Imperial College London

Gaussian Processes

Recommended reading:
Rasmussen/Williams: Chapters 1, 2, 4, 5
Deisenroth & Ng (2015)[3]

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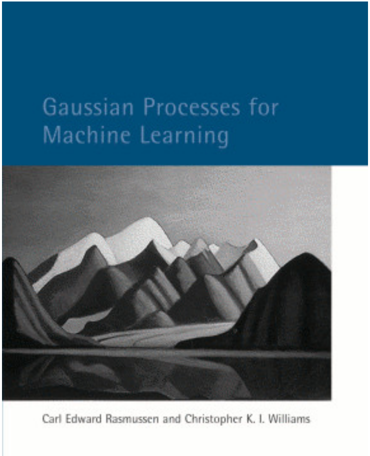
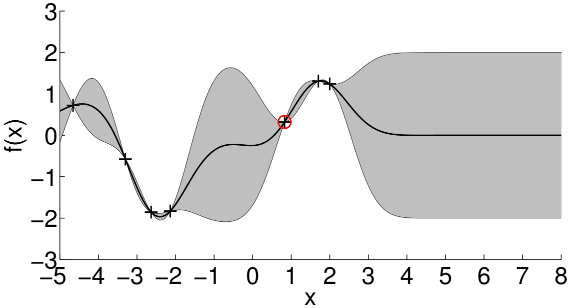
Department of Computing
Imperial College London

February 13, 2018



http://www.gaussianprocess.org/

Problem Setting



Objective

For a set of observations $y_i = f(\boldsymbol{x}_i) + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$, find a distribution over functions $p(f)$ that explains the data

▶▶ Probabilistic regression problem

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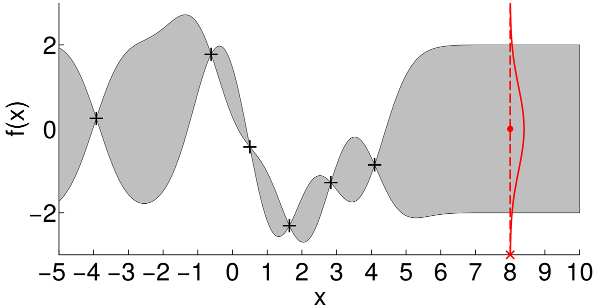

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Linear Regression (Recap from CO-496)

$$y = \boldsymbol{\theta}^\top \phi(\boldsymbol{x}) + \epsilon, \qquad \epsilon \sim \mathcal{N}\big(0,\, \sigma_n^2\big)$$

Finding good parameters $\boldsymbol{\theta}$:

- Maximum likelihood estimate (least squares)
- Maximum a posteriori estimate (regularized least squares)

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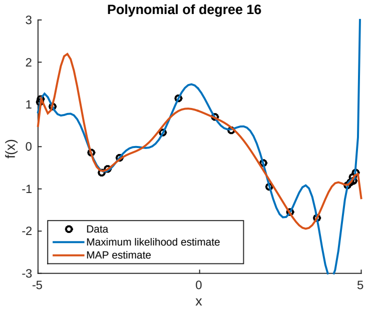
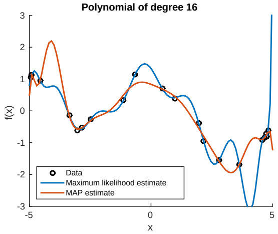


Bayesian Linear Regression (Recap from CO-496)

- Place a prior $p(\boldsymbol{\theta})$ on parameters $\boldsymbol{\theta}$



Likelihood: $p(y|\boldsymbol{x}, \boldsymbol{\theta}) = \mathcal{N}\big(y \mid \boldsymbol{\theta}^\top \phi(\boldsymbol{x}),\, \sigma_n^2\big)$

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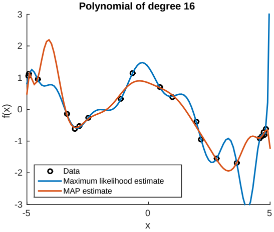

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$$p(y|\boldsymbol{x}) = \int p(y|\boldsymbol{x}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$$

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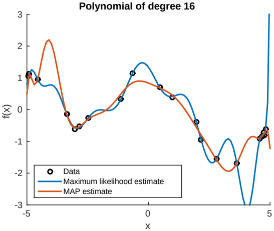
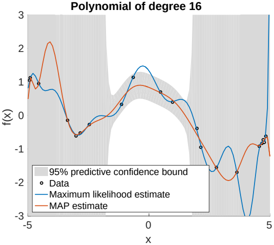
$$p(y|\boldsymbol{x}) = \int p(y|\boldsymbol{x}, \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

- Induce a distribution over functions:

$$p(y|\cdot) = \int \mathcal{N}\big(y \,|\, \boldsymbol{\theta}^\top \phi(\cdot),\, \sigma_n^2\big) \mathcal{N}\big(\boldsymbol{\mu},\, \boldsymbol{\Sigma}\big) d\boldsymbol{\theta}$$

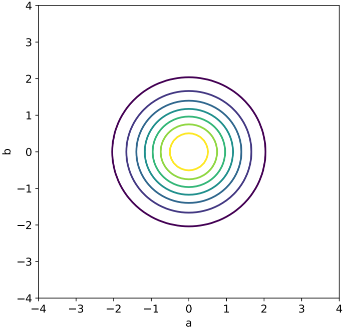




Sampling from the Prior over Functions

Consider a linear regression setting

$$y = f(x) + \epsilon = a + bx + \epsilon\,, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_n^2\big)$$
$$p(a, b) = \mathcal{N}\big(\mathbf{0},\, \boldsymbol{I}\big)$$



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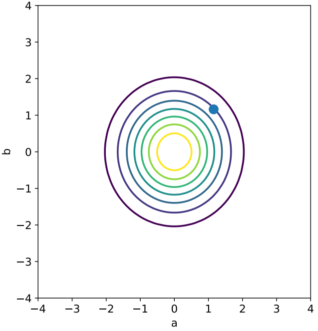
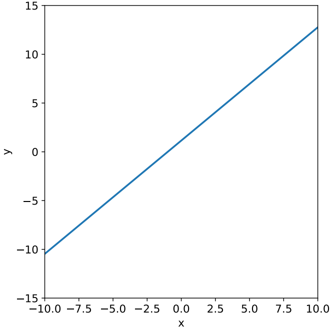
$$p(a, b) = \mathcal{N}\big(\mathbf{0},\, \boldsymbol{I}\big)$$
$$f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$$





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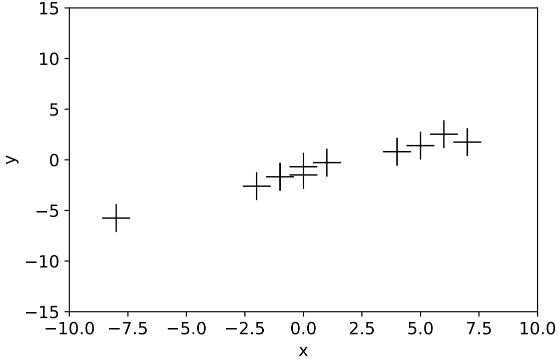
$$\boldsymbol{X} = [x_1, \ldots, x_N],\ \boldsymbol{y} = [y_1, \ldots, y_N] \quad \text{Training inputs/targets}$$



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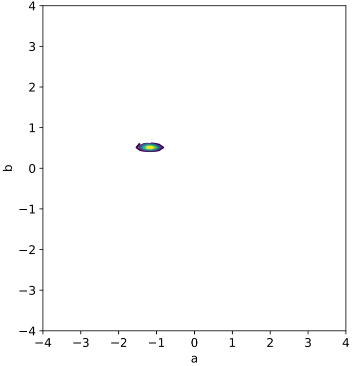
$$p(a, b|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}\big(\boldsymbol{m}_N,\, \boldsymbol{S}_N\big) \qquad \text{Posterior}$$



