

Gaussian Processes

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- 1 Motivation
- 2 Gaussian Process model
- 3 GP regression
- 4 Learning Gaussian Process model
- 5 Gaussian Process classification
- 6 Take-home messages
- 7 Afterword: Random Features. Numerical Stability. Non-stationary GP

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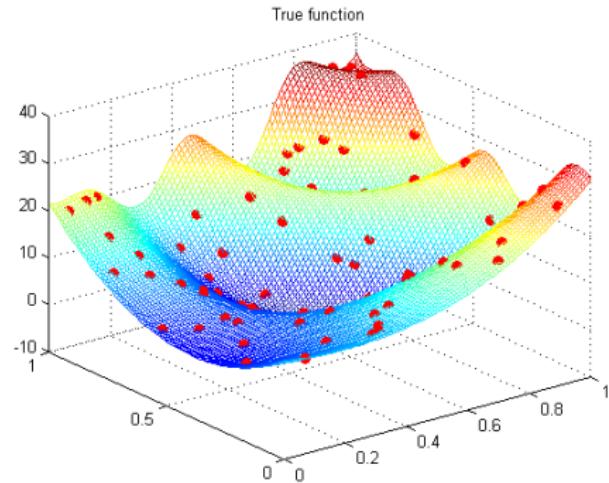
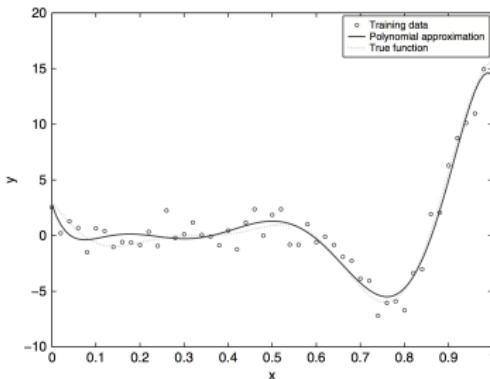
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- Learn scalar function $f(\mathbf{x})$ of vector \mathbf{x}
- We have (possibly noisy) sample $S_m = \{\mathbf{X}, \mathbf{y}\} = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$



- **Real-valued regression:**

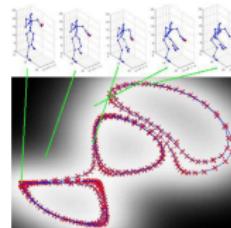
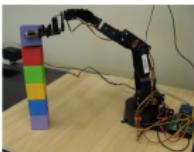
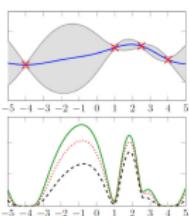
- Model-based predictive control: predict yield, quality, losses, etc.
- Surrogate surfaces for optimization or simulation
- Robotics: target state → required torques

- **Classification:**

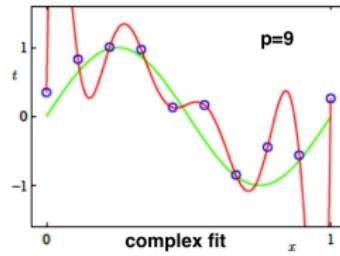
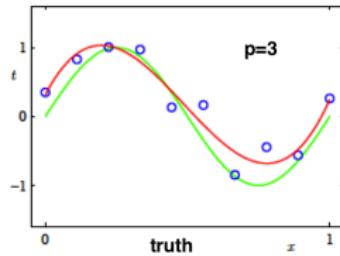
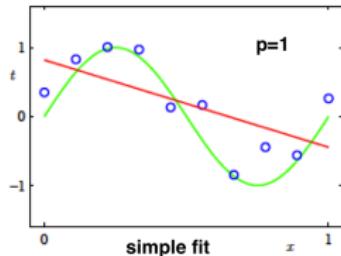
- Recognition: handwritten digits on payment docs, etc.
- Detection: fraud, screening in chemoinformatics

- **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?
- Uncertainty of predictions?

