}|x - x'|}{\lambda} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu}|x - x'|}{\lambda} \right),$$

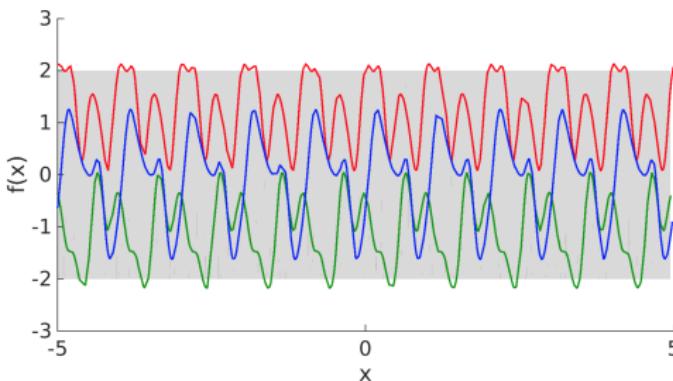
where  $K_\nu$  is a modified Bessel function

- Stationary, isotropic
- $\nu \rightarrow \infty$ : squared-exponential covariance
- Finite  $\nu$ : much rougher sample functions
- $\nu = 1/2$ :  $K(x, x') = \sigma_f^2 \exp(-|x - x'|/r)$ , very rough sample functions (**seminar**)

## Example: Nonstationary covariances

- Linear covariance:  $K(x, x') = \sigma_f^2 \cdot xx' + \sigma_1^2$
- Periodic covariance (**seminar**):

$$K(x, x') = \sigma_f^2 \cdot \exp\left(-\frac{2 \sin^2\left(\frac{x-x'}{2}\right)}{r^2}\right)$$



- Neural network covariance

There are several ways to combine covariances (**seminar**)

- **Sum:**  $K(x, x') = K_1(x, x') + K_2(x, x')$
- **Product:**  $K(x, x') = K_1(x, x') \cdot K_2(x, x')$
- **Convolution:**  $K(x, x') = \int dz dz' h(x, z) K(z, z') h(x', z')$  (blurring of process with kernel  $h$ )

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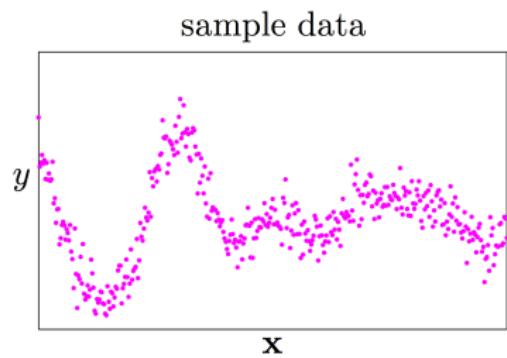
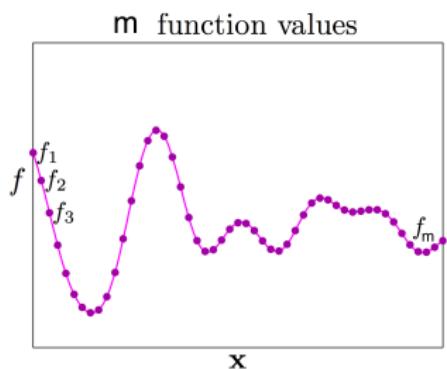
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- Training data set  $S_m = \{\mathbf{X}, \mathbf{y}\} = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
- Model:

$$y_i = f(\mathbf{x}_i) + \varepsilon_i,$$

$$f \sim \mathcal{GP}(\cdot | 0, K)$$

$\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$  is a white noise



- Training data set  $S_m = \{\mathbf{X}, \mathbf{y}\} = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$
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- The prior is

$$p(\mathbf{f}) = \mathcal{N}(\mathbf{f} | \mathbf{0}, \mathbf{K})$$

- The noise model, or likelihood is

$$p(\mathbf{y} | \mathbf{f}) = \mathcal{N}(\mathbf{y} | \mathbf{f}, \sigma^2 \mathbf{I}_m)$$

- Integrating over the function variables  $\mathbf{f}$  we get the marginal likelihood

$$p(\mathbf{y}) = \int d\mathbf{f} p(\mathbf{y} | \mathbf{f}) p(\mathbf{f}) d\mathbf{f} = \mathcal{N}(\mathbf{0}, \mathbf{K} + \sigma^2 \mathbf{I}_m)$$

- Let us denote input test point as  $\mathbf{x}_*$ , and output

$$y_* = f_* + \varepsilon_*, \quad f_* = f(\mathbf{x}_*)$$

- Consider joint training and test marginal likelihood

$$p(\mathbf{y}, f_*) = \mathcal{N} \left( \mathbf{0}, \begin{bmatrix} \mathbf{K} + \sigma^2 \mathbf{I}_m & \mathbf{k}_* \\ \mathbf{k}_*^\top & K_{**} \end{bmatrix} \right),$$

where  $\mathbf{k}_* = \{K(\mathbf{x}_*, \mathbf{x}_i)\}_{i=1}^m$  and  $K_{**} = K(\mathbf{x}_*, \mathbf{x}_*)$

- What we know about noiseless value  $f(\mathbf{x}_*)$ ?

- Joint training and test marginal likelihood

$$p(\mathbf{y}, f_*) = \mathcal{N} \left( \mathbf{0}, \begin{bmatrix} \mathbf{K} + \sigma^2 \mathbf{I}_m & \mathbf{k}_* \\ \mathbf{k}_*^\top & K_{**} \end{bmatrix} \right),$$

where  $\mathbf{k}_* = \{K(\mathbf{x}_*, \mathbf{x}_i)\}_{i=1}^m$  and  $K_{**} = K(\mathbf{x}_*, \mathbf{x}_*)$

- Condition on training outputs we get

$$p(f_* | \mathbf{y}) = \mathcal{N} (f_* | \mu_*, \sigma_*^2),$$

$$\mu_* = \mathbf{k}_*^\top [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{y}, \quad \sigma_*^2 = K_{**} - \mathbf{k}_*^\top [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{k}_*$$

- In fact  $\mu_*$  has the form

$$\mu_* = \sum_{i=1}^m \alpha_i K(\mathbf{x}, \mathbf{x}_i), \quad \boldsymbol{\alpha} = [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{y}$$

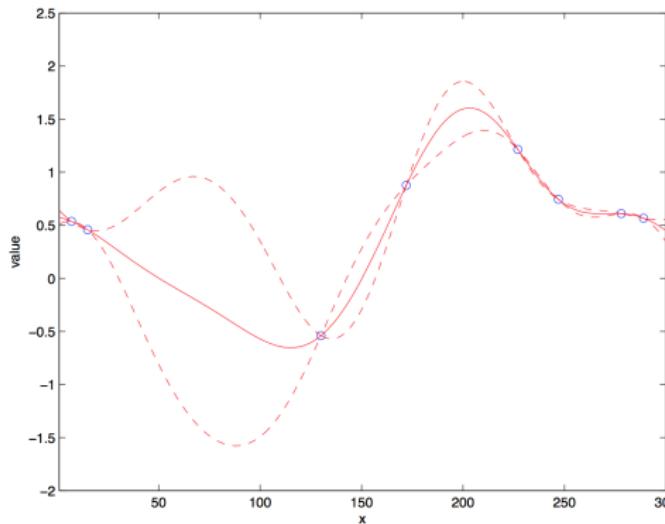
- Computational complexity:  $O(m^3)$  for inversion in  $\boldsymbol{\alpha}$ ,  $O(m)$  for  $\mu_*$  and  $O(m^2)$  for  $\sigma_*^2$

- Conditional distribution

$$p(f_* | \mathbf{y}) = \mathcal{N}(f_* | \mu_*, \sigma_*^2),$$

$$\mu_* = \mathbf{k}_*^T [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{y}, \quad \sigma_*^2 = K_{**} - \mathbf{k}_*^T [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{k}_*$$

- What we know about noiseless value  $f_* = f(\mathbf{x}_*)$ ? Let us assume that  $\sigma = 0$  (interpolation)

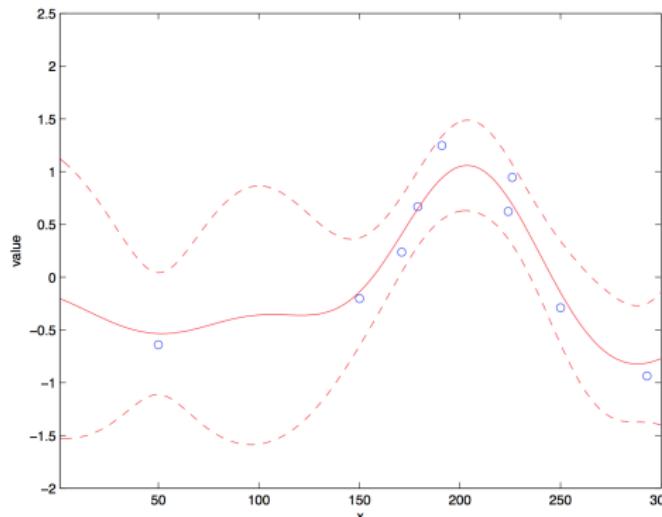


- Conditional distribution

$$p(f_* | \mathbf{y}) = \mathcal{N}(f_* | \mu_*, \sigma_*^2),$$

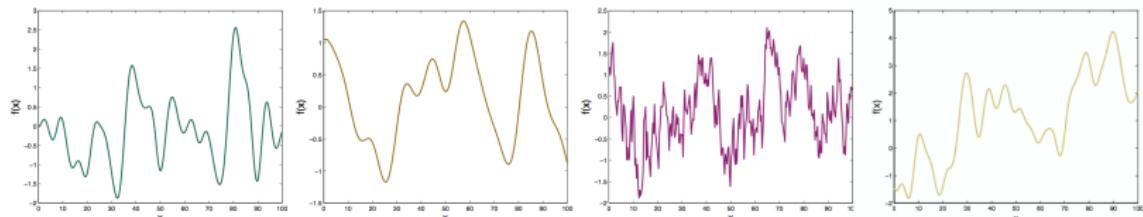
$$\mu_* = \mathbf{k}_*^T [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{y}, \quad \sigma_*^2 = K_{**} - \mathbf{k}_*^T [\mathbf{K} + \sigma^2 \mathbf{I}_m]^{-1} \mathbf{k}_*$$

- What we know about noiseless value  $f_* = f(\mathbf{x}_*)$ ?

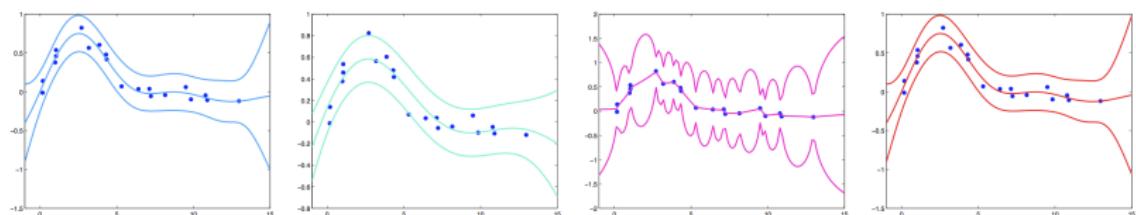


- $p(y_* | \mathbf{y}) = \mathcal{N}(y_* | \mu_*, \sigma_*^2 + \sigma^2)$  predicts what we'll see next

A sample from the prior for each covariance function:



Corresponding predictions, mean with two standard deviations:



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- Advantage of the probabilistic GP framework — ability to choose hyperparameters and covariances directly from the training data
- Other models, e.g. SVMs, require cross-validation
- **GP:** minimize negative log marginal likelihood  $\mathcal{L}(\theta)$  wrt covariance function parameters and noise level  $\theta$ . Since

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{0}, \mathbf{K} + \sigma^2 \mathbf{I}_m),$$

then

$$\mathcal{L} = -\log p(\mathbf{y}|\theta) = \underbrace{\frac{1}{2} \log \det \mathbf{C}(\theta)}_{\text{regularization}} + \underbrace{\frac{1}{2} \mathbf{y}^T \mathbf{C}^{-1}(\theta) \mathbf{y}}_{\text{data-fit}} + \frac{m}{2} \log(2\pi),$$

where  $\mathbf{C} = \mathbf{K} + \sigma^2 \mathbf{I}_m$

- Uncertainty in function variables  $\mathbf{f}$  is taken into account

- Minimization of  $\mathcal{L}(\theta)$  is a **non-convex optimization** problem
- Standard gradient based techniques, such as CG or quasi-Newton
- Gradients:**

$$\frac{\partial \mathcal{L}}{\partial \theta_i} = \frac{1}{2} \text{tr} \left( \mathbf{C}^{-1} \frac{\partial \mathbf{C}}{\partial \theta_i} \right) - \frac{1}{2} \mathbf{y}^T \mathbf{C}^{-1} \frac{\partial \mathbf{C}}{\partial \theta_i} \mathbf{C}^{-1} \mathbf{y}$$

- Local minima, but usually not much of a problem with few parameters, and/or using restarts
- Use weighted sums of covariances and let ML choose
- Each iteration of optimization costs  $O(m^3)$