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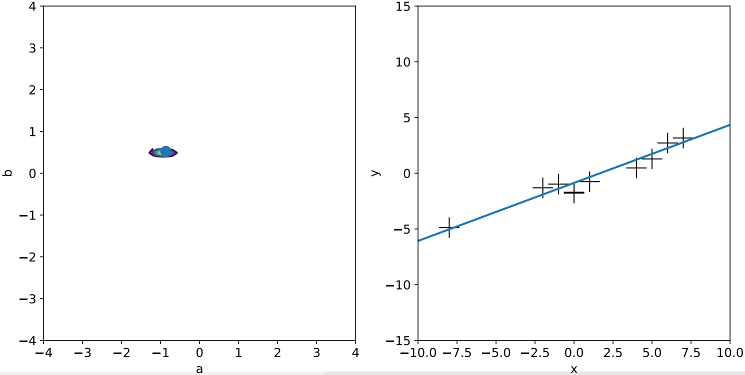
$$[a_i, b_i] \sim p(a, b|\boldsymbol{X}, \boldsymbol{y})$$
$$f_i = a_i + b_i x$$



Fitting Nonlinear Functions

- Fit nonlinear functions using (Bayesian) linear regression: Linear combination of nonlinear features
- Example: Radial-basis-function (RBF) network

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} w_i \phi_i(\boldsymbol{x}), \quad w_i \sim \mathcal{N}\big(0, \sigma_p^2\big)$$

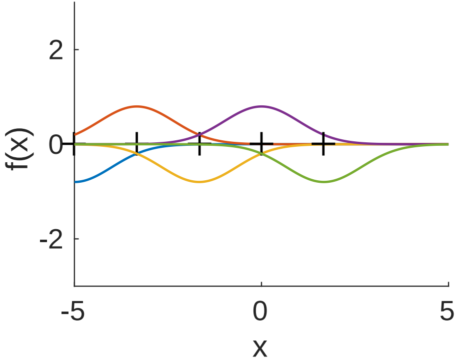
where

$$\phi_i(\boldsymbol{x}) = \exp\big(-\tfrac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_i)^\top(\boldsymbol{x}-\boldsymbol{\mu}_i)\big)$$

for given "centers" $\boldsymbol{\mu}_i$

Illustration: Fitting a Radial Basis Function Network

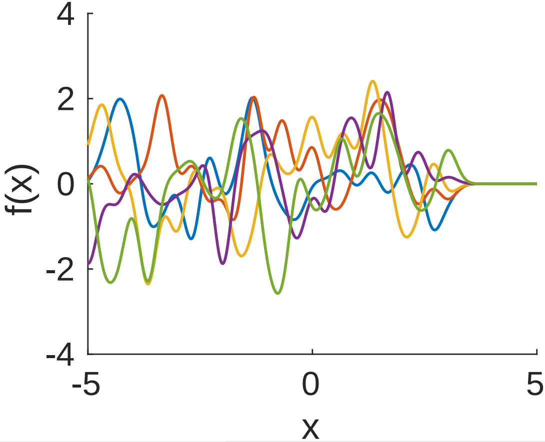
$$\phi_i(\boldsymbol{x}) = \exp\left(-\tfrac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_i)^\top(\boldsymbol{x}-\boldsymbol{\mu}_i)\right)$$



- Place Gaussian-shaped basis functions ϕ_i at 25 input locations μ_i, linearly spaced in the interval $[-5, 3]$

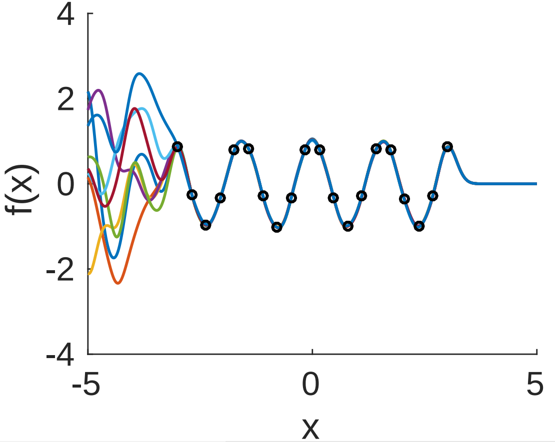
Samples from the RBF Prior

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} w_i \phi_i(\boldsymbol{x}), \quad p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

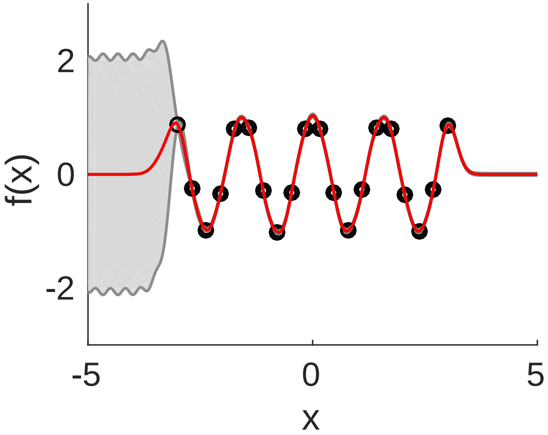


Samples from the RBF Posterior

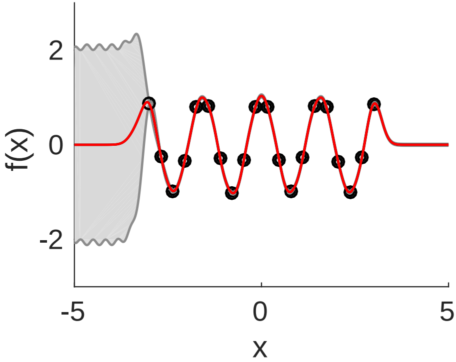
$$f(\boldsymbol{x}) = \sum_{i=1}^{n} w_i \phi_i(\boldsymbol{x}), \quad p(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}\big(\boldsymbol{m}_N, \boldsymbol{S}_N\big)$$



RBF Posterior



Limitations



- Feature engineering
- Finite number of features:
    - Above: Without basis functions on the right, we cannot express any variability of the function
    - Ideally: Add more (infinitely many) basis functions

Approach

- Instead of sampling parameters, which induce a distribution over functions, sample functions directly

  ⏩ Make assumptions on the distribution of functions

- **Intuition:** function = infinitely long vector of function values

  ⏩ Make assumptions on the distribution of function values

Gaussian Process

- We will place a distribution $p(f)$ on functions f
- Informally, a function can be considered an infinitely long vector of function values $f = [f_1, f_2, f_3, ...]$
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Definition (Rasmussen & Williams, 2006)

A Gaussian process (GP) is a collection of random variables $f_1, f_2, \dots,$ any finite number of which is Gaussian distributed.