- **Problem:**

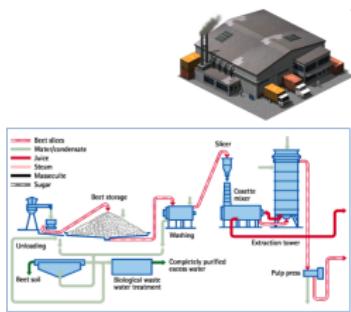
- **Object:** production of one batch of a product
- **Input x :** beet chips shape, temperature; wash water temperature, pH and flux, etc.
- **Output y :** costs, losses, efficiency

- **Challenges:**

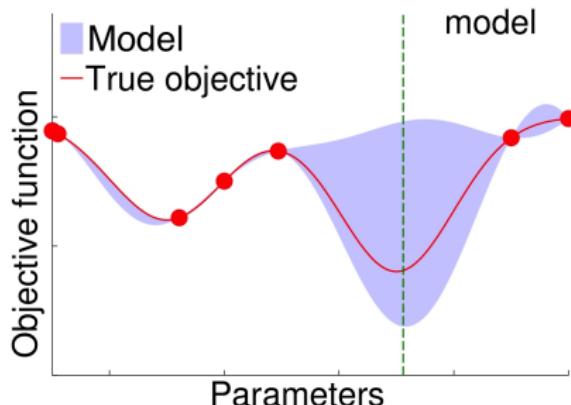
- Heterogeneous data and noise,
- Large volumes of high-dimensional stream data,
- Missing values, outliers, etc.

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

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



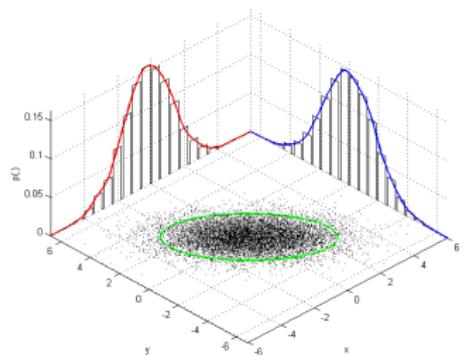
- In high-dimensional case we need many functions evaluations
- Often each evaluation is costly, e.g. in case of experiments



- 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?

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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?

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

What is a Gaussian process?

- **Continuous stochastic process** — random function — 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

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- 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

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

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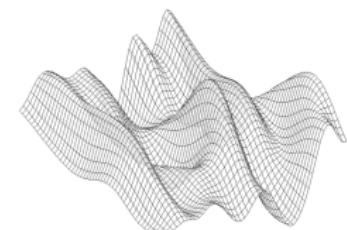
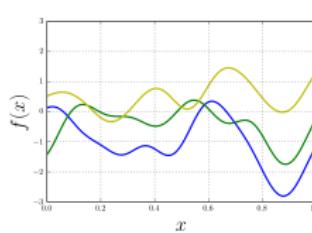
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$$f(\mathbf{x}) \sim \mathcal{GP}(\cdot | \mu(\mathbf{x}), K(\mathbf{x}, \mathbf{x}'))$$



- The most commonly-used kernel in machine learning

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

- 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 σ_f^2

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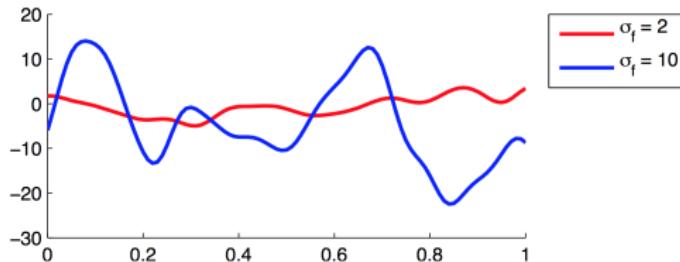
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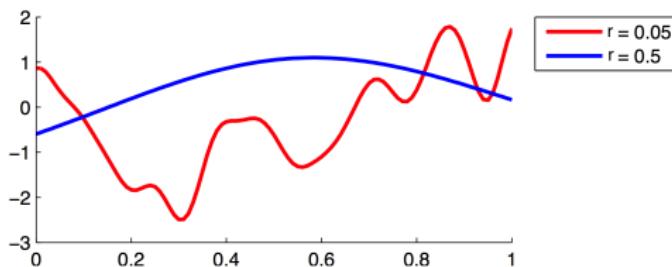
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- More general example of covariance function

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

- As usual covariance function parameters are **interpretable**
 - σ_f^2 — marginal function variance
 - σ_1^2 — variance of bias
 - σ_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