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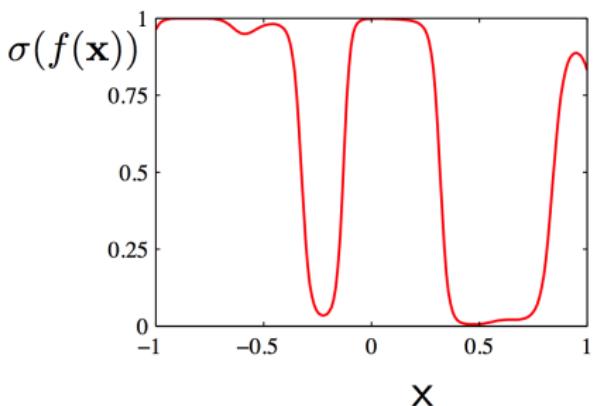
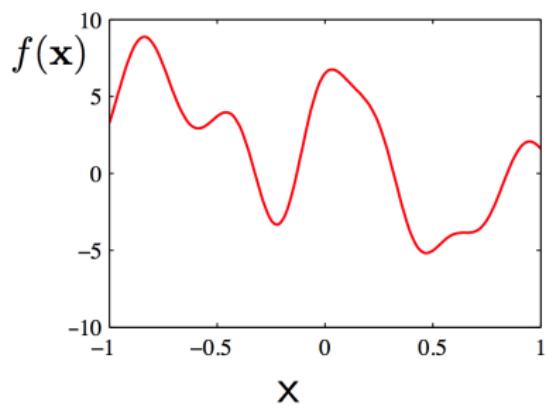
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- **Binary classification task:**  $y = \pm 1$
- GLM likelihood:  $p(y = +1 | \mathbf{x}, \mathbf{w}) = \pi(\mathbf{x}) = \sigma(\mathbf{x}^T \mathbf{w})$
- $\sigma(z)$  — **sigmoid** function such as the logistic or cumulative normal
- **Weight space viewpoint:** prior  $p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \Sigma_w)$
- **Function space viewpoint:** let  $f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$ , then likelihood  $\pi(\mathbf{x}) = \sigma(f(\mathbf{x}))$ , Gaussian prior on  $\mathbf{f}$



- Place a GP prior directly on  $f(\mathbf{x})$
- Use a sigmoidal likelihood:  $p(y = +1|f) = \sigma(f)$
- Non-Gaussian likelihood makes integrating over  $\mathbf{f}$  intractable:

$$p(f_*|\mathbf{y}) = \int d\mathbf{f} p(f_*|\mathbf{f})p(\mathbf{f}|\mathbf{y}),$$

where the posterior  $p(\mathbf{f}|\mathbf{y}) \sim p(\mathbf{y}|\mathbf{f})p(\mathbf{f})$

- Make tractable by using a Gaussian approximation to posterior.  
Then prediction:

$$p(y_* = +1|\mathbf{y}) = \int df_* \sigma(f_*) p(f_*|\mathbf{y})$$

Two common ways to make Gaussian approximation to posterior:

1. **Laplace approximation**. Second order Taylor approximation about mode of posterior
  2. **Expectation propagation (EP)**. EP can be thought of as approximately minimizing  $\text{KL}[p(\mathbf{f}|\mathbf{y})||q(\mathbf{f}|\mathbf{y})]$  by an iterative procedure
- Kuss and Rasmussen [2005] evaluate both methods experimentally and find **EP to be often better**
  - Classification accuracy on digits data sets comparable to SVMs
  - **Advantages**: uncertainty quantification, probabilistic predictions, kernel parameters by ML

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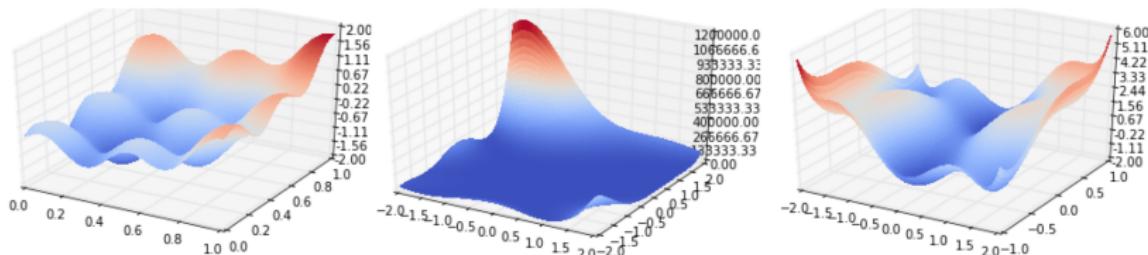
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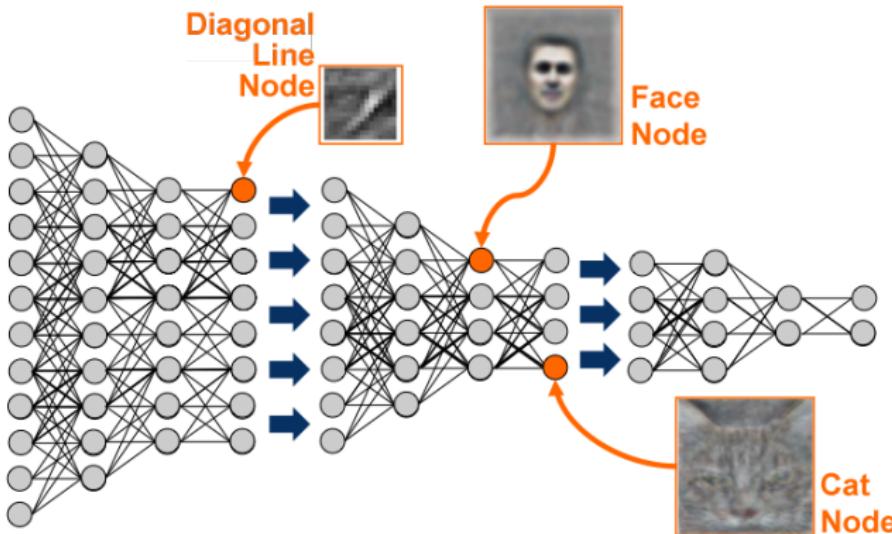
Consider a “well behaved” function  $f : \mathcal{X} \rightarrow \mathbb{R}$ , with  $\mathcal{X} \subseteq \mathbb{R}^d$  being a compact set

$$\mathbf{x}_{\min} = \arg \min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$



- $f$  is explicitly unknown and multimodal
- Evaluations of  $f$  may be perturbed
- Evaluations of  $f$  are expensive ⇒
  - Gradient and Hessian are not computable
  - Grid search is not possible

## Parameter tuning in ML algorithms



- Number of layers/units per layer
- Types of each layer
- Regularization coefficients
- Learning rates, etc.

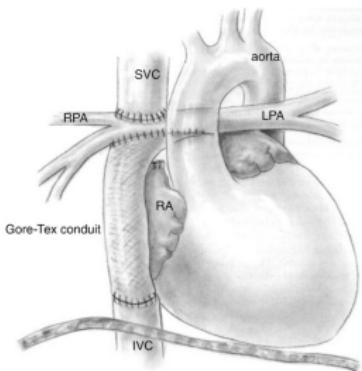
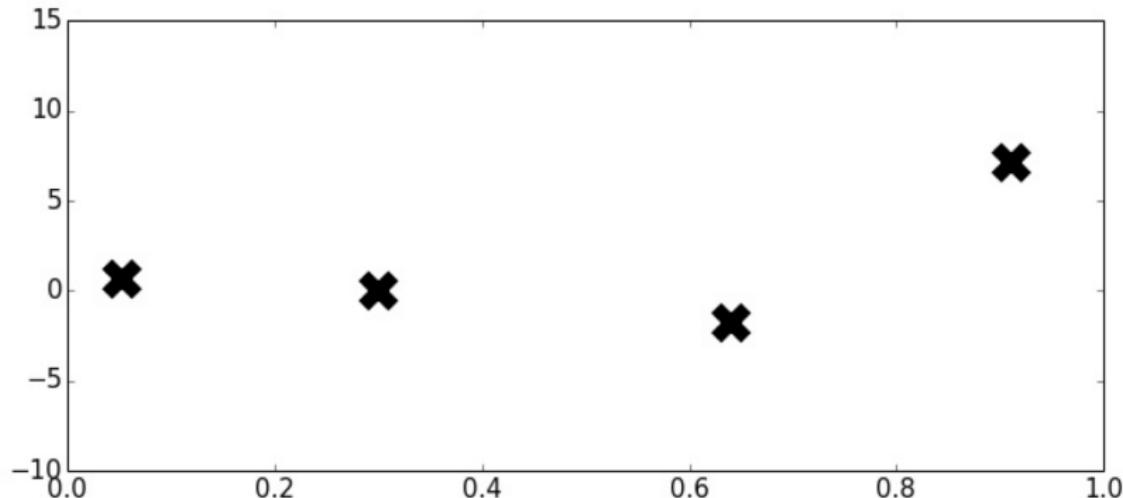


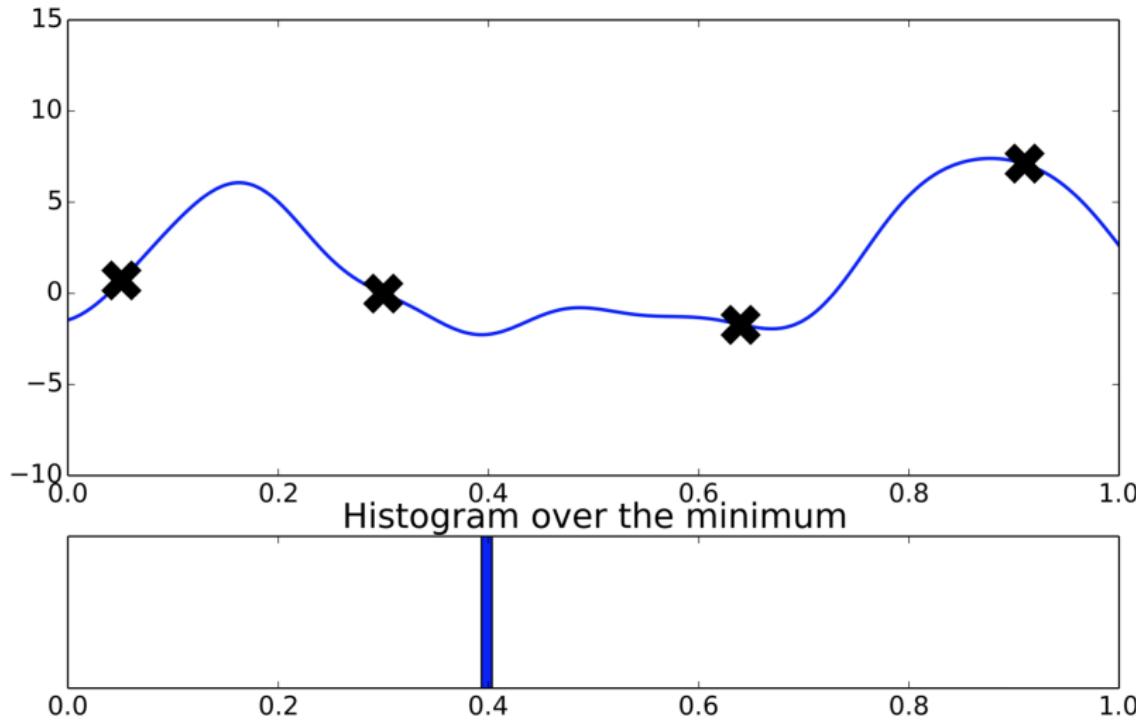
Fig. 1. Extracardiac total cavopulmonary connection. The IVC is disconnected from the right atrium (RA) and connected to the PAs via a Gore-Tex conduit. Figure taken from Reddy et al. [13].

- Design of grafts to be used in heart surgery
- Design of aerodynamic structures, e.g., cars, airplanes
- Calibrating parameters of complex physical models to experimental data
- A/B testing data to optimize the web design to maximize sign-ups, downloads, purchases, etc.

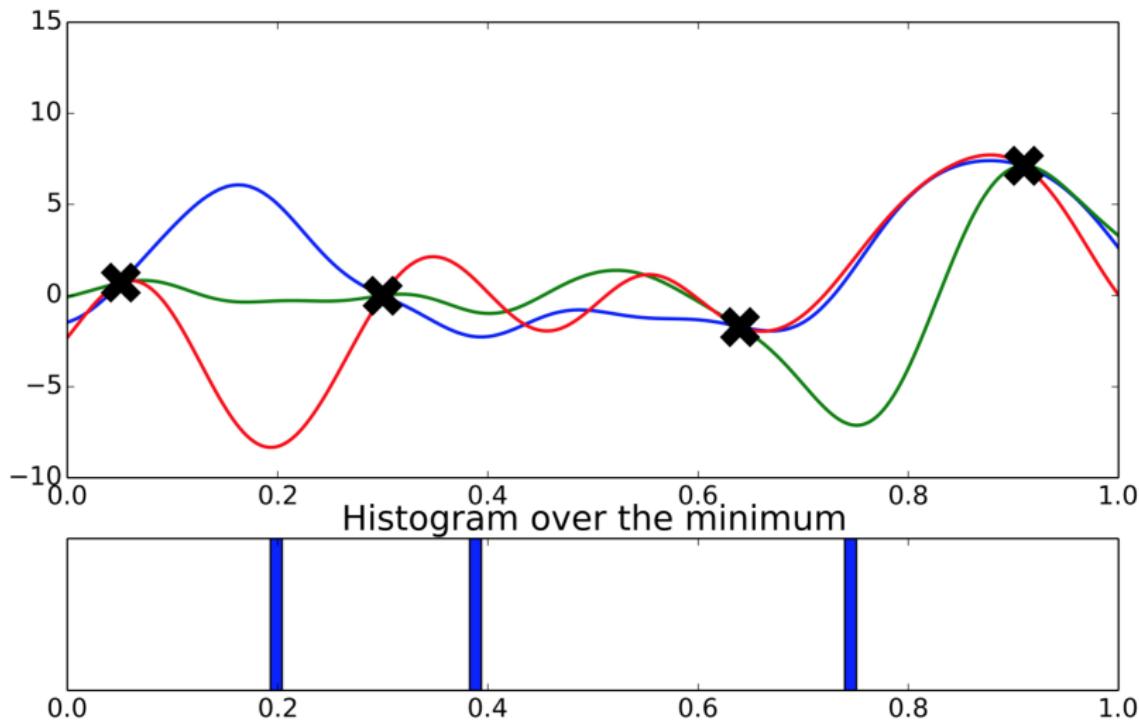
**NB!** There exists commercial services for optimizing black-box functions: SIGOPT, Google Vizier, etc.