- A Gaussian distribution is specified by a mean vector $\boldsymbol{\mu}$ and a covariance matrix $\boldsymbol{\Sigma}$
- A Gaussian process is specified by a mean function $m(\cdot)$ and a covariance function (kernel) $k(\cdot, \cdot)$

Covariance Function

- The covariance function (kernel) is symmetric and positive semi-definite
- It allows us to compute covariances between (unknown) function values by just looking at the corresponding inputs:

$$\mathrm{Cov}[f(\boldsymbol{x}_i), f(\boldsymbol{x}_j)] = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

▶▶ Kernel trick (Schölkopf & Smola, 2002)

GP Regression as a Bayesian Inference Problem

Objective

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Training data: $\boldsymbol{X}, \boldsymbol{y}$. Bayes' theorem yields

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Posterior: $p(f|\boldsymbol{y}, \boldsymbol{X}) = GP(m_{\text{post}}, k_{\text{post}})$

Prior over Functions

- Treat a function as a long vector of function values:

$$f = [f_1, f_2, \dots]$$

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- Consider a finite number of N function values $\boldsymbol{f}$ and all other (infinitely many) function values $\tilde{\boldsymbol{f}}$. Informally:

$$p(\boldsymbol{f}, \tilde{\boldsymbol{f}}) = \mathcal{N}\left(\begin{bmatrix}\boldsymbol{\mu}_f \\ \boldsymbol{\mu}_{\tilde{f}}\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{ff} & \boldsymbol{\Sigma}_{f\tilde{f}} \\ \boldsymbol{\Sigma}_{\tilde{f}f} & \boldsymbol{\Sigma}_{\tilde{f}\tilde{f}}\end{bmatrix}\right)$$

where $\boldsymbol{\Sigma}_{\tilde{f}\tilde{f}} \in \mathbb{R}^{m\times m}$ and $\boldsymbol{\Sigma}_{f\tilde{f}} \in \mathbb{R}^{N\times m}$, $m \to \infty$.

- $\Sigma_{ff}^{(i,j)} = \mathrm{Cov}[f(\boldsymbol{x}_i), f(\boldsymbol{x}_j)] = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$

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- $\Sigma_{ff}^{(i,j)} = \mathrm{Cov}[f(\boldsymbol{x}_i), f(\boldsymbol{x}_j)] = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$
- Key property: The marginal remains finite

$$p(\boldsymbol{f}) = \int p(\boldsymbol{f}, \tilde{\boldsymbol{f}}) d\tilde{\boldsymbol{f}} = \mathcal{N}(\boldsymbol{\mu}_f, \boldsymbol{\Sigma}_{ff})$$

Training and Test Marginal

- In practice, we always have finite training and test inputs $\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}$.
- Define $f_* := f_{\text{test}}, f := f_{\text{train}}$.

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- Define $\boldsymbol{f}_* := \boldsymbol{f}_{\text{test}}, \boldsymbol{f} := \boldsymbol{f}_{\text{train}}$.
- Then, we obtain the finite marginal

$$p(\boldsymbol{f}, \boldsymbol{f}_*) = \int p(\boldsymbol{f}, \boldsymbol{f}_*, \boldsymbol{f}_{\text{other}}) d\boldsymbol{f}_{\text{other}} = \mathcal{N}\left(\begin{bmatrix}\boldsymbol{\mu}_f \\ \boldsymbol{\mu}_*\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{ff} & \boldsymbol{\Sigma}_{f*} \\ \boldsymbol{\Sigma}_{*f} & \boldsymbol{\Sigma}_{**}\end{bmatrix}\right)$$

GP Regression as a Bayesian Inference Problem (ctd.)

Posterior over functions (with training data $\boldsymbol{X}, \boldsymbol{y}$):

$$p(f|\boldsymbol{X}, \boldsymbol{y}) = \frac{p(\boldsymbol{y}|f, \boldsymbol{X})\, p(f|\boldsymbol{X})}{p(\boldsymbol{y}|\boldsymbol{X})}$$

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Using the properties of Gaussians, we obtain

$$p(\boldsymbol{y}|f, \boldsymbol{X})\, p(f|\boldsymbol{X}) = \mathcal{N}\big(\boldsymbol{y}\,|\,f(\boldsymbol{X}),\, \sigma_n^2 \boldsymbol{I}\big)\, \mathcal{N}\big(f(\boldsymbol{X})\,|\,m(\boldsymbol{X}),\, \boldsymbol{K}\big)$$

$\boldsymbol{K} = k(\boldsymbol{X}, \boldsymbol{X})$

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$$= Z\mathcal{N}\big(f(\boldsymbol{X}) \,|\, \underbrace{m(\boldsymbol{X}) + \boldsymbol{K}(\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1}(\boldsymbol{y} - m(\boldsymbol{X}))}_{\text{posterior mean}}, \, \underbrace{\boldsymbol{K} - \boldsymbol{K}(\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1}\boldsymbol{K}}_{\text{posterior covariance}}\big)$$

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Marginal likelihood:

$$Z = p(\boldsymbol{y}|\boldsymbol{X}) = \int p(\boldsymbol{y}|f, \boldsymbol{X})\; p(f|\boldsymbol{X})\, df = \mathcal{N}\big(\boldsymbol{y} \,|\, m(\boldsymbol{X}), \boldsymbol{K} + \sigma_n^2 \boldsymbol{I}\big)$$

GP Predictions (1)

$$y = f(\boldsymbol{x}) + \epsilon, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_n^2\big)$$

- **Objective:** Find $p(f(\boldsymbol{X}_*)|\boldsymbol{X}, \boldsymbol{y})$ for training data $\boldsymbol{X}, \boldsymbol{y}$ and test inputs $\boldsymbol{X}_*$.
- GP prior: $p(f|\boldsymbol{X}) = \mathcal{N}\big(m(\boldsymbol{X}),\, \boldsymbol{K}\big)$
- Gaussian Likelihood: $p(\boldsymbol{y}|f(\boldsymbol{X})) = \mathcal{N}\big(f(\boldsymbol{X}),\, \sigma_n^2\boldsymbol{I}\big)$

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- GP prior: $p(f|\boldsymbol{X}) = \mathcal{N}\big(m(\boldsymbol{X}),\, \boldsymbol{K}\big)$
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- With $f \sim GP$ it follows that $\boldsymbol{f}, \boldsymbol{f}_*$ are jointly Gaussian distributed:

$$p(\boldsymbol{f}, \boldsymbol{f}_*|\boldsymbol{X}, \boldsymbol{X}_*) = \mathcal{N}\left(\begin{bmatrix} m(\boldsymbol{X}) \\ m(\boldsymbol{X}_*) \end{bmatrix}, \begin{bmatrix} \boldsymbol{K} & k(\boldsymbol{X}, \boldsymbol{X}_*) \\ k(\boldsymbol{X}_*, \boldsymbol{X}) & k(\boldsymbol{X}_*, \boldsymbol{X}_*) \end{bmatrix}\right)$$

GP Predictions (1)

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- Due to the Gaussian likelihood, we also get ($\boldsymbol{f}$ is unobserved)

$$p(\boldsymbol{y}, \boldsymbol{f}_*|\boldsymbol{X}, \boldsymbol{X}_*) = \mathcal{N}\left(\begin{bmatrix} m(\boldsymbol{X}) \\ m(\boldsymbol{X}_*) \end{bmatrix}, \begin{bmatrix} \boldsymbol{K} + \sigma_n^2\boldsymbol{I} & k(\boldsymbol{X}, \boldsymbol{X}_*) \\ k(\boldsymbol{X}_*, \boldsymbol{X}) & k(\boldsymbol{X}_*, \boldsymbol{X}_*) \end{bmatrix}\right)$$

GP Predictions (2)

Prior:

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Posterior predictive distribution $p(f_* | \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*)$ at test inputs $\boldsymbol{X}_*$

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$$p(f_* | \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*) = \mathcal{N}\big(\mathbb{E}[f_* | \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*],\ \mathbb{V}[f_* | \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*]\big)$$

$$\mathbb{E}[f_* | \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*] = m_{\text{post}}(\boldsymbol{X}_*) = \underbrace{m(\boldsymbol{X}_*)}_{\text{prior mean}} + \underbrace{k(\boldsymbol{X}_*, \boldsymbol{X})(\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1}}_{\text{“Kalman gain”}} \underbrace{(\boldsymbol{y} - m(\boldsymbol{X}))}_{\text{error}}$$

$$\begin{aligned} \mathbb{V}[f_* | \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*] &= k_{\text{post}}(\boldsymbol{X}_*, \boldsymbol{X}_*) \\ &= \underbrace{k(\boldsymbol{X}_*, \boldsymbol{X}_*)}_{\text{prior variance}} - \underbrace{k(\boldsymbol{X}_*, \boldsymbol{X})(\boldsymbol{K} + \sigma_n^2 \boldsymbol{I})^{-1} k(\boldsymbol{X}, \boldsymbol{X}_*)}_{\geqslant 0} \end{aligned}$$