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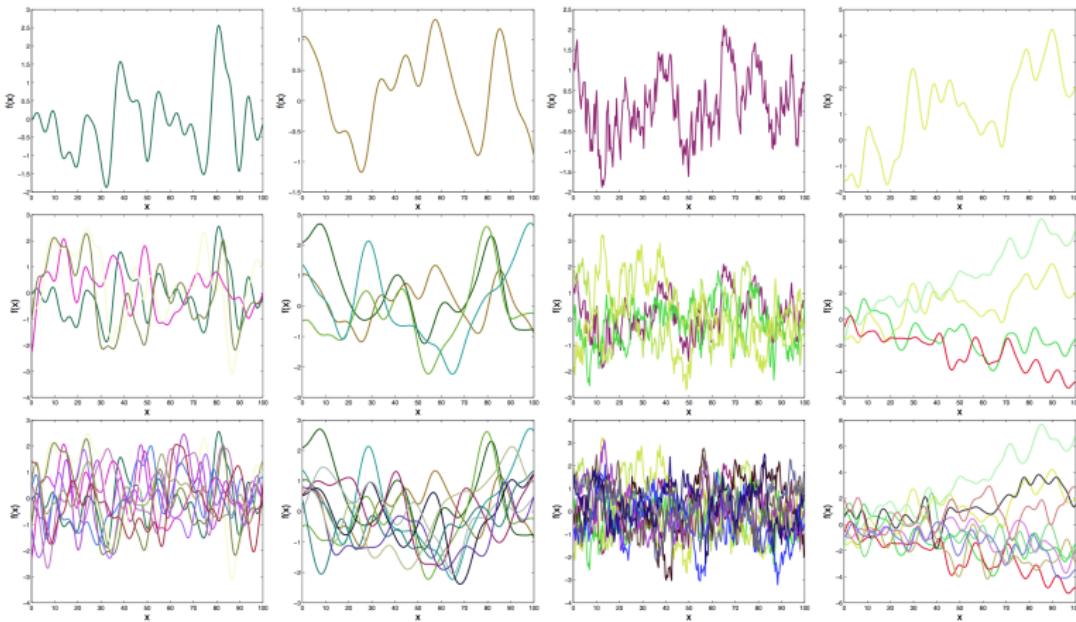
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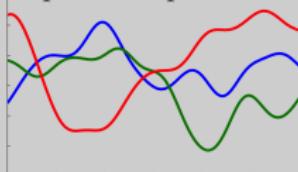
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Samples from GPs with different $K(x, x')$



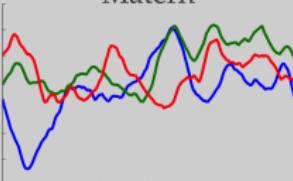
Comparison of GP realizations vs. different covariance functions

Squared-Exponential



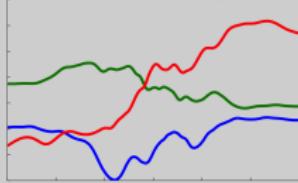
$$K(x, x') = \alpha \exp \left\{ -\frac{1}{2} \sum_{d=1}^D \left(\frac{x_d - x'_d}{\ell_d} \right)^2 \right\}$$

Matérn



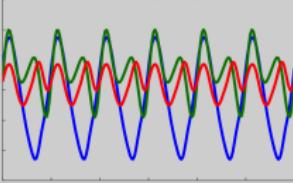
$$K(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}r}{\ell} \right)^\nu K_\nu \left(\frac{\sqrt{2\nu}r}{\ell} \right)$$

"Neural Network"



$$K(x, x') = \frac{2}{\pi} \sin^{-1} \left\{ \frac{2x^T \Sigma x'}{\sqrt{(1 + 2x^T \Sigma x)(1 + 2x'^T \Sigma x')}} \right\}$$

Periodic



$$K(x, x') = \exp \left\{ -\frac{2 \sin^2 \left(\frac{1}{2}(x - x') \right)}{\ell^2} \right\}$$

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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- 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