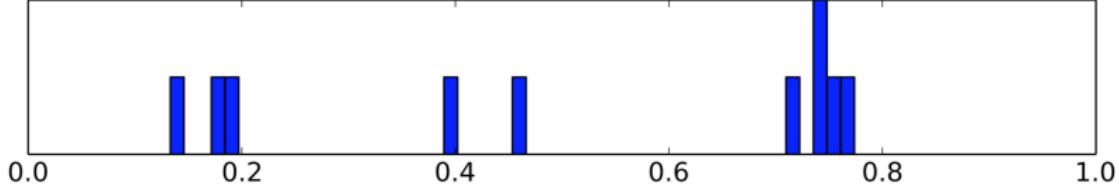
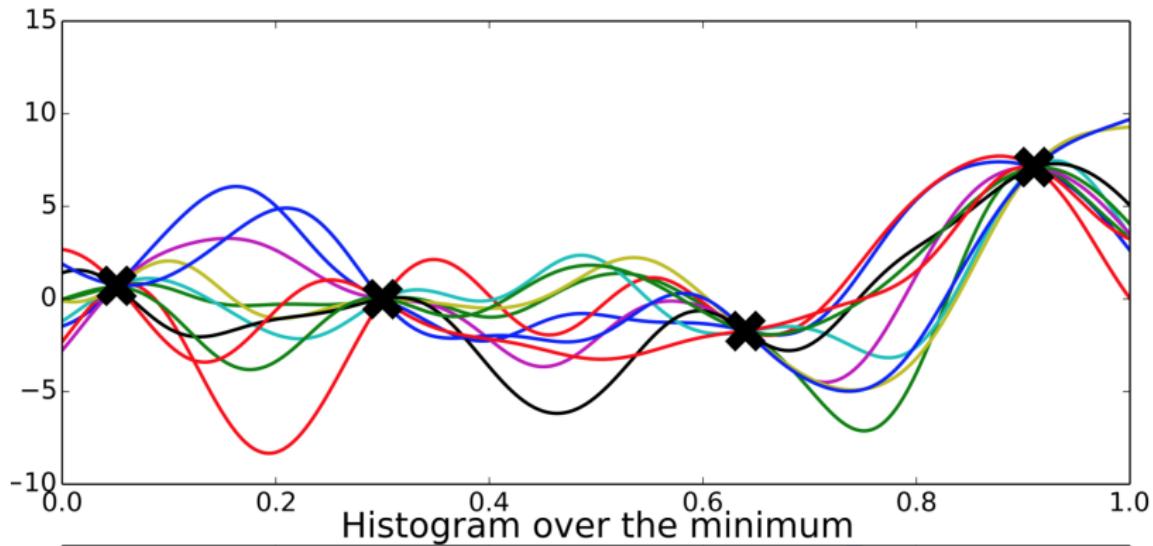
Where is the minimum of  $f$ ?  
Where should we evaluate the function next?



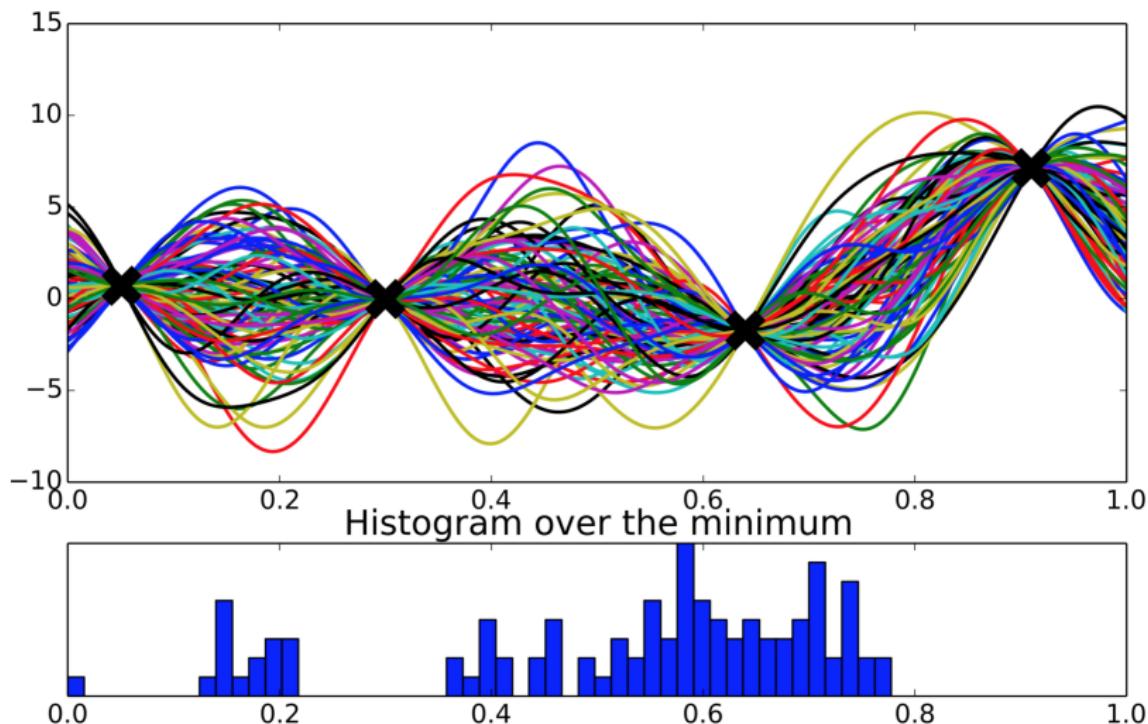
## Intuition: three curves

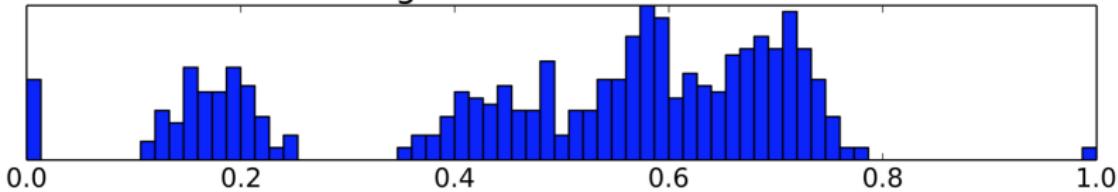
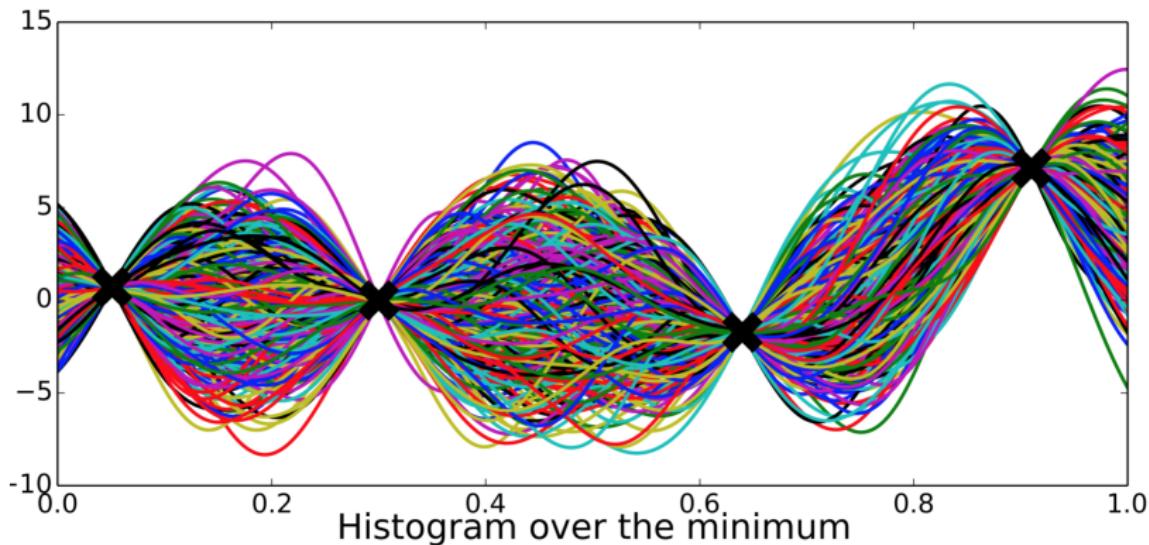


## Intuition: ten curves

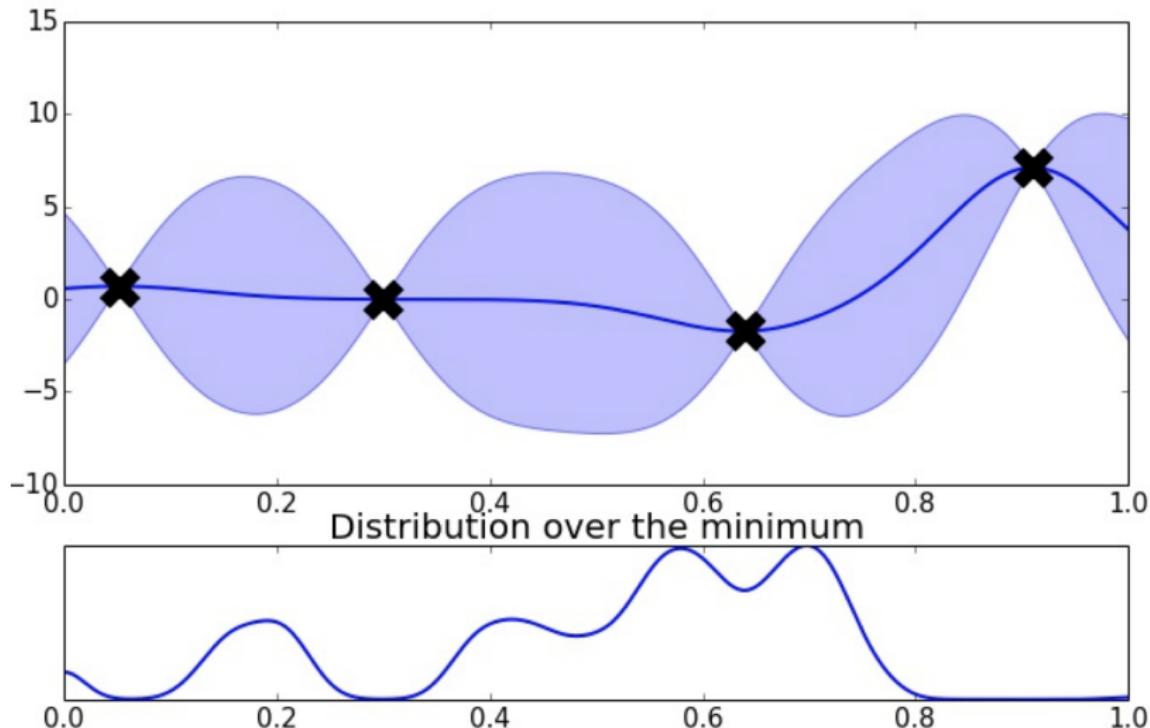


# Intuition: hundred curves





## Intuition: infinite number of curves



- We made prior assumption about  $f$
- Information about the minimum is now encoded in a new function (the probability distribution  $p_{\min}$  over the minimum in this case)
- We can use  $p_{\min}$  (or a functional of it) to decide where to sample next
- Other functions to encode relevant information about the minimum are possible, e. g. the “marginal expected gain” at each location.

Methodology to perform global optimization of multimodal black-box functions

1. Choose some **prior measure** over the space of possible objectives  $f$
2. Combine prior and the likelihood to get a **posterior** over the objective given some observations
3. Use the posterior to decide where to take the next evaluation according to some **acquisition function**
4. Augment the data set

Iterate between 2 and 4 until the evaluation budget is over

**Comment:** BO can be theoretically formalized in the framework of dynamic programming principle

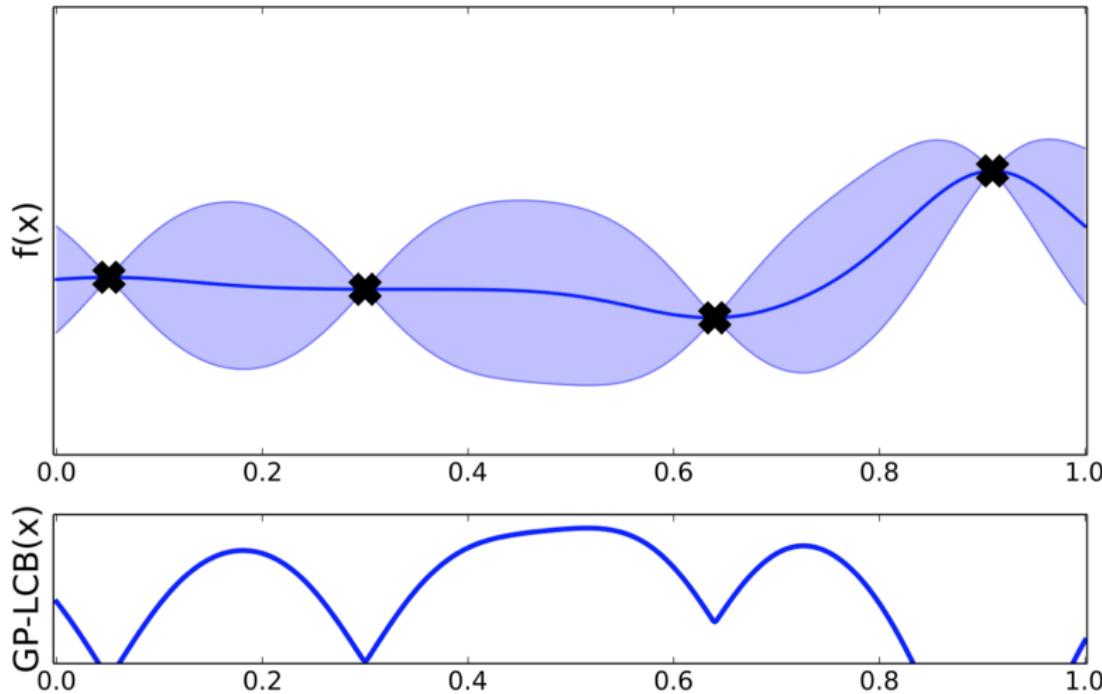
- Use GP  $\mathcal{GP}(\cdot | \mu(\mathbf{x}), K(\mathbf{x}, \mathbf{x}'))$  as a prior for  $f(\cdot)$
- GP has marginal closed-form for the posterior mean  $\mu_*(\mathbf{x})$  and variance  $\sigma_*^2(\mathbf{x}) \Rightarrow$  efficient calculation of acquisition function
  - **Exploration:** Evaluate in places where the variance is large
  - **Exploitation:** Evaluate in places where the mean is low