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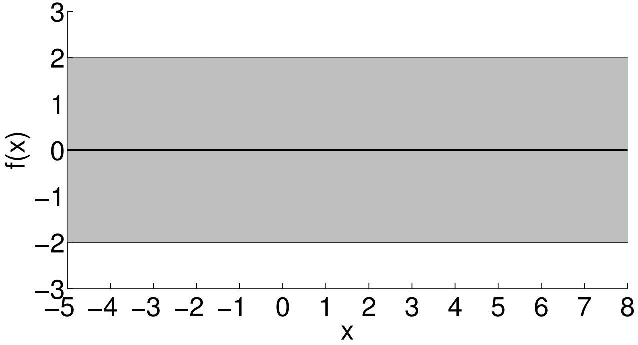
From now: Set prior mean function $m \equiv 0$

Illustration: Inference with Gaussian Processes



Prior belief about the function

Predictive (marginal) mean and variance:

$$\mathbb{E}[f(\boldsymbol{x}_*)|\boldsymbol{x}_*, \varnothing] = m(\boldsymbol{x}_*) = 0$$
$$\mathbb{V}[f(\boldsymbol{x}_*)|\boldsymbol{x}_*, \varnothing] = \sigma^2(\boldsymbol{x}_*) = k(\boldsymbol{x}_*, \boldsymbol{x}_*)$$

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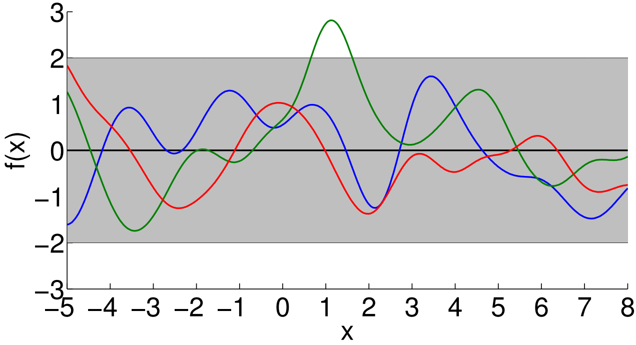

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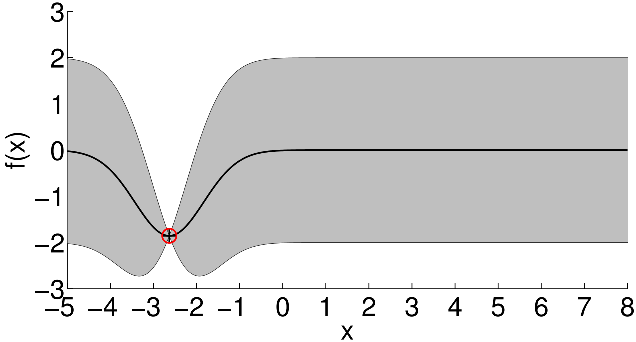

Posterior belief about the function

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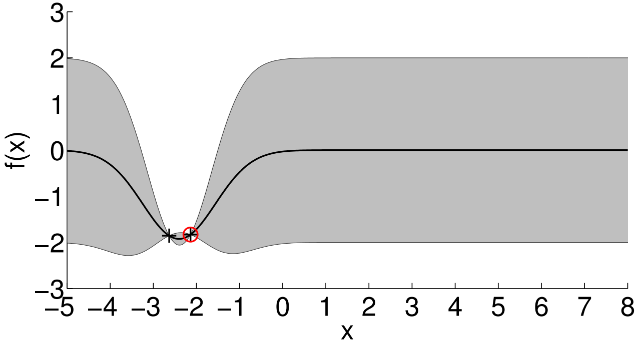

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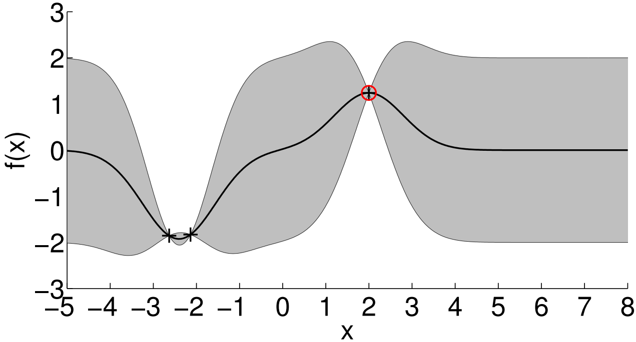

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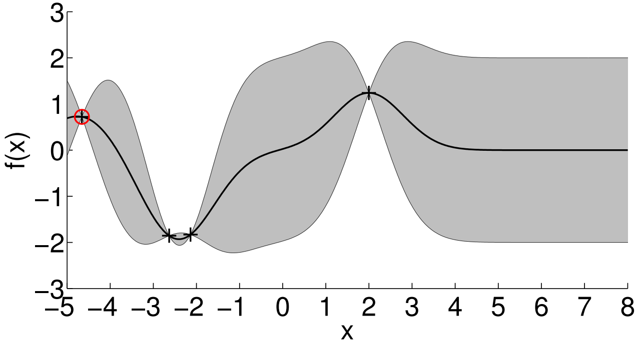

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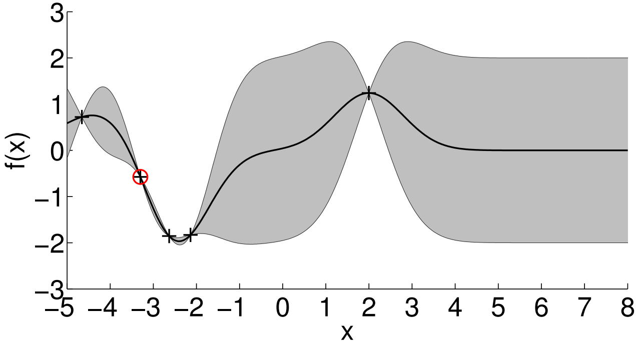

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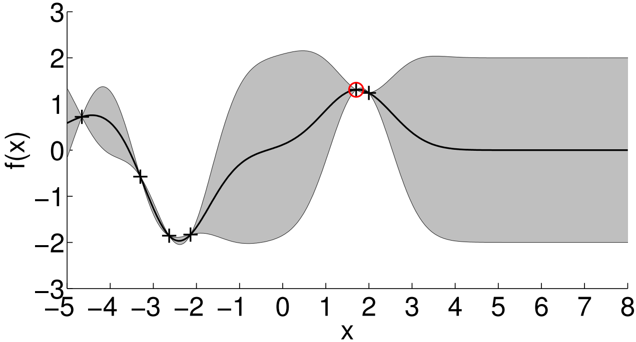

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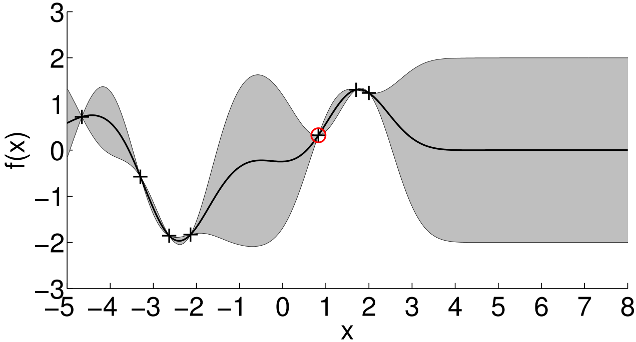