- We can use heteroscedastic noise and/or non-Gaussian noise models

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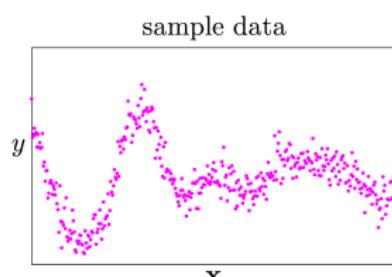
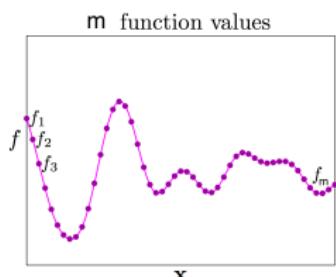
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- The noise model, or likelihood is

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

- 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

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

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

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

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- 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 $K_{**} = K(\mathbf{x}_*, \mathbf{x}_*)$

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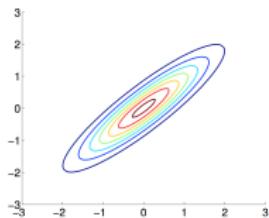
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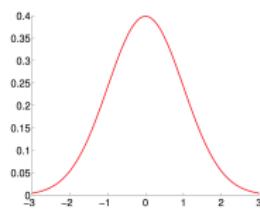
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The Gaussian Distribution



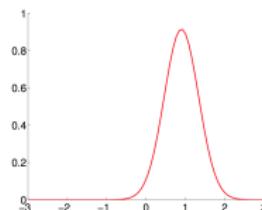
$$p(\mathbf{f}_1, \mathbf{f}_2) \sim \mathcal{N}(\mathbf{f}_1, \mathbf{f}_2 | \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Joint



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

Marginal



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

Conditional

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

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

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

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

- 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

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

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

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- In fact μ_* 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 μ_* and $O(m^2)$ for σ_*^2

- Joint training and test marginal likelihood

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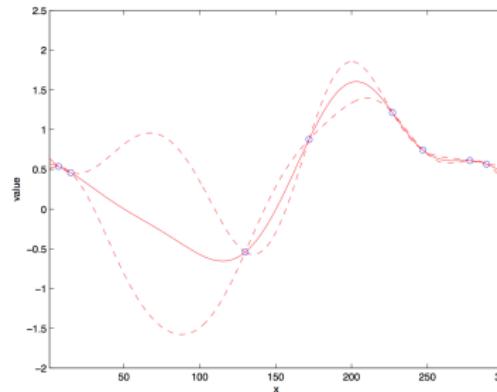
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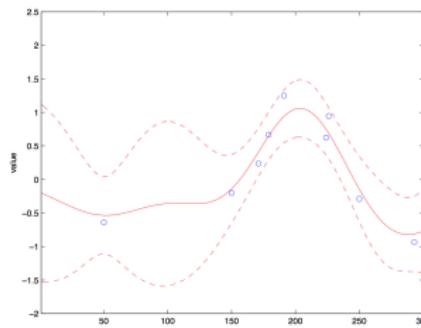
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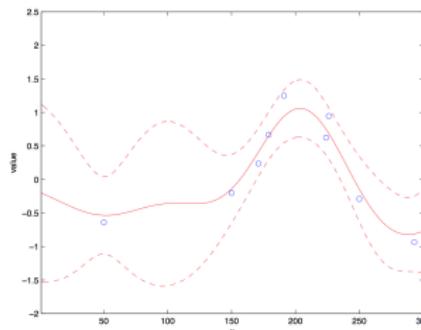
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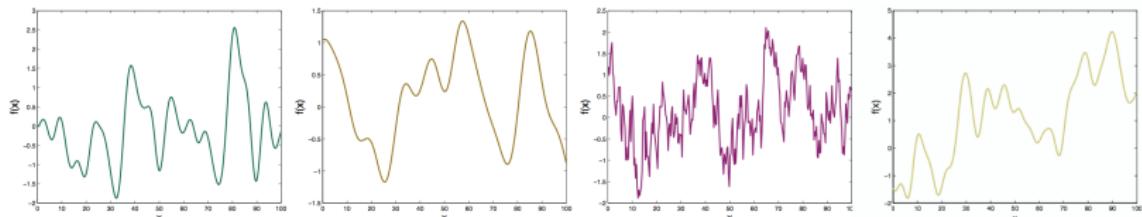
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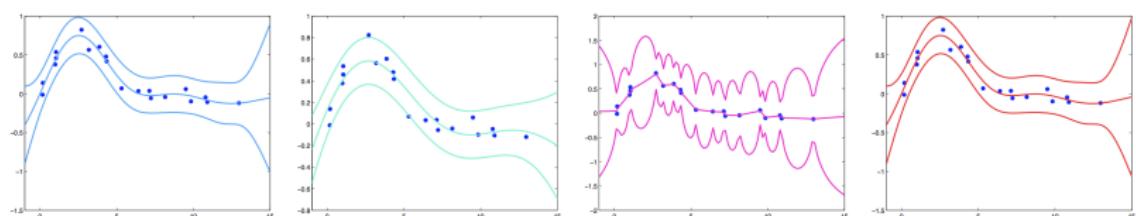