**Acquisition functions balance these two factors to determine where to evaluate next**

## GP Upper (lower) Confidence Band

Direct balance between exploration and exploitation:

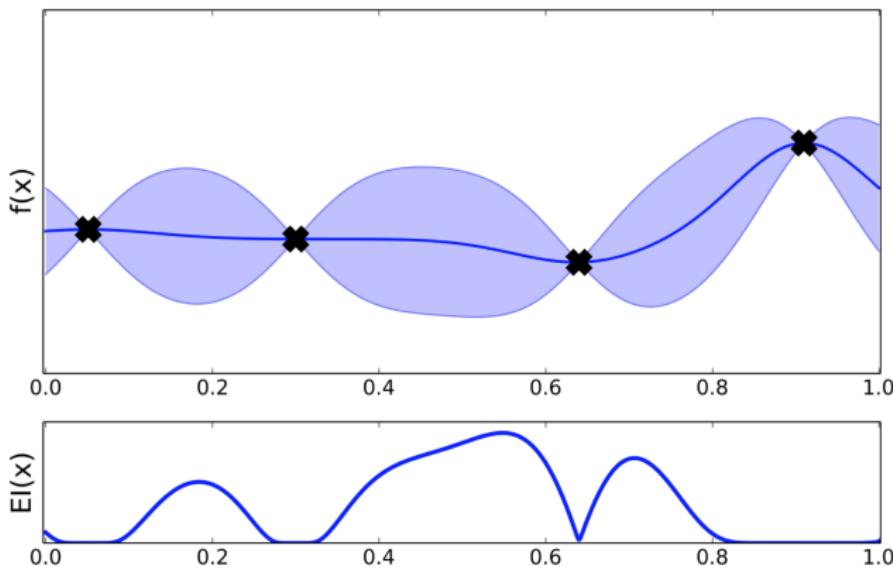
$$\alpha_{LCB}(\mathbf{x}) = -\mu_*(\mathbf{x}) + \zeta\sigma_*(\mathbf{x})$$



## Expected Improvement

Let us denote by  $\Delta(\mathbf{x}) = y_{\text{best}} - \mu_*(\mathbf{x})$ , then

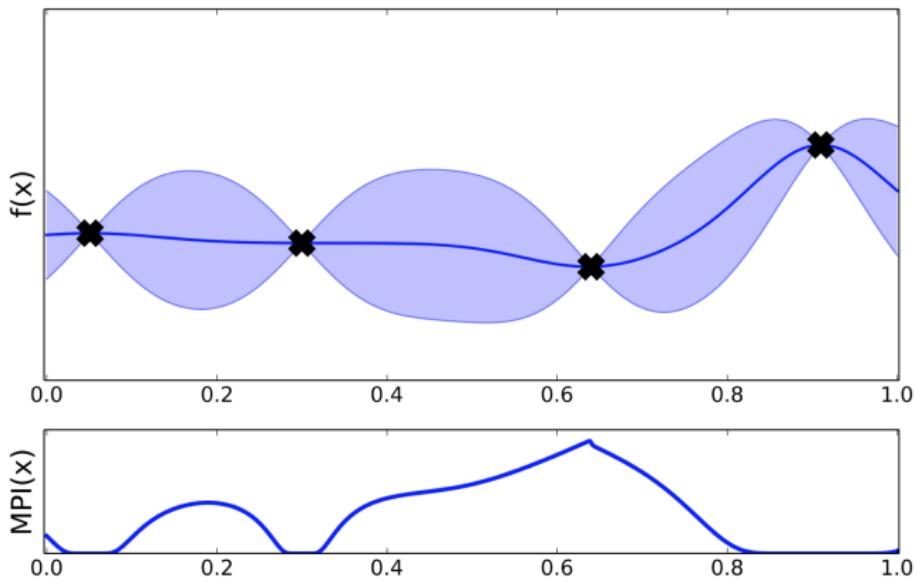
$$\begin{aligned}\alpha_{EI}(\mathbf{x}) &= \int_y \max(0, y_{\text{best}} - y_*) p(y_* | \mathbf{x}) dy_* = \\ &= \max(0, \Delta(\mathbf{x})) - \sigma_*(\mathbf{x}) \varphi \left( \frac{\Delta(\mathbf{x})}{\sigma_*(\mathbf{x})} \right) + |\Delta(\mathbf{x})| \Phi \left( -\frac{|\Delta(\mathbf{x})|}{\sigma_*(\mathbf{x})} \right)\end{aligned}$$



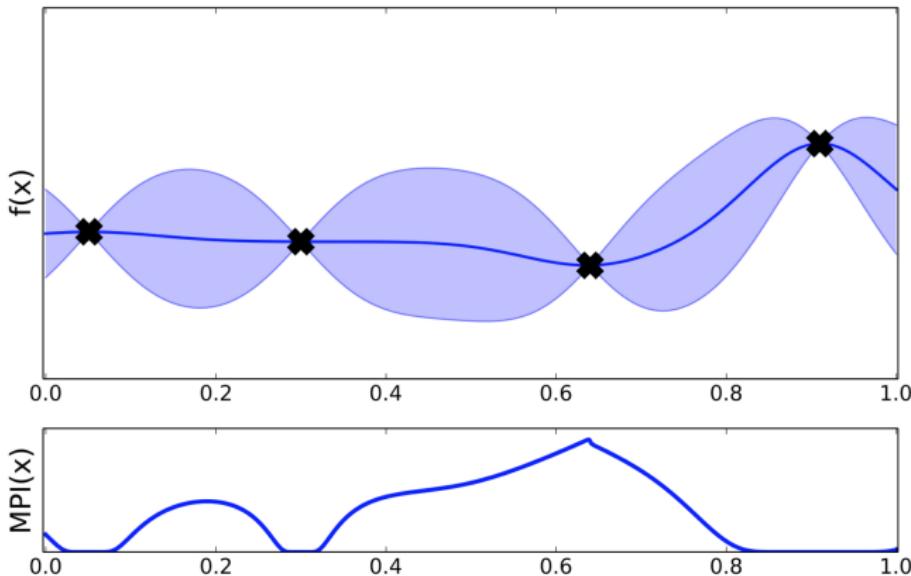
# Maximum Probability of Improvement

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

$$\alpha_{MPI}(\mathbf{x}) = \mathbb{P}(f(\mathbf{x}) < y_{\text{best}}) = \Phi(\gamma(\mathbf{x}))$$



$$\alpha_{ES}(\mathbf{x}) = \mathcal{H}[p(\mathbf{x}_{\min}|\mathbf{y})] - \mathbb{E}_{p(y|\mathbf{y}, \mathbf{x})}[\mathcal{H}[p(\mathbf{x}_{\min}|\mathbf{y} \cup \{\mathbf{x}, y\})]]$$



- BO is an strategy to transform the problem

$$\mathbf{x}_{\min} = \arg \min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

unsolvable!

into a series of problems

$$\mathbf{x}_{t+1} = \arg \max_{\mathbf{x} \in \mathcal{X}} \alpha(\mathbf{x}|S_t),$$

solvable!

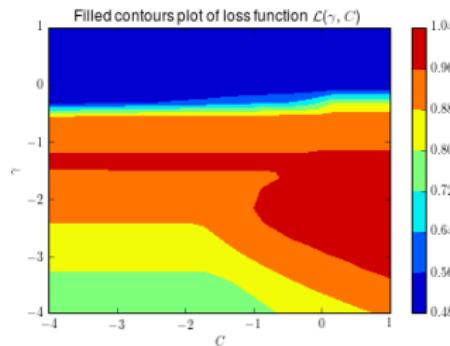
where

- $\alpha(\mathbf{x})$  is not so expensive to evaluate
- Gradients of  $\alpha(\mathbf{x})$  are typically available
- Still need to find  $\mathbf{x}_{t+1}$ : DIRECT, gradient methods, SA

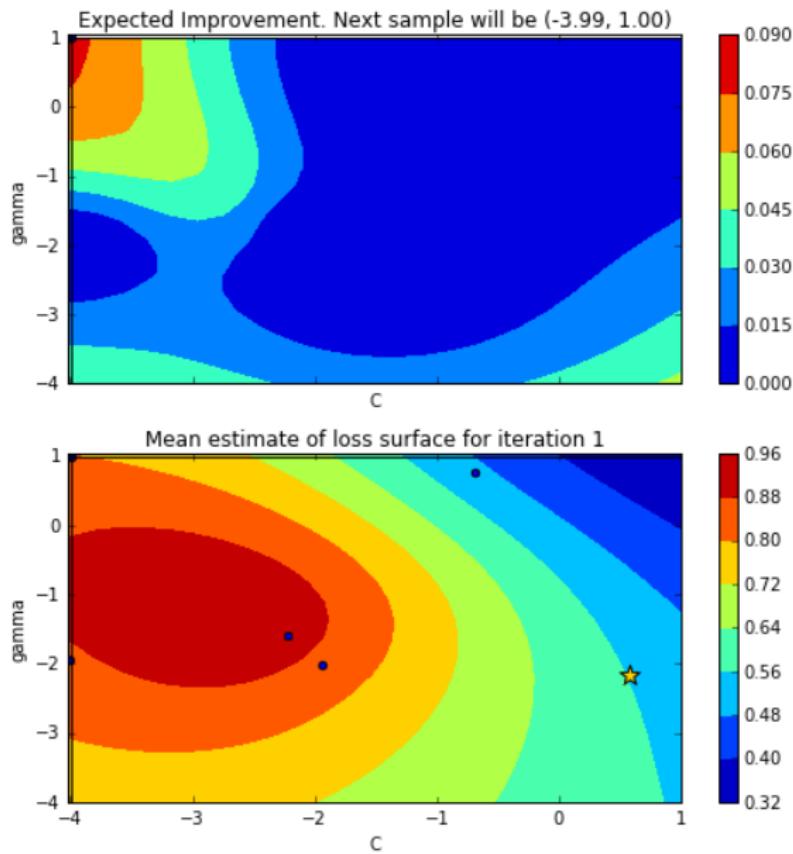
- Scikit-learn dummy data for testing classifiers:

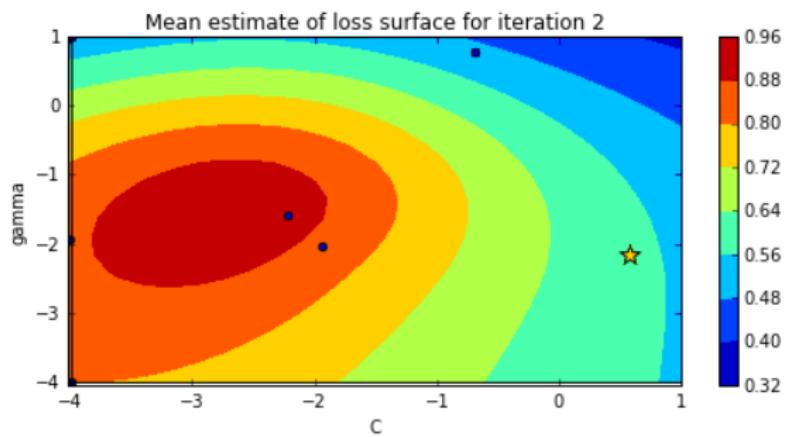
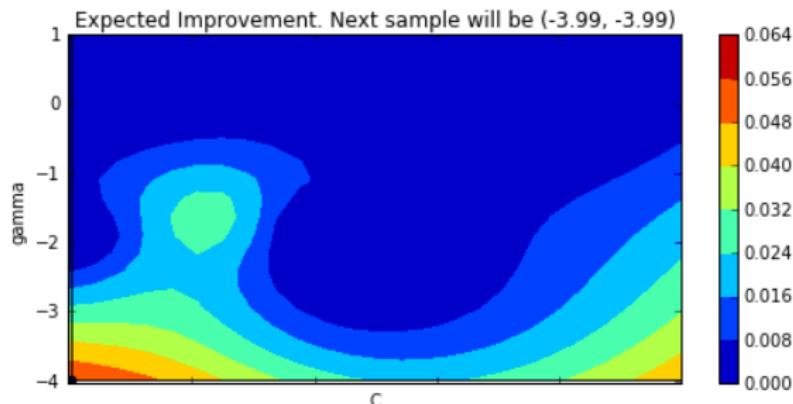
`n_samples=2500, n_features=45, n_informative=15,  
n_redundant=5`