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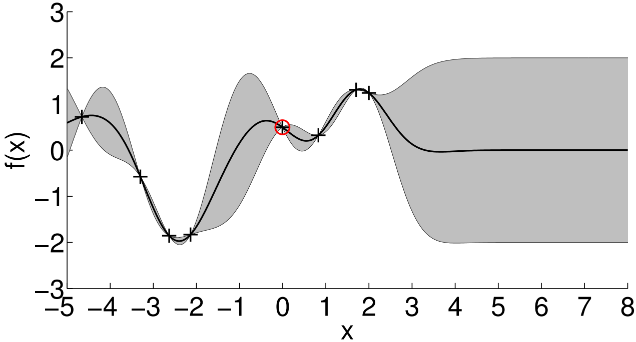

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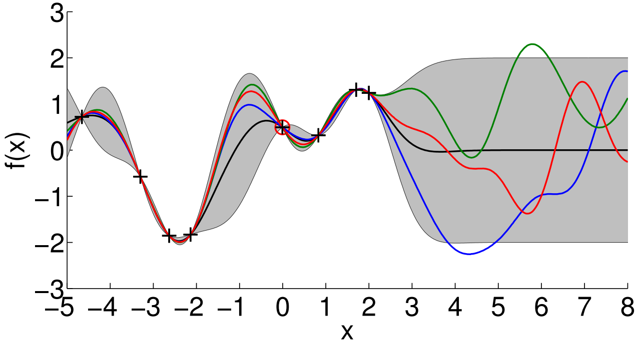

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Covariance Function

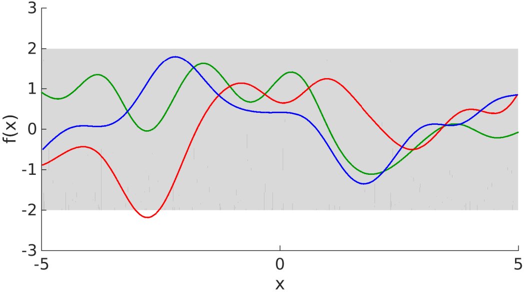
- A Gaussian process is fully specified by a mean function m and a kernel/covariance function k
- The covariance function (kernel) is symmetric and positive semi-definite
- Covariance function encodes high-level structural assumptions about the latent function f (e.g., smoothness, differentiability, periodicity)

Gaussian Covariance Function

$$k_{Gauss}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sigma_f^2 \exp\left(-(\boldsymbol{x}_i - \boldsymbol{x}_j)^\top(\boldsymbol{x}_i - \boldsymbol{x}_j)/\ell^2\right)$$

- σ_f: Amplitude of the latent function
- ℓ: Length scale. How far do we have to move in input space before the function value changes significantly

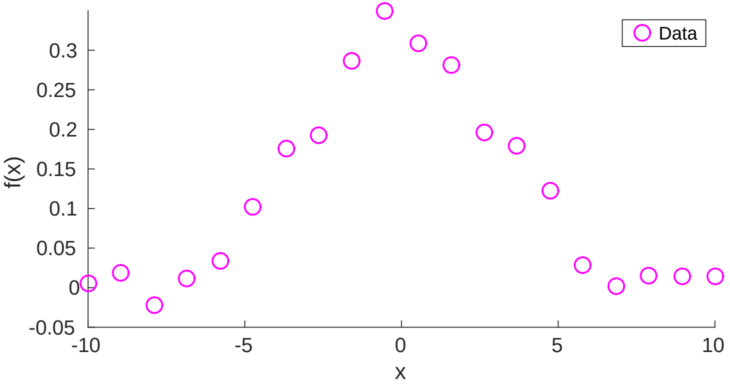
  ▶▶ **Smoothness parameter**



- Assumption on latent function: Smooth (∞ differentiable)

Length-Scales

Length scales determine how wiggly the function is and how much information we can transfer to other function values



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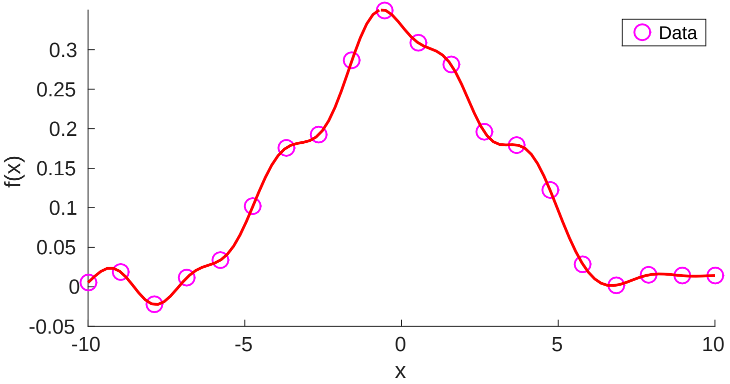

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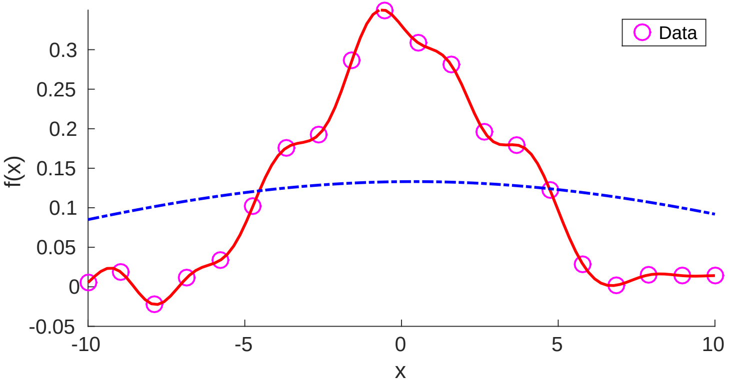

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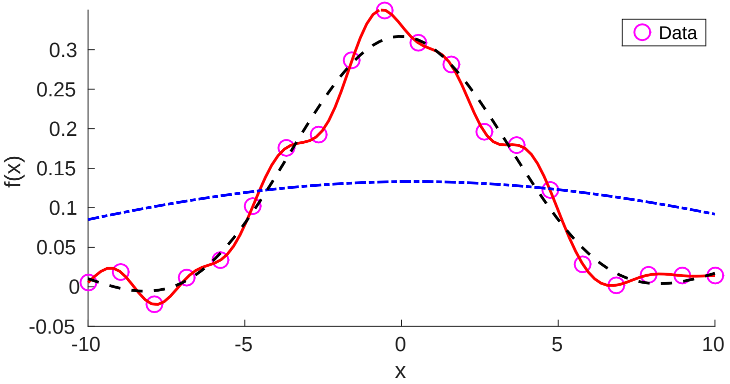
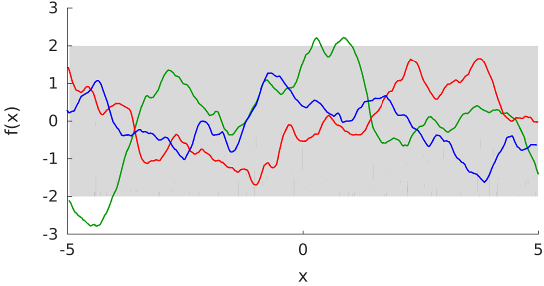


Matérn Covariance Function

$$k_{Mat,3/2}(x_i, x_j) = \sigma_f^2\left(1 + \frac{\sqrt{3}\|\boldsymbol{x}_i - \boldsymbol{x}_j\|}{\ell}\right)\exp\left(-\frac{\sqrt{3}\|\boldsymbol{x}_i - \boldsymbol{x}_j\|}{\ell}\right)$$

- σ_f: Amplitude of the latent function
- ℓ: Length scale. How far do we have to move in input space before the function value changes significantly?