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A sample from the prior for each covariance function:



Corresponding predictions, mean with two standard deviations:



- 1 Motivation
- 2 Gaussian Process model
- 3 GP regression
- 4 Learning Gaussian Process model
- 5 Gaussian Process classification
- 6 Take-home messages
- 7 Afterword: Random Features. Numerical Stability. Non-stationary GP

- 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 θ . Since

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

then

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

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

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

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

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- Advantage of the probabilistic GP framework — ability to choose hyperparameters and covariances directly from the training data
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- Minimization of $\mathcal{L}(\theta)$ is a **non-convex optimization** problem
- Standard gradient based techniques, such as CG or quasi-Newton
- **Gradients:**

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

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- **Binary classification task:** $y = \pm 1$
- GLM likelihood: $p(y = +1|\mathbf{x}, \mathbf{w}) = \pi(\mathbf{x}) = \sigma(\mathbf{w} \cdot \mathbf{x}^\top)$
- $\sigma(z)$ — 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 $f(\mathbf{x}) = \mathbf{w} \cdot \phi(\mathbf{x})^\top$, then likelihood $\pi(\mathbf{x}) = \sigma(f(\mathbf{x}))$, Gaussian prior on \mathbf{f}

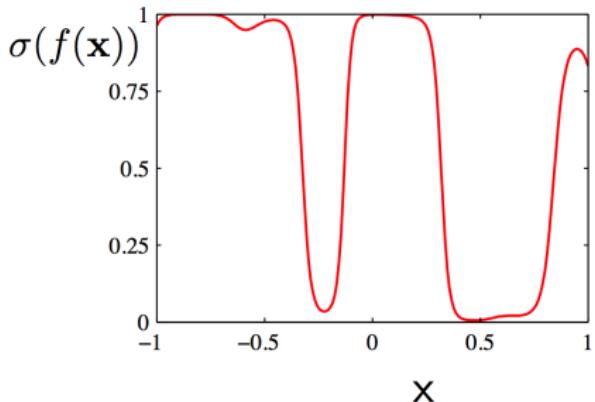
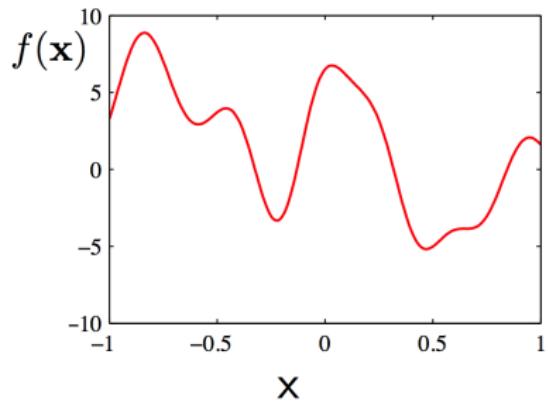
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Two common ways to make Gaussian approximation to posterior:

1. **Laplace approximation**. Second order Taylor approximation about mode of posterior
2. **Expectation propagation (EP)**. EP can be thought of as approximately minimizing $\text{KL}[p(f|y)||q(f|y)]$ by an iterative procedure
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My message...



- **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

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- 1 Motivation
- 2 Gaussian Process model
- 3 GP regression
- 4 Learning Gaussian Process model
- 5 Gaussian Process classification
- 6 Take-home messages
- 7 Afterword: Random Features. Numerical Stability. Non-stationary GP

What else?