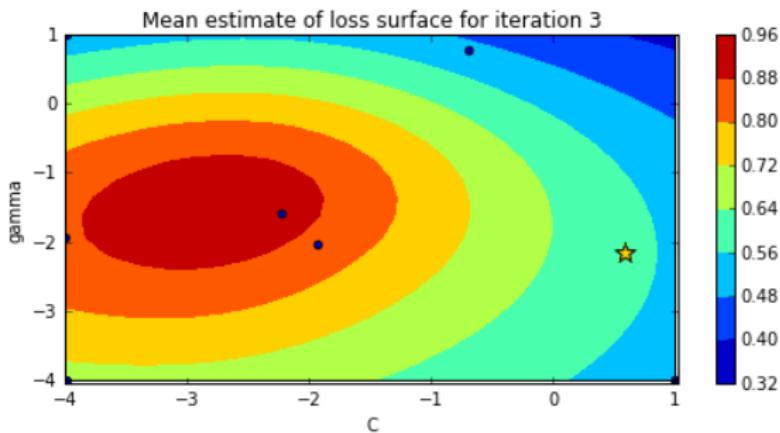
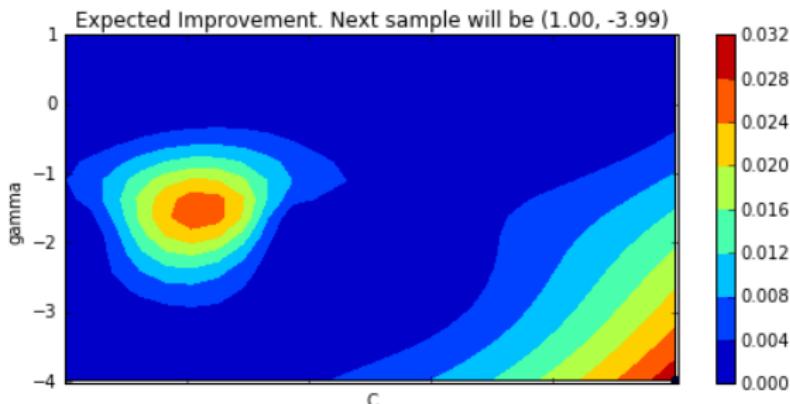
- Optimize penalization parameter  $C$ , and kernel width parameter  $\gamma$
- The loss function is the cross-validated area under the curve (AUC), based on three folds
- We computed the loss surface as a function of  $C$  and  $\gamma$  to get an accurate estimate of where the true optimum of the loss surface is

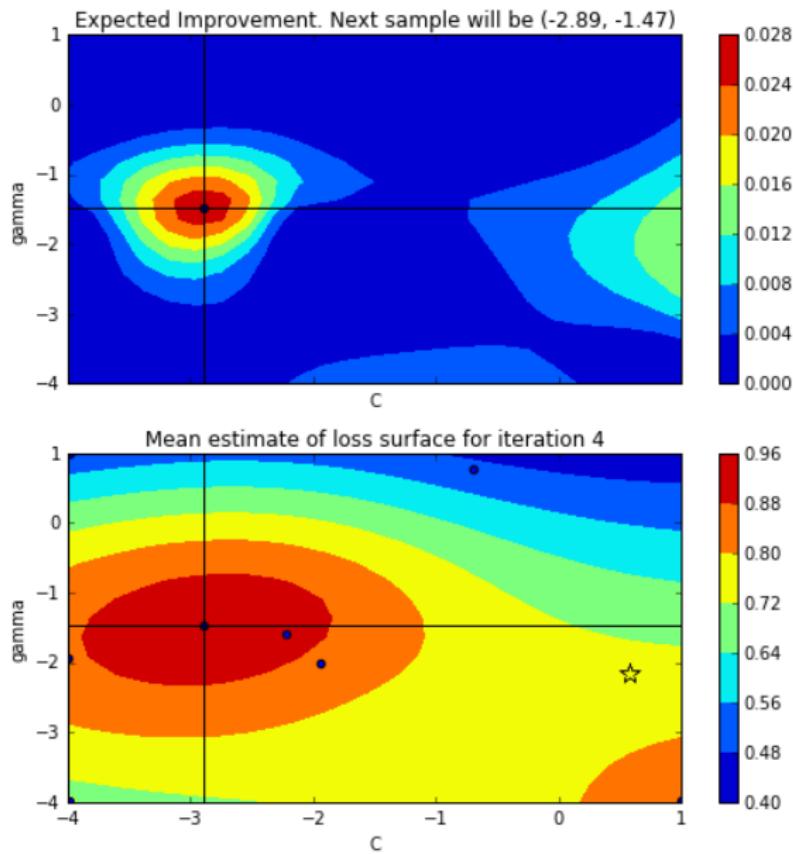


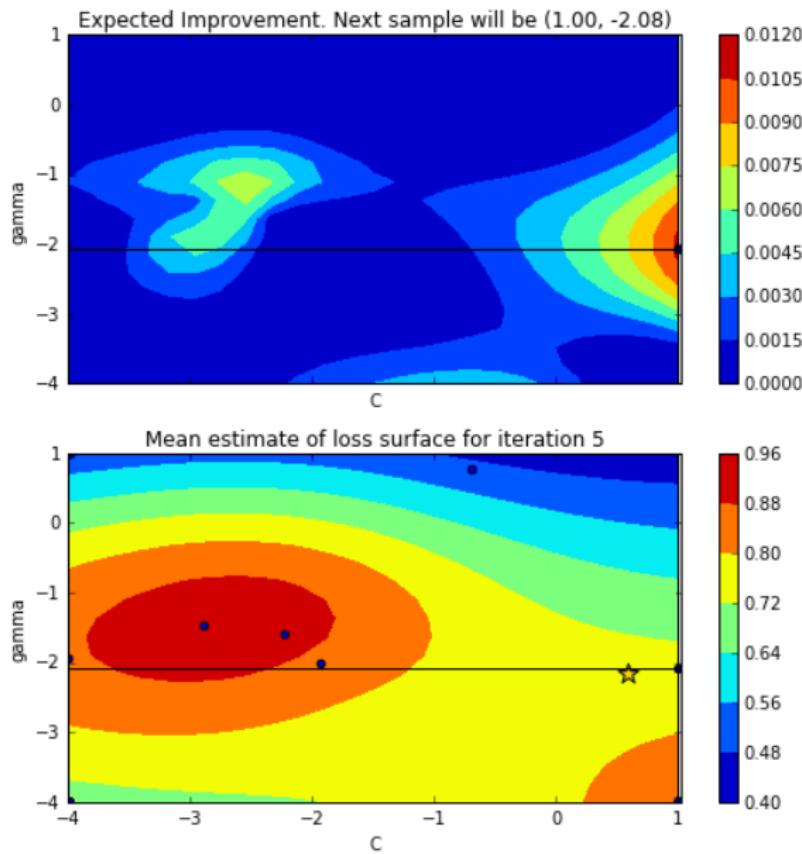
- The figures below show the sequence of points selected, if we run the Bayesian optimization algorithm in this setting

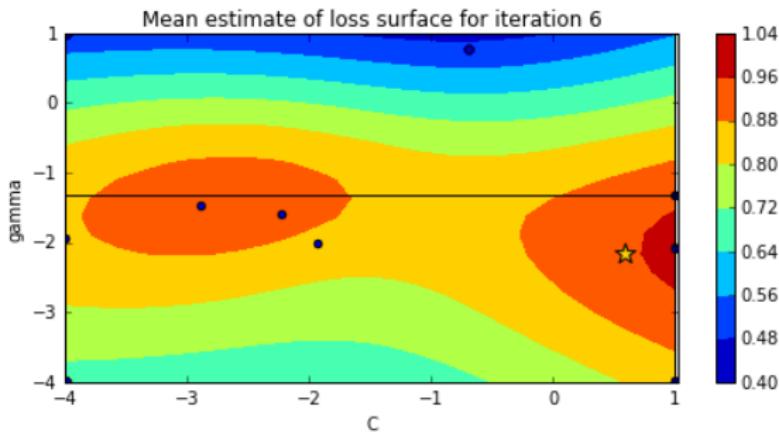
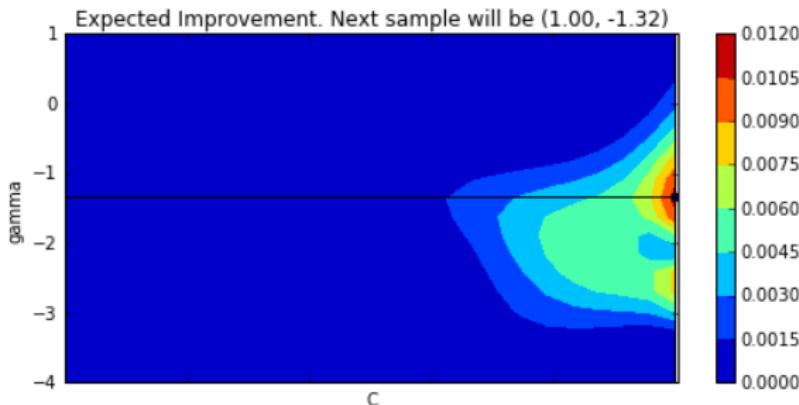


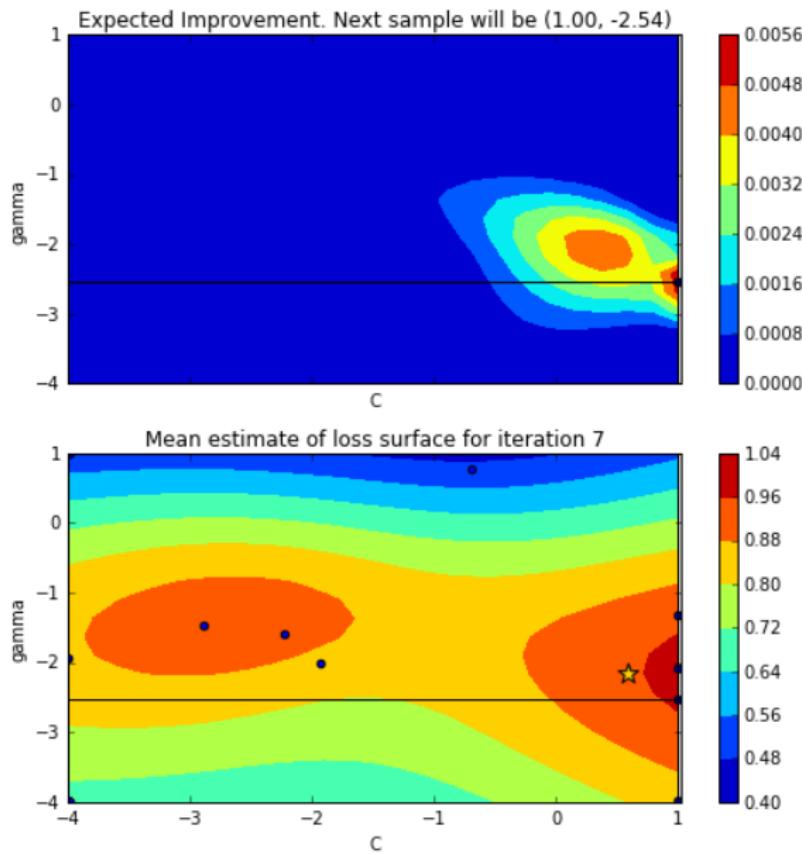


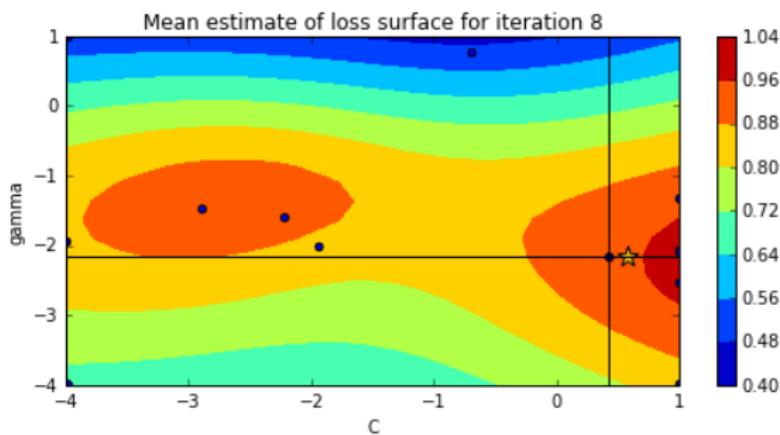
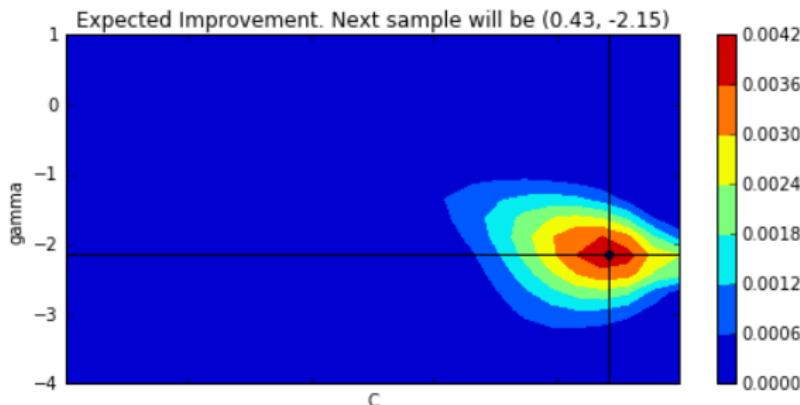


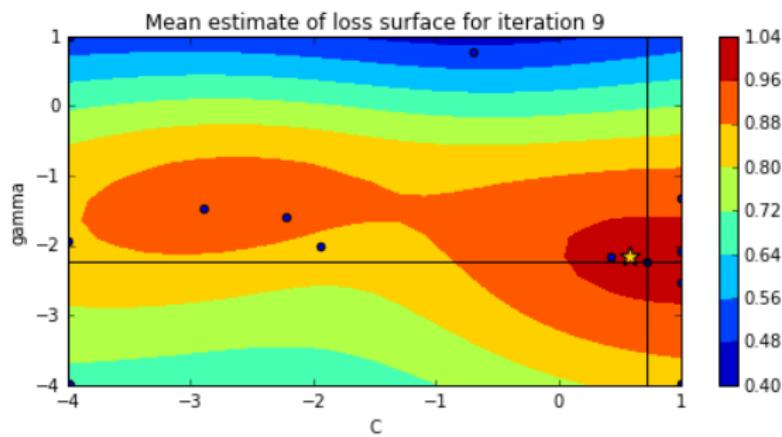
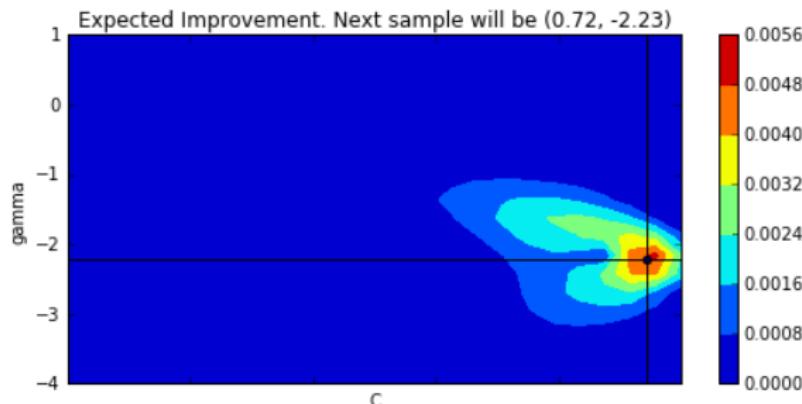