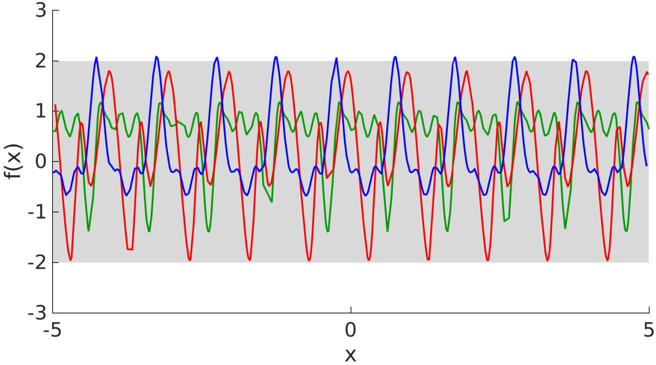
- Assumption on latent function: 1-times differentiable

Periodic Covariance Function

$$k_{per}(x_i, x_j) = \sigma_f^2 \exp\left(-\frac{2\sin^2\left(\frac{\kappa(x_i - x_j)}{2\pi}\right)}{\ell^2}\right)$$

$$= k_{Gauss}(\boldsymbol{u}(x_i), \boldsymbol{u}(x_j)), \quad \boldsymbol{u}(x) = \begin{bmatrix}\cos(\kappa x)\\ \sin(\kappa x)\end{bmatrix}$$

κ: Periodicity parameter



Meta-Parameters of a GP

The GP possesses a set of hyper-parameters:

- Parameters of the mean function
- Hyper-parameters of the covariance function (e.g., length-scales and signal variance)
- Likelihood parameters (e.g., noise variance σ_n^2)

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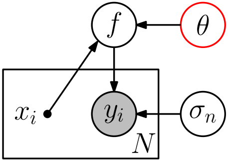
▶▶ Train a GP to find a good set of hyper-parameters

▶▶ Model selection to find good mean and covariance functions
(can also be automated: Automatic Statistician (Lloyd et al., 2014))

Gaussian Process Training: Hyper-Parameters

GP Training

Find good GP hyper-parameters $\boldsymbol{\theta}$ (kernel and mean function parameters)



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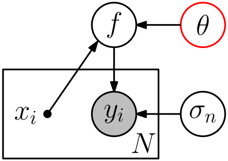

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$$p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) = \frac{p(\boldsymbol{\theta})\, p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{X})}, \quad p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) = \int p(\boldsymbol{y}|f(\boldsymbol{X}))p(f|\boldsymbol{X}, \boldsymbol{\theta})df$$

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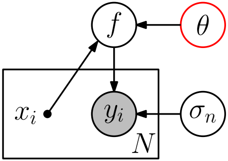

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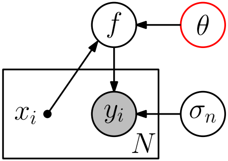

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▶▶ Maximize marginal likelihood if $p(\boldsymbol{\theta}) = \mathcal{U}$ (uniform prior)

Training via Marginal Likelihood Maximization

GP Training

Maximize the evidence/marginal likelihood (probability of the data given the hyper-parameters, where the unwieldy f has been integrated out) ⏩ Also called Maximum Likelihood Type-II

Marginal likelihood:

$$
\begin{aligned}
p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta}) &= \int p(\boldsymbol{y}|f(\boldsymbol{X}))p(f|\boldsymbol{X},\boldsymbol{\theta})df \\
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\end{aligned}
$$

Training via Marginal Likelihood Maximization

GP Training

Maximize the evidence/marginal likelihood (probability of the data given the hyper-parameters, where the unwieldy f has been integrated out) ⏩ Also called Maximum Likelihood Type-II

Marginal likelihood:

$$
\begin{aligned}
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\end{aligned}
$$

Learning the GP hyper-parameters:

$$
\boldsymbol{\theta}^* \in \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})
$$

$$
\log p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta}) = -\tfrac{1}{2}\boldsymbol{y}^\top\boldsymbol{K}_{\boldsymbol{\theta}}^{-1}\boldsymbol{y} - \tfrac{1}{2}\log|\boldsymbol{K}_{\boldsymbol{\theta}}| + \text{const}\,, \quad \boldsymbol{K}_{\boldsymbol{\theta}} := \boldsymbol{K} + \sigma_n^2\boldsymbol{I}
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Training via Marginal Likelihood Maximization

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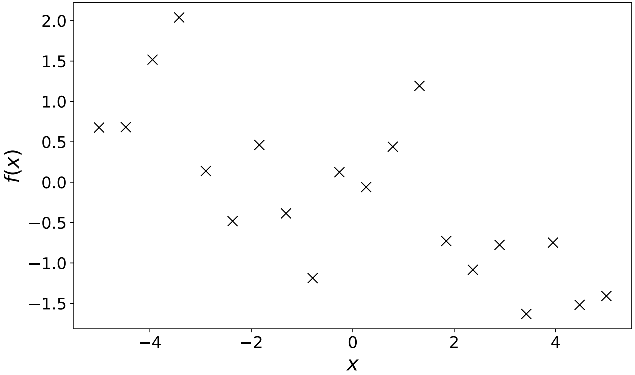
- Automatic trade-off between data fit and model complexity
- Gradient-based optimization of hyper-parameters $\boldsymbol{\theta}$:

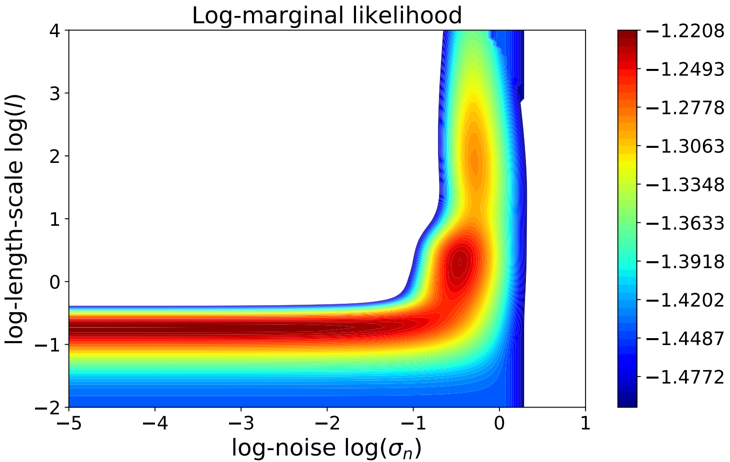
$$\begin{aligned}\frac{\partial \log p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})}{\partial\theta_i} &= \tfrac{1}{2}\boldsymbol{y}^\top\boldsymbol{K}_{\boldsymbol{\theta}}^{-1}\frac{\partial\boldsymbol{K}_{\boldsymbol{\theta}}}{\partial\theta_i}\boldsymbol{K}_{\boldsymbol{\theta}}^{-1}\boldsymbol{y} - \tfrac{1}{2}\mathrm{tr}\big(\boldsymbol{K}_{\boldsymbol{\theta}}^{-1}\frac{\partial\boldsymbol{K}_{\boldsymbol{\theta}}}{\partial\theta_i}\big)\\ &= \tfrac{1}{2}\mathrm{tr}\big((\boldsymbol{\alpha}\boldsymbol{\alpha}^\top - \boldsymbol{K}_{\boldsymbol{\theta}}^{-1})\frac{\partial\boldsymbol{K}_{\boldsymbol{\theta}}}{\partial\theta_i}\big)\,,\end{aligned}$$

$$\boldsymbol{\alpha} := \boldsymbol{K}_{\boldsymbol{\theta}}^{-1}\boldsymbol{y}$$

Example: Training Data



Example: Marginal Likelihood Contour



- Three local optima. What do you expect?