- **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 $O(m)$

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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
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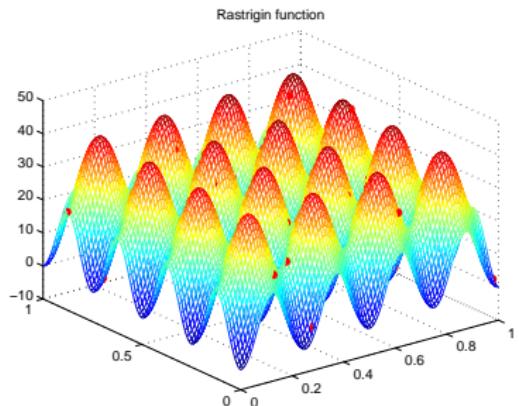


Figure – Rastrigin function

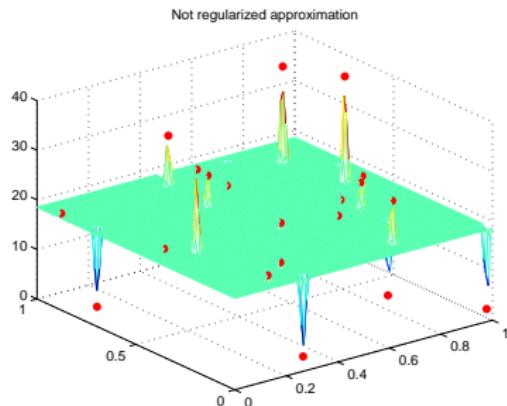


Figure – An approximation of Rastrigin function

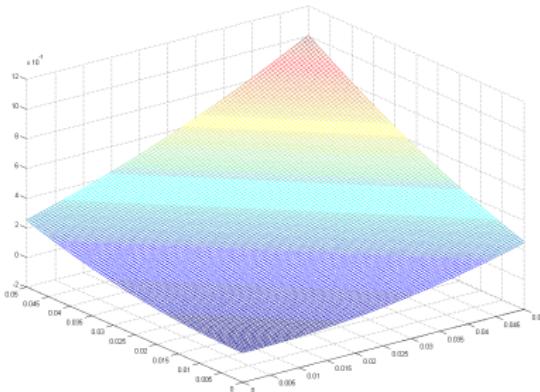
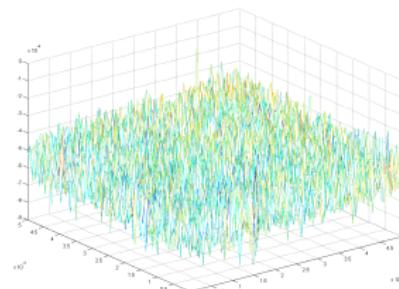
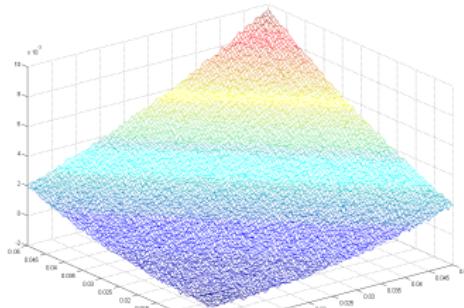


Figure – $y(\mathbf{x}) = (x_1 + x_2)^2$



Let us introduce the following priors on covariance function parameters:

$$\begin{aligned}\theta_i^2 &\in \Gamma(\alpha, \beta), i = 1, \dots, d \\ \sigma^2 &\in \Gamma(\alpha_\sigma, \beta_\sigma)\end{aligned}$$

Thus log-prior of parameters has the form

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

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

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

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Regularized approximation vs. degeneracy