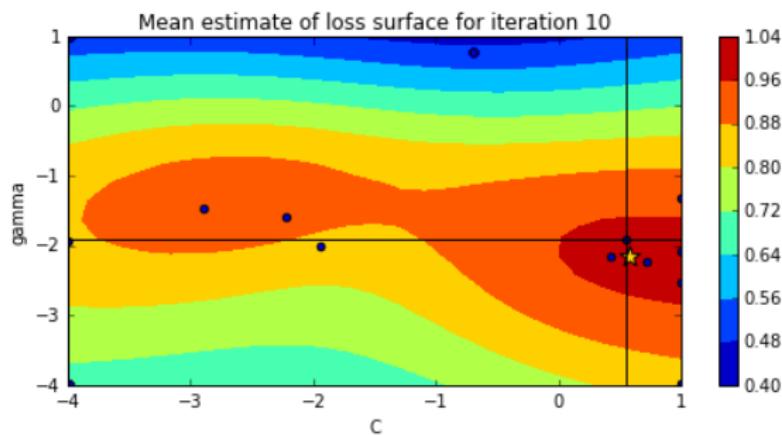
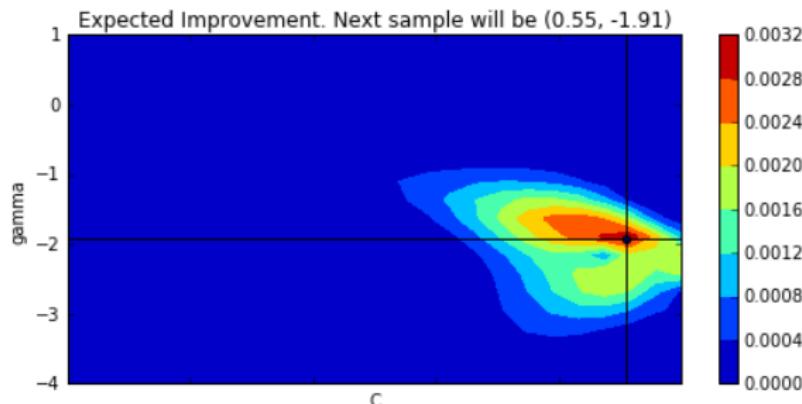


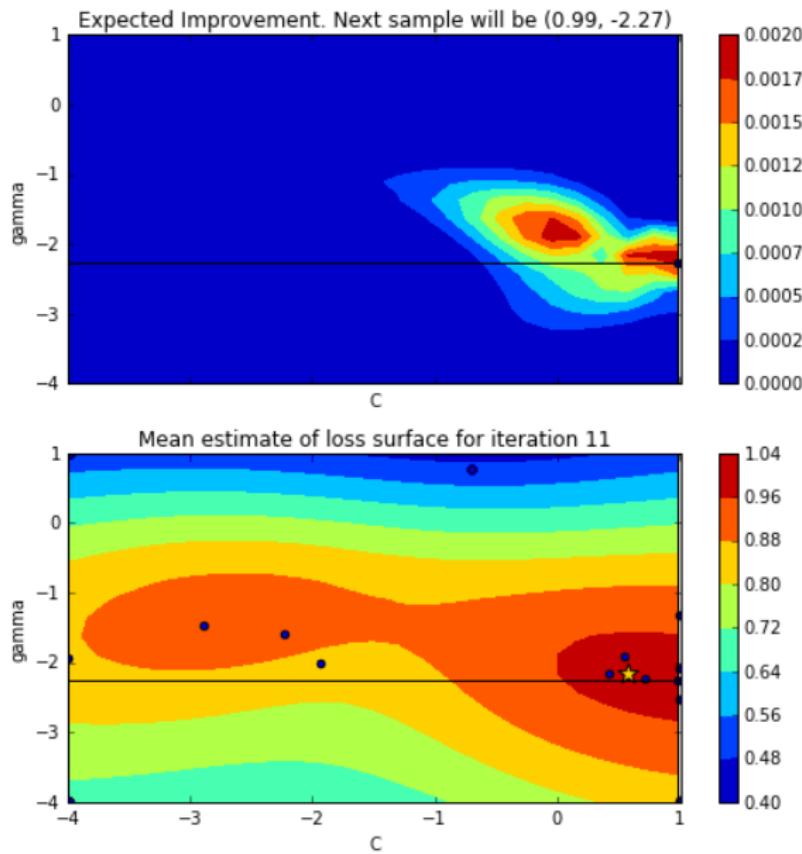


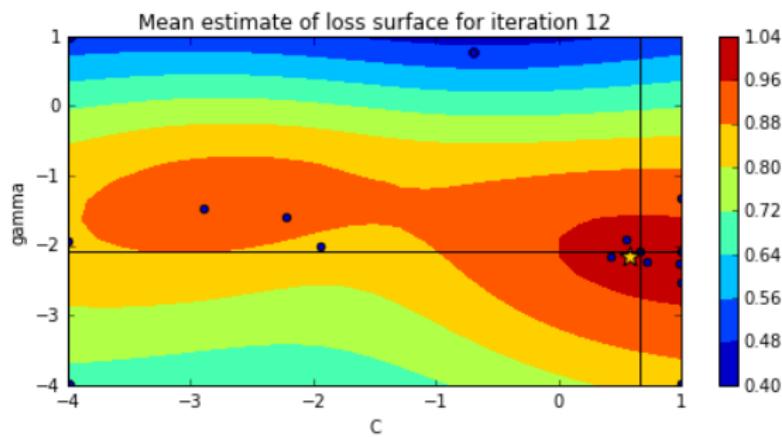
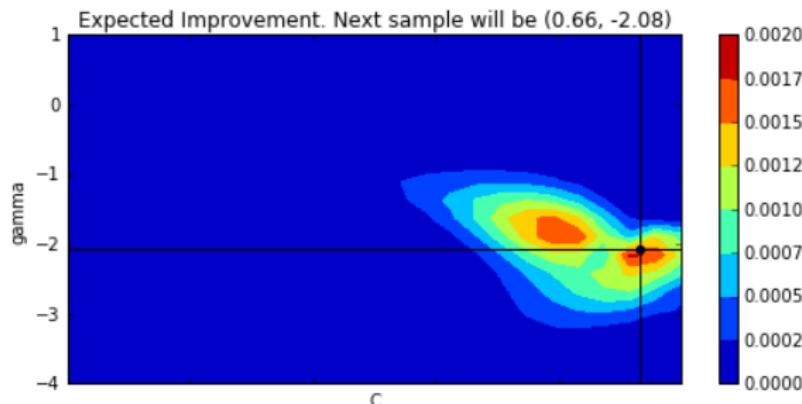


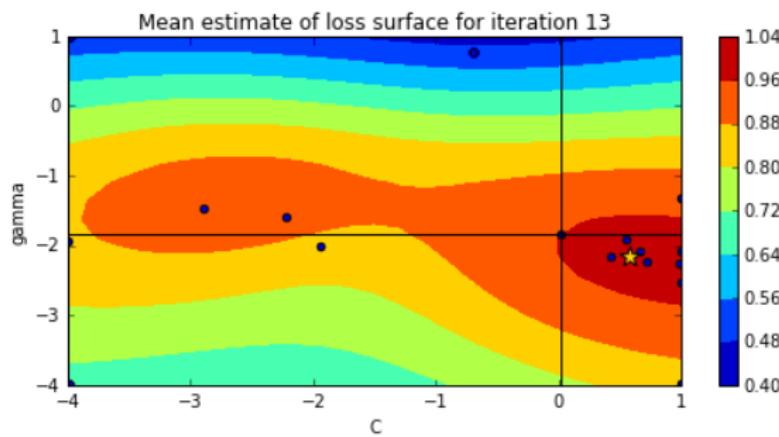
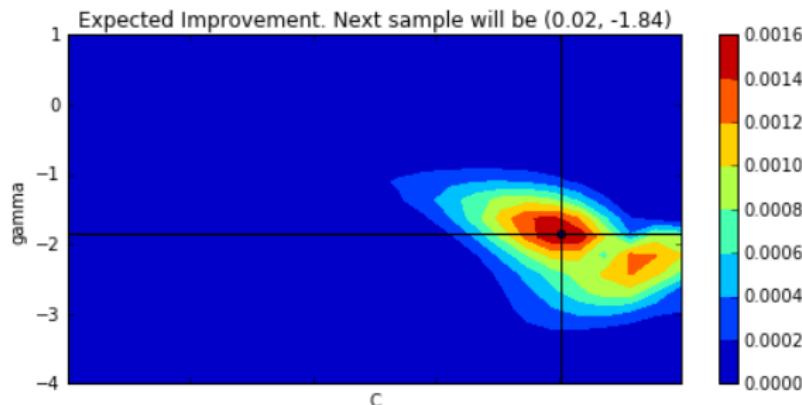


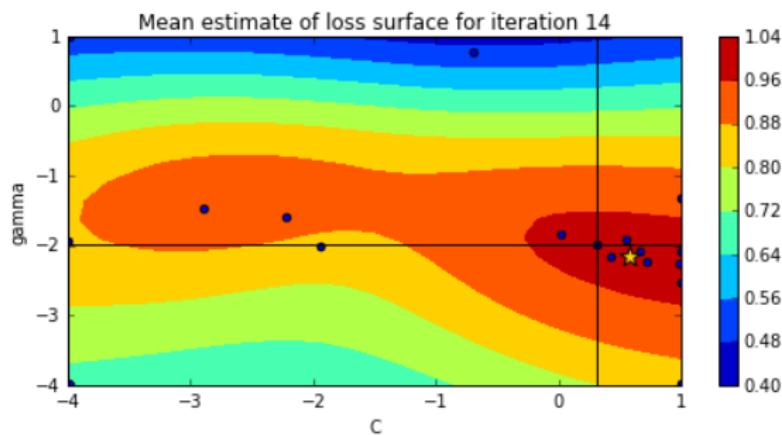
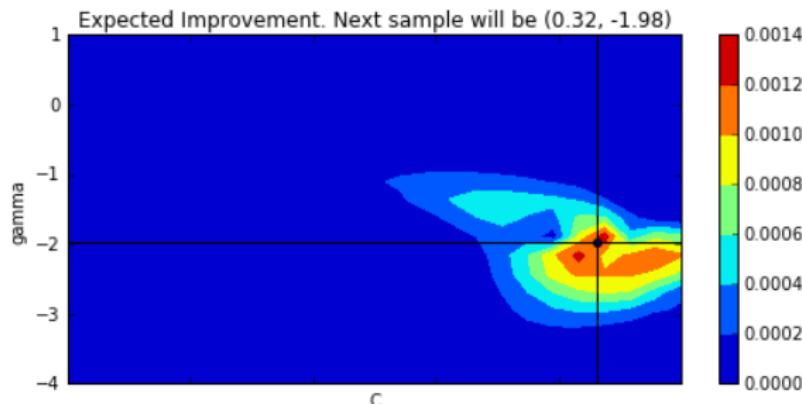


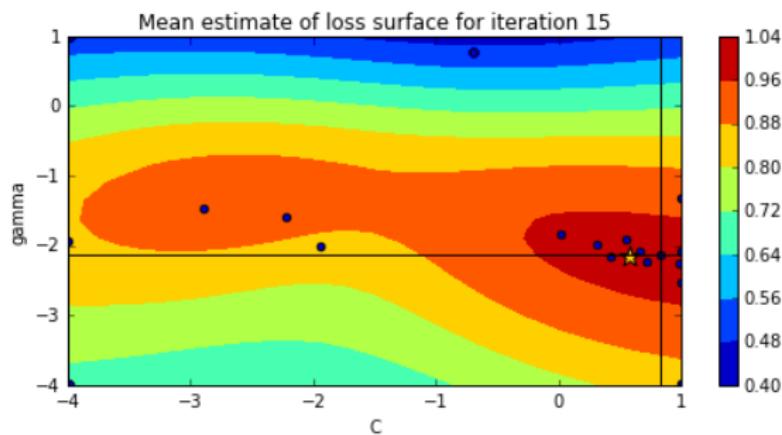
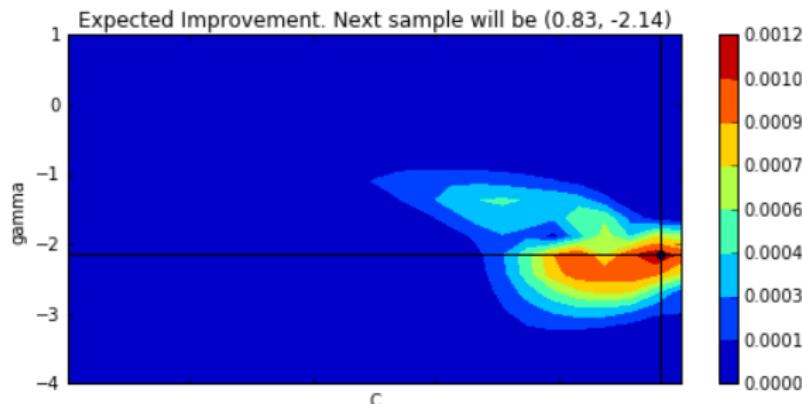