Demo

https://drafts.distill.pub/gp/

Marginal Likelihood and Parameter Learning

- The marginal likelihood is non-convex

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- With increasing data set size the GP typically ends up in the "good-fit" mode. Overfitting (indicator: small length-scales and small noise variance) is unlikely.
- Ideally, we would integrate the hyper-parameters out
  Why can we do not do this easily?

Model Selection—Mean Function and Kernel

- Assume we have a finite set of models M_i, each one specifying a mean function m_i and a kernel k_i. How do we find the best one?

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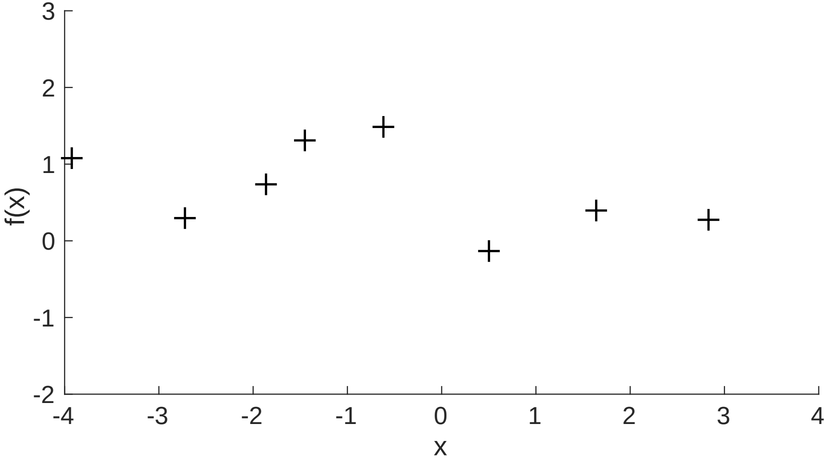
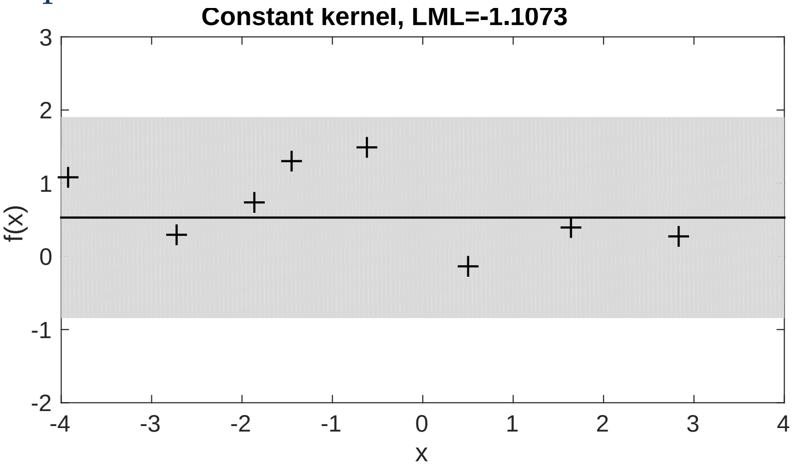
- Some options:
  - BIC, AIC (see CO-496)
  - Compare marginal likelihood values (assuming a uniform prior on the set of models)

Example



- Four different kernels (mean function fixed to $m \equiv 0$)
- MAP hyper-parameters for each kernel
- Log-marginal likelihood values for each (optimized) model

Example



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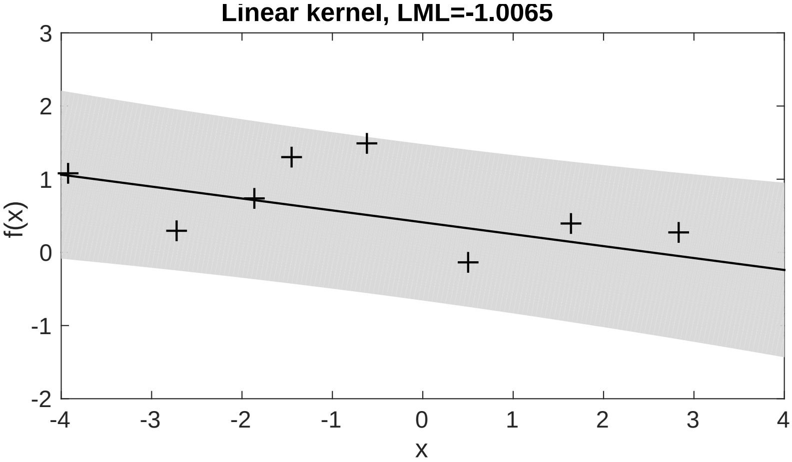

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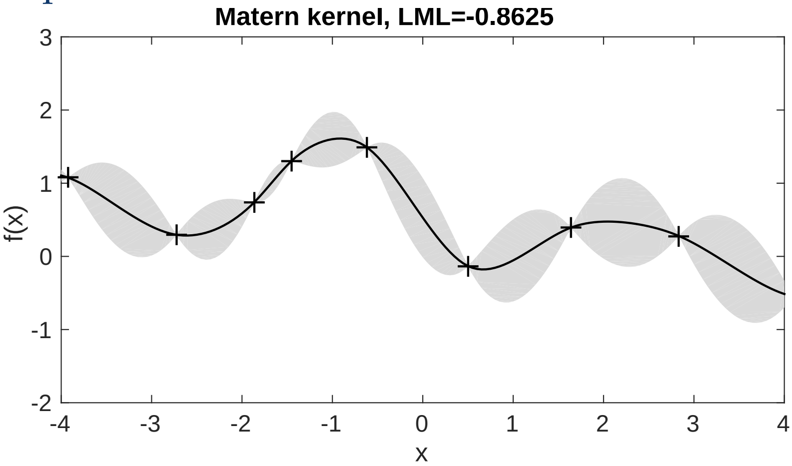

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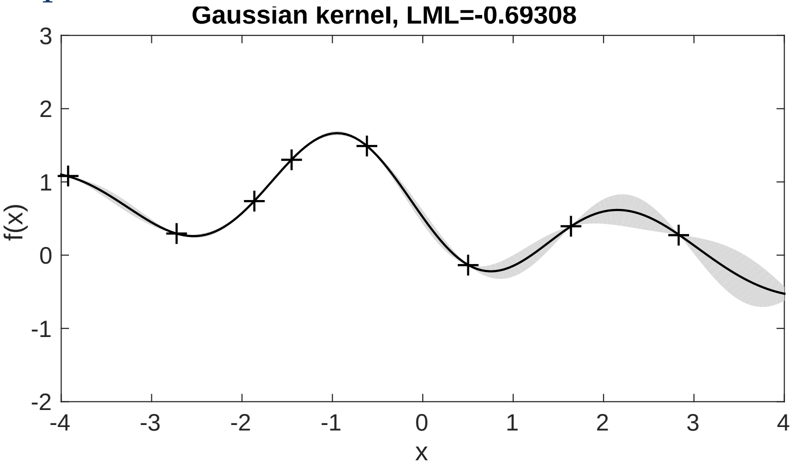

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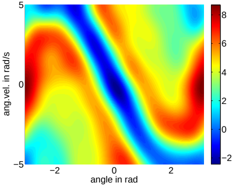
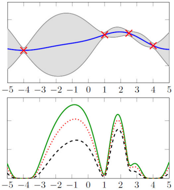
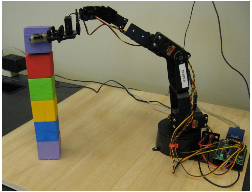
Application Areas