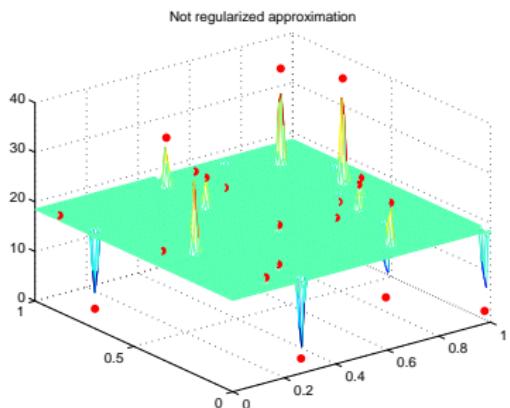


Figure – Degenerate approximation

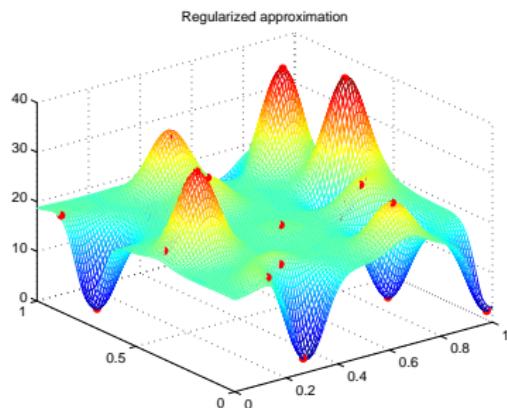
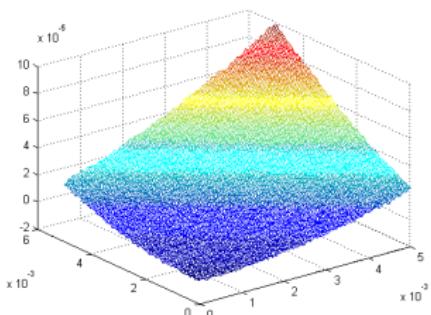
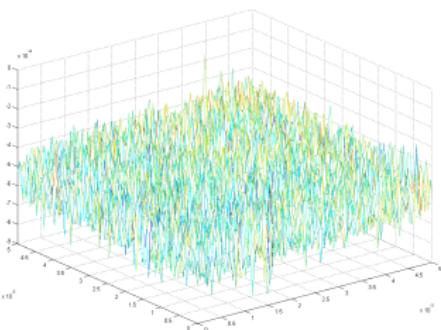
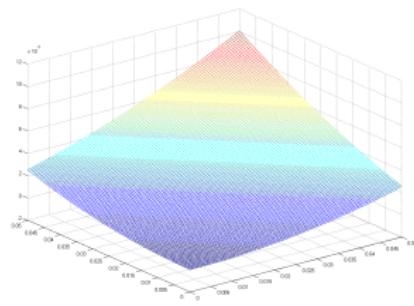
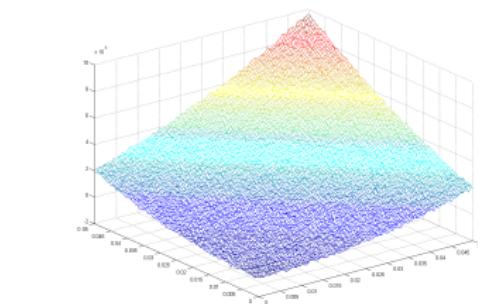
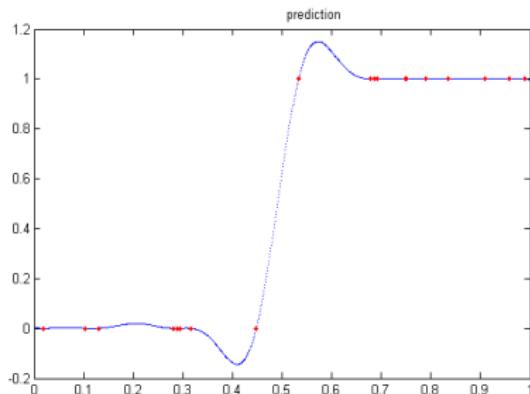


Figure – Approximation with imposed Bayesian regularization

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 $\frac{\sigma_0^2}{Q}$,
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Thus the covariance function of $y(\mathbf{x})$ has the form:

$$\bar{K}(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}, \mathbf{x}') + \sigma_0^2 \psi^\top(\mathbf{x}) \psi(\mathbf{x}') + \sigma^2 \delta(\mathbf{x}, \mathbf{x}'),$$

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

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- $\Psi = \{\psi(\mathbf{x}_i), i = 1, \dots, m\}$,
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$$-\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) = \frac{1}{2}\mathbf{y}^\top \bar{\mathbf{K}}^{-1} \mathbf{y} + \frac{1}{2} \log |\bar{\mathbf{K}}| - \frac{m}{2} \log 2\pi,$$

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

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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.

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

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Approximation of Heaviside function

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