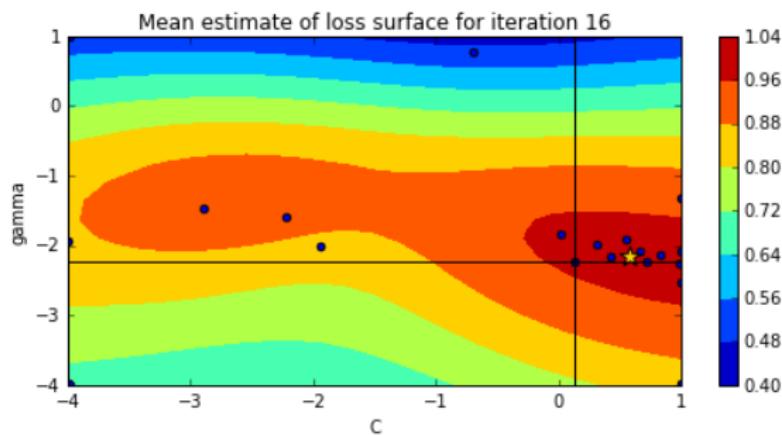
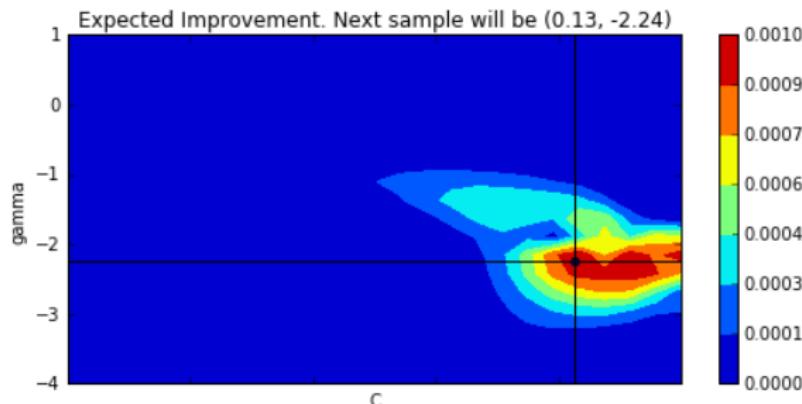


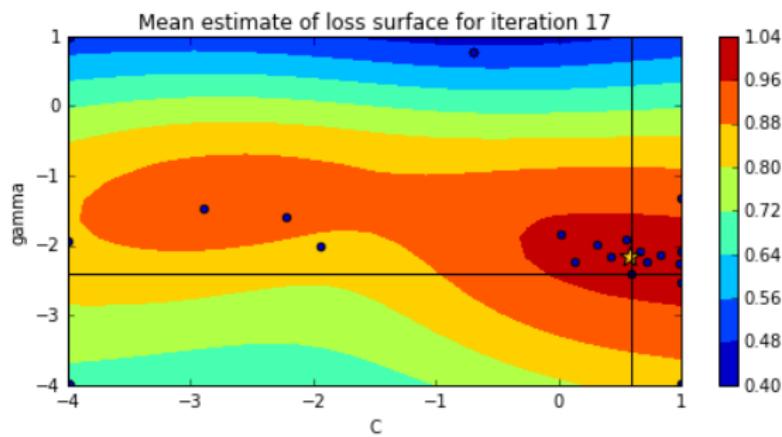
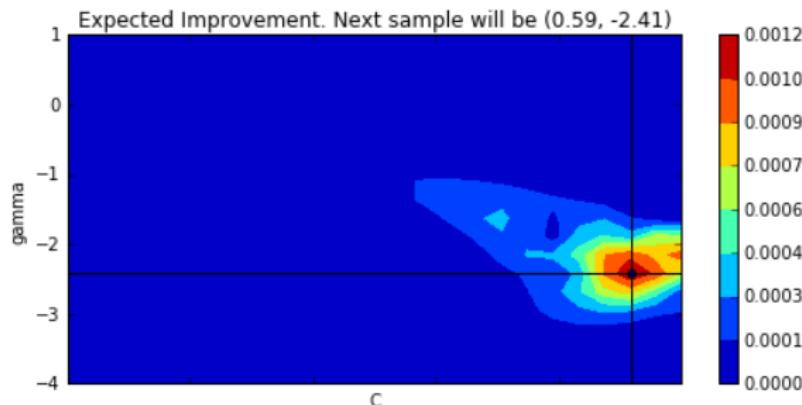


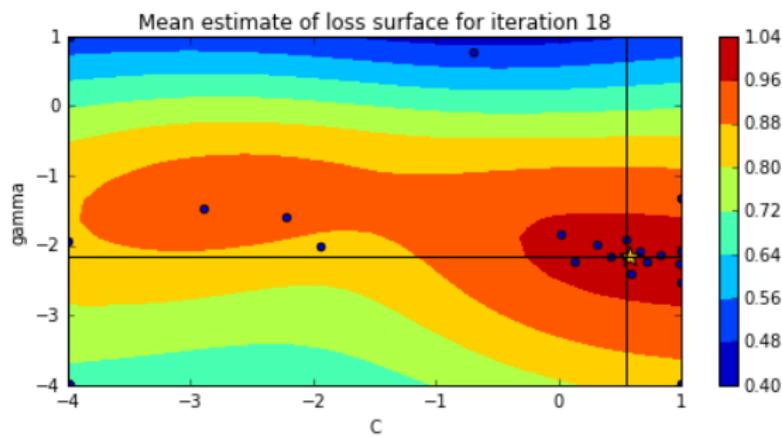
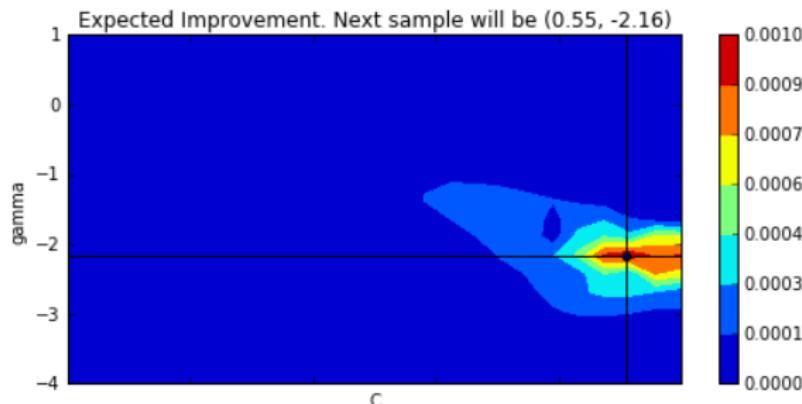


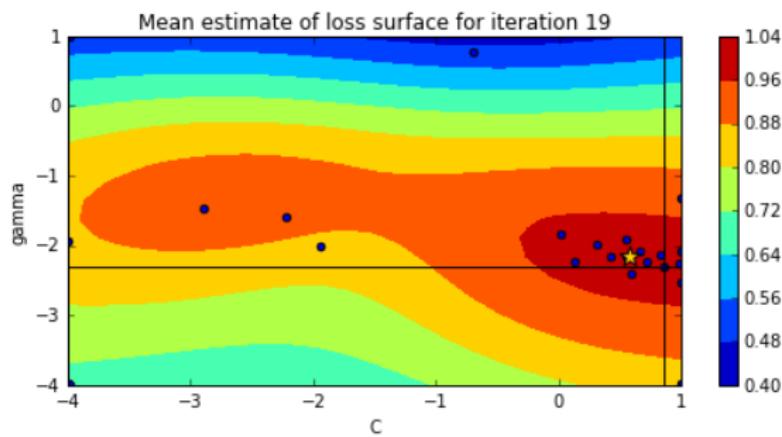
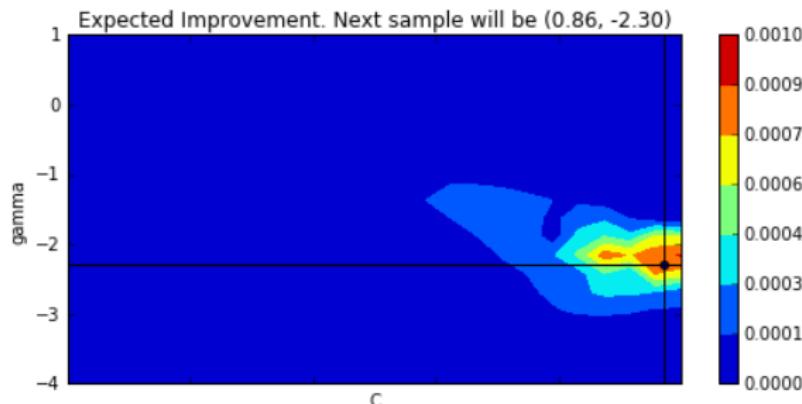


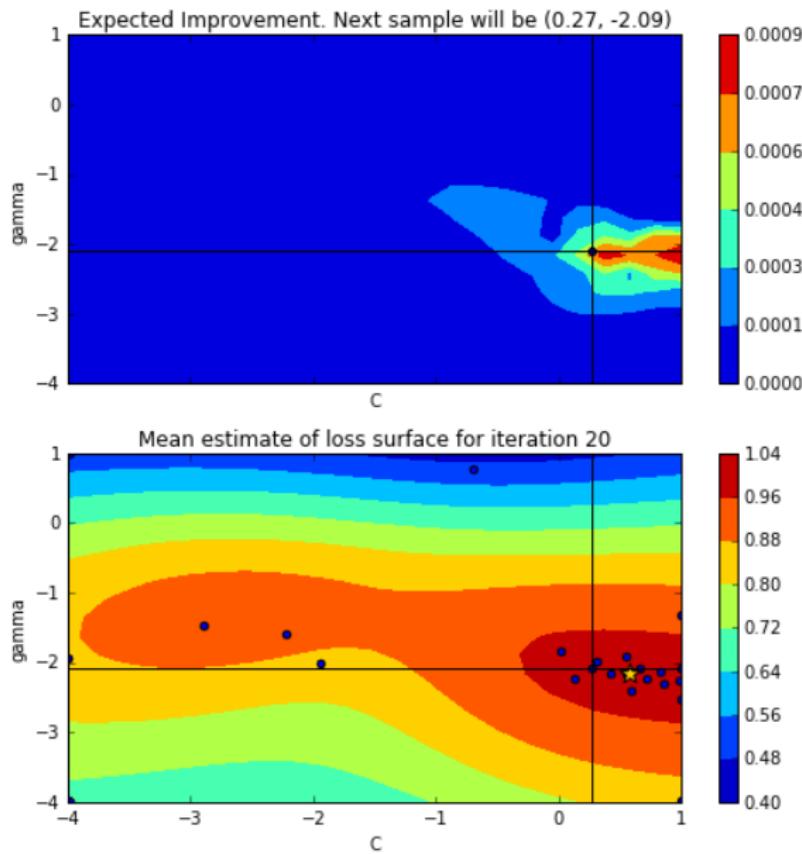












1 Motivation

2 Gaussian Process model

3 GP regression

4 Learning Gaussian Process model

5 Gaussian Process classification

6 Bayesian Optimization

7 Take-home messages

8 Afterword

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My message...

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- **Simple to use**
  - Just matrix operations (if likelihoods are Gaussian)
  - Few parameters: relatively easy to set or sample over
  - Predictions are often very good
  - Handle uncertainty in unknown function  $f$
  - Can learn kernel parameters automatically from data, no matter how flexible we wish to make the kernel
  - Can incorporate interpretable noise models and priors over functions
  - Can combine automatic feature selection with learning using ARD
- **No magic bullet:** best results need (at least) careful data scaling, which could be modelled or done by hand
- **The need for approximate inference:**
  - Sometimes Gaussian likelihoods aren't enough
  - $O(m^3)$  and  $O(m^2)$  costs are bad news for big problems

- Multi-task and structured GP learning
- Large scale GP based on Random Fourier features
- Deep GP based on random Fourier features
- Deep GP with Deep NN input features
- Multi-fidelity and multi-criteria Bayesian optimization
- Learning to optimize
- Other probabilistic models, e.g. modeling and optimization based on point processes

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What else?

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- **Mercer's theorem:** can always decompose covariance function into eigenfunctions and eigenvalues

$$K(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{\infty} \lambda_i \psi_i(\mathbf{x}) \psi_i(\mathbf{x}')$$

- If sum is finite — back to linear regression. Often sum is infinite, and no analytical expression for eigenfunctions
- However, a lot of kernels can be represented as

$$K(\mathbf{x}, \mathbf{x}') = \int_{\mathbb{R}^d} \phi(\mathbf{x}, \mathbf{w}) \phi(\mathbf{x}', \mathbf{w}) p(\mathbf{w}) d\mathbf{w}$$

Thus we can approximate kernels using random sampling and get approximate non-linear kernel models in linear time  $O(m)$

Let us consider the squared exponential covariance function

$$K(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\sum_{i=1}^d \theta_i^2 (x_i - x'_i)^2\right)$$

When optimizing the likelihood wrt covariance function parameters  $\{\boldsymbol{\theta} = (\theta_1, \dots, \theta_d), \sigma_f, \sigma\}$ , the following weird behavior can occur

- MLE optimum is located in the area where  $\|\boldsymbol{\theta}\| \sim 0$ , and the conditional number of  $\mathbf{K}$  is big
- For  $\|\boldsymbol{\theta}\| \rightarrow \infty$  matrix  $\mathbf{K} \rightarrow \mathbf{I}_m$ . Thus, we have a degenerate approximation
- Dependence of the likelihood  $\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})$  on  $\boldsymbol{\theta}$  can be weak

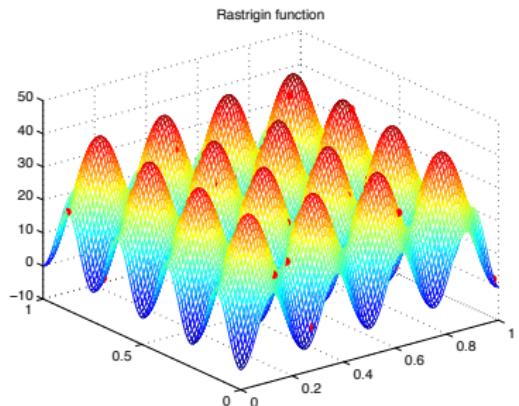


Figure – Rastrigin function

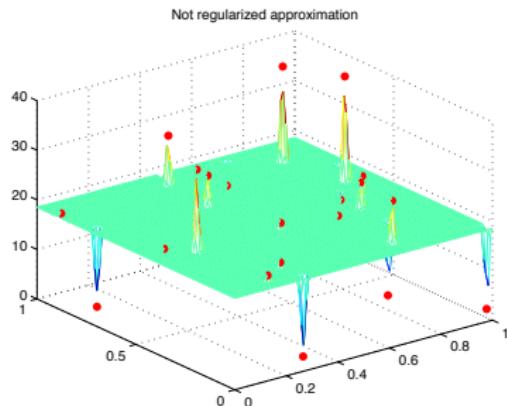


Figure – An approximation of Rastrigin function

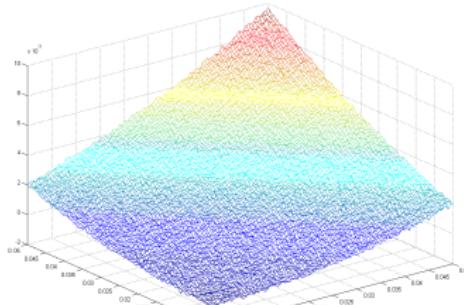
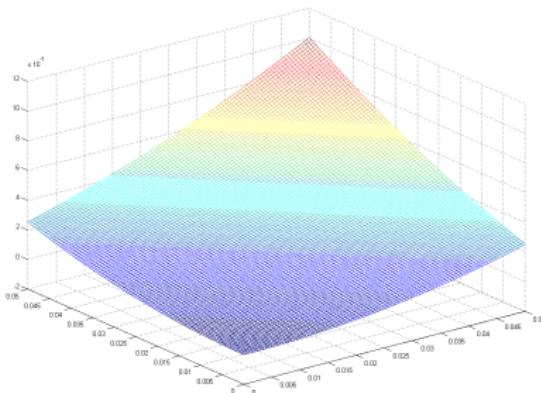
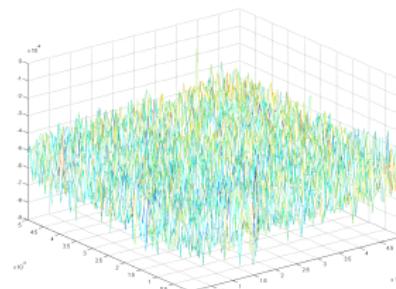


Figure –  $y(\mathbf{x}) = (x_1 + x_2)^2$



Let us introduce the following priors on covariance function parameters:

$$\theta_i^2 \in \Gamma(\alpha, \beta), i = 1, \dots, d$$
$$\sigma^2 \in \Gamma(\alpha_\sigma, \beta_\sigma)$$

Thus log-prior of parameters has the form

$$\log p(\{\boldsymbol{\theta}, \sigma\}) = m(\alpha \log \beta - \log \Gamma(\alpha)) + 2(\alpha - 1) \sum_{i=1}^m \log \theta_i +$$
$$- \beta \sum_{i=1}^m \theta_i^2 + (\alpha_\sigma \log \beta_\sigma - \log \Gamma(\alpha_\sigma)) + 2(\alpha_\sigma - 1) \log \sigma - \beta_\sigma \sigma^2$$

We obtain MAP estimates for  $\{\boldsymbol{\theta}, \sigma\}$ :

$$\log p(\mathbf{y}|\mathbf{X}, \{\boldsymbol{\theta}, \sigma\}) + \log p_{\alpha, \beta, \alpha_\sigma, \beta_\sigma}(\{\boldsymbol{\theta}, \sigma\})$$
$$+ \log p(\alpha, \beta, \alpha_\sigma, \beta_\sigma) \rightarrow \max_{\{\boldsymbol{\theta}, \sigma\}, \{\alpha, \beta, \alpha_\sigma, \beta_\sigma\}}$$

Here parameters  $\{\alpha, \beta, \alpha_\sigma, \beta_\sigma\}$  are also optimized along with imposed hyper-prior  $p(\alpha, \beta, \alpha_\sigma, \beta_\sigma)$ , parameters of which are fixed to some constants

# Regularized approximation vs. degeneracy

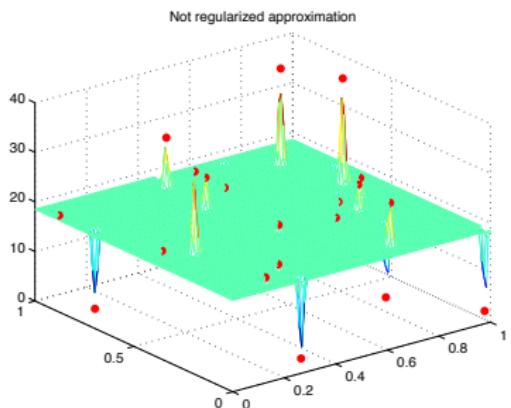


Figure – Degenerate approximation

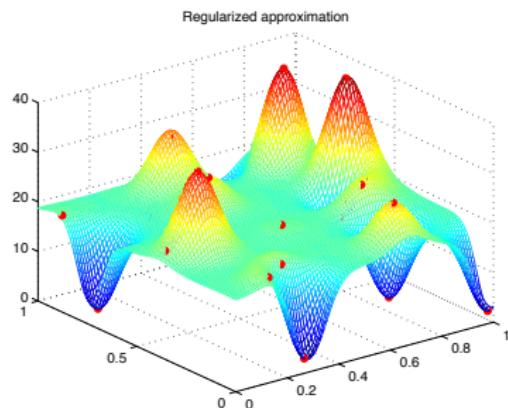
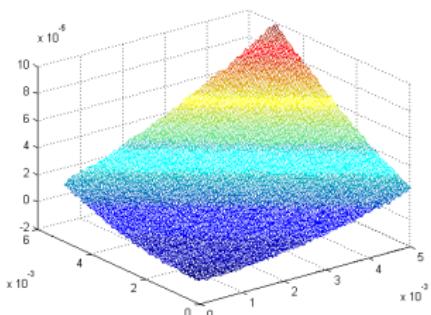
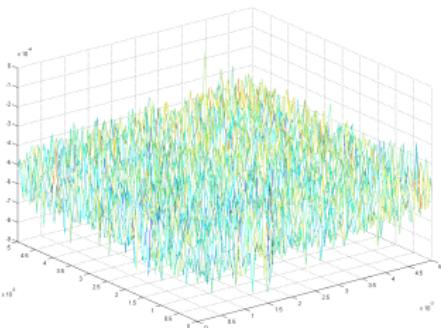
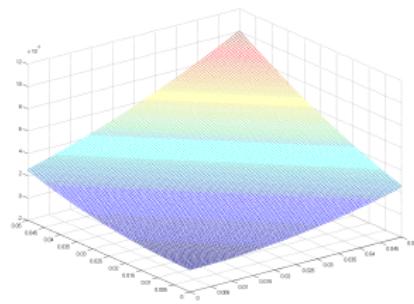
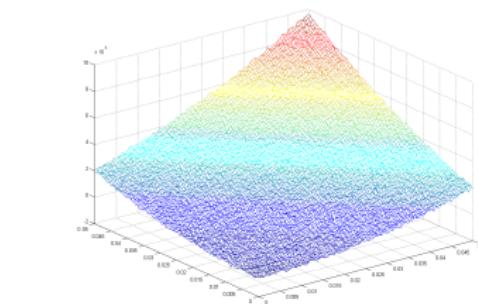
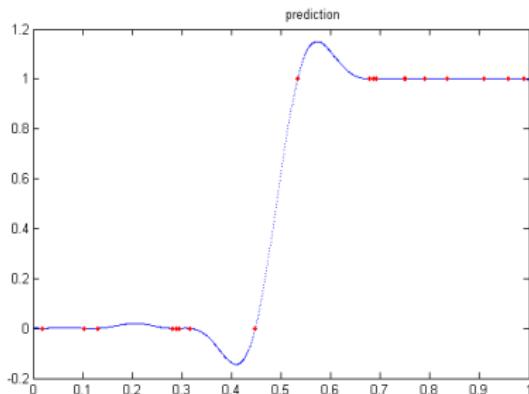


Figure – Approximation with imposed Bayesian regularization

# Regularized approximation vs. numerical noise



Approximation of Heaviside function for  $x \in [0, 1]$ , training sample size  $m = 20$



Let us assume that

$$y(\mathbf{x}) = \sum_{i=1}^Q \alpha_i \psi_i(\mathbf{x}) + f(\mathbf{x}) + \varepsilon(\mathbf{x}),$$

where

- $f(\mathbf{x})$  is a GP,
- $\varepsilon(\mathbf{x})$  is a Gaussian white noise,
- $\{\alpha_i\}_{i=1}^Q$  are i.i.d. r.v. with zero mean and variance  $\frac{\sigma_0^2}{Q}$ ,
- $\{\psi_i(\mathbf{x})\}_{i=1}^Q$  is a set of functions

Thus the covariance function of  $y(\mathbf{x})$  has the form:

$$\overline{K}(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}, \mathbf{x}') + \sigma_0^2 \boldsymbol{\psi}^T(\mathbf{x}) \boldsymbol{\psi}(\mathbf{x}') + \sigma^2 \delta(\mathbf{x}, \mathbf{x}'),$$

where  $\boldsymbol{\psi}(\mathbf{x}) = \{\psi_i(\mathbf{x}), i = 1, \dots, Q\}$

Posterior mean of  $y(\mathbf{x})$  has the form:

$$\mu_*(\mathbf{x}) = \bar{\mathbf{k}}(\mathbf{x}) \bar{\mathbf{K}}^{-1} \mathbf{y},$$

where

- $\Psi = \{\psi(\mathbf{x}_i), i = 1, \dots, m\}$ ,
- $\bar{\mathbf{k}}(\mathbf{x}) = \mathbf{k}(\mathbf{x}) + \sigma_0^2 \psi^T(\mathbf{x}) \Psi$ ,
- $\bar{\mathbf{K}} = \mathbf{K} + \sigma_0^2 \Psi^T \Psi + \sigma^2 \mathbf{I}_m$

Posterior variance has the form:

$$\sigma_*^2(\mathbf{x}) = K(\mathbf{x}, \mathbf{x}) + \sigma^2 + \sigma_0^2 \psi^T(\mathbf{x}) \psi(\mathbf{x}) - \bar{\mathbf{k}}^T(\mathbf{x}) \bar{\mathbf{K}}^{-1} \bar{\mathbf{k}}(\mathbf{x})$$

Minus log-likelihood has a similar structure compared to a stationary process, but we should replace  $\mathbf{K}$  by  $\bar{\mathbf{K}}$ :

$$-\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = \frac{1}{2}\mathbf{y}^T\bar{\mathbf{K}}^{-1}\mathbf{y} + \frac{1}{2}\log |\bar{\mathbf{K}}| - \frac{m}{2}\log 2\pi,$$

where  $\{\boldsymbol{\theta}, \sigma_0, \sigma\}$  are parameters

If the set of functions is fixed, then estimates of parameters can be obtained via usual maximization of the log-likelihood

$$\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) \rightarrow \max_{\boldsymbol{\theta}}$$

Let us consider three families of functions:

## 1. Sigmoid functions

$$\psi_j(\mathbf{x}) = \sigma \left( \sum_{i=1}^d \beta_{j,i} x_i \right),$$

where  $\sigma(x) = \frac{e^x - 1}{e^x + 1}$ ,  $\beta_{j,i} \in \mathbb{R}$  are parameters

## 2. Radial basis functions (RBF)

$$\psi_j(\mathbf{x}) = \exp \left( -\frac{\|\mathbf{x} - \mathbf{c}_j\|_2^2}{r_j^2} \right),$$

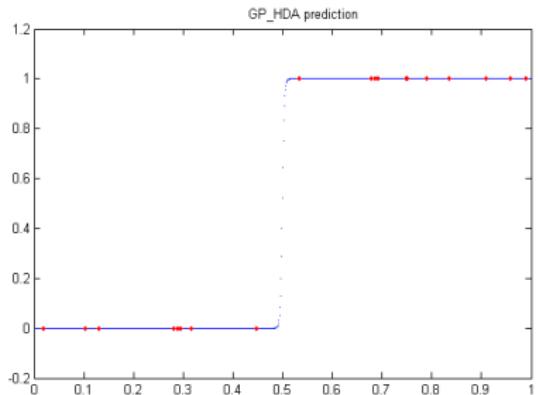
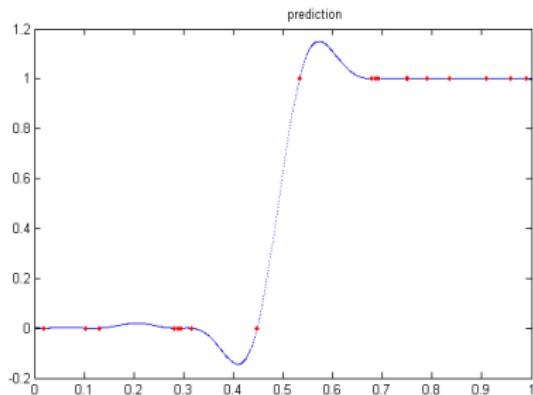
where  $\mathbf{c}_j \in \mathbb{R}^d$ ,  $r_j \in \mathbb{R}$  are parameters of the function.

## 3. Linear basis functions

$$\psi_j(\mathbf{x}) = x_j, j = 1, 2, \dots, d$$

# Approximation of Heaviside function

Approximation of Heaviside function for  $x \in [0, 1]$ , training sample size  $m = 20$



1 Motivation

2 Gaussian Process model

3 GP regression

4 Learning Gaussian Process model

5 Gaussian Process classification

6 Bayesian Optimization

7 Take-home messages

8 Afterword

9 Bibliography

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## Bibliography: additional reading

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