- Reinforcement learning and robotics
  - ⏩ Model value functions and/or dynamics with GPs
- Bayesian optimization (Experimental Design)
  - ⏩ Model unknown utility functions with GPs
- Geostatistics
  - ⏩ Spatial modeling (e.g., landscapes, resources)
- Sensor networks
- Time-series modeling and forecasting

Limitations of Gaussian Processes

Computational and memory complexity

Training set size: N

- Training scales in $\mathcal{O}(N^3)$
- Prediction (variances) scales in $\mathcal{O}(N^2)$
- Memory requirement: $\mathcal{O}(ND + N^2)$

▶▶ **Practical limit** $N \approx 10,000$

Tips and Tricks for Practitioners

- To set initial hyper-parameters, use domain knowledge.
- Standardize input data and set initial length-scales ℓ to ≈ 0.5.
- Standardize targets y and set initial signal variance to $\sigma_f \approx 1$.
- Often useful: Set initial noise level relatively high (e.g., $\sigma_n \approx 0.5 \times \sigma_f$ amplitude, even if you think your data have low noise. The optimization surface for your other parameters will be easier to move in.
- When optimizing hyper-parameters, try random restarts or other tricks to avoid local optima are advised.
- Mitigate the problem of numerical instability (Cholesky decomposition of $\boldsymbol{K} + \sigma_n^2 \boldsymbol{I}$) by penalizing high signal-to-noise ratios σ_f / σ_n

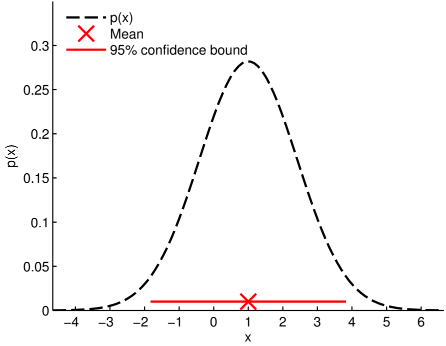
▶▶ `https://drafts.distill.pub/gp`

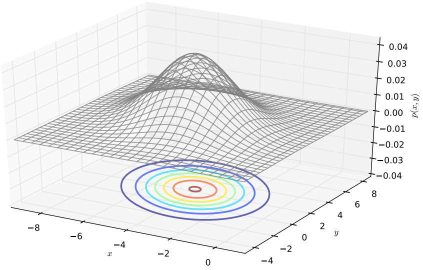
Appendix

The Gaussian Distribution

$$p(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}}|\boldsymbol{\Sigma}|^{-\frac{1}{2}}\exp\big(-\tfrac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\big)$$

- Mean vector $\boldsymbol{\mu}$ ⏩ Average of the data
- Covariance matrix $\boldsymbol{\Sigma}$ ⏩ Spread of the data





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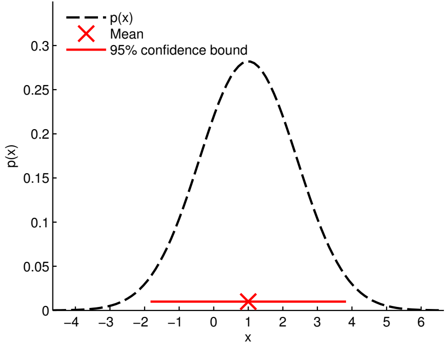

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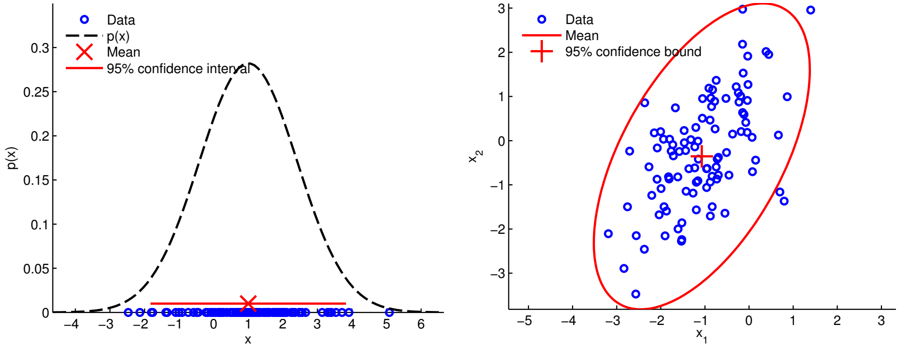

Sampling from a Multivariate Gaussian

Objective

Generate a random sample $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ from a D-dimensional joint Gaussian with covariance matrix $\boldsymbol{\Sigma}$ and mean vector $\boldsymbol{\mu}$.

However, we only have access to a random number generator that can sample $\boldsymbol{x}$ from $\mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$...

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Exploit that affine transformations $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$ of a Gaussian random variable $\boldsymbol{x}$ remain Gaussian

- Mean: $\mathbb{E}_{\boldsymbol{x}}[\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}] = \boldsymbol{A}\mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x}] + \boldsymbol{b}$
- Covariance: $\mathbb{V}_{\boldsymbol{x}}[\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}] = \boldsymbol{A}\mathbb{V}_{\boldsymbol{x}}[\boldsymbol{x}]\boldsymbol{A}^{\top}$

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1. Find conditions for $\boldsymbol{A}, \boldsymbol{b}$ to match the mean of $\boldsymbol{y}$
2. Find conditions for $\boldsymbol{A}, \boldsymbol{b}$ to match the covariance of $\boldsymbol{y}$

Sampling from a Multivariate Gaussian (2)

Objective

Generate a random sample $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ from a D-dimensional joint Gaussian with covariance matrix $\boldsymbol{\Sigma}$ and mean vector $\boldsymbol{\mu}$.

```
x = randn(D,1);          Sample x ~ N(0, I)
y = chol(Σ)'*x + μ;      Scale x and add offset
```

Here `chol(Σ)` is the Cholesky factor $\boldsymbol{L}$, such that $\boldsymbol{L}^\top \boldsymbol{L} = \boldsymbol{\Sigma}$

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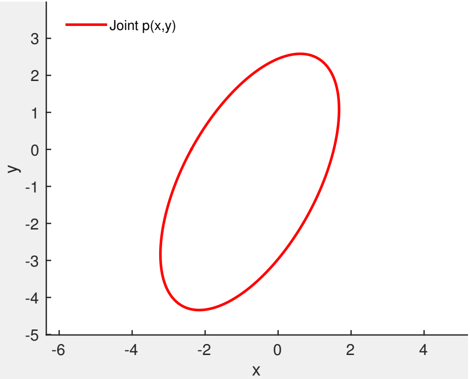
Therefore, the mean and covariance of $\boldsymbol{y}$ are

$$\mathbb{E}[\boldsymbol{y}] = \bar{\boldsymbol{y}} = \mathbb{E}[\boldsymbol{L}^\top \boldsymbol{x} + \boldsymbol{\mu}] = \boldsymbol{L}^\top \mathbb{E}[\boldsymbol{x}] + \boldsymbol{\mu} = \boldsymbol{\mu}$$

$$\mathrm{Cov}[\boldsymbol{y}] = \mathbb{E}[(\boldsymbol{y} - \bar{\boldsymbol{y}})(\boldsymbol{y} - \bar{\boldsymbol{y}})^\top] = \mathbb{E}[\boldsymbol{L}^\top \boldsymbol{x}\boldsymbol{x}^\top \boldsymbol{L}] = \boldsymbol{L}^\top \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^\top]\boldsymbol{L} = \boldsymbol{L}^\top \boldsymbol{L} = \boldsymbol{\Sigma}$$

Conditional



$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix}\right)$$

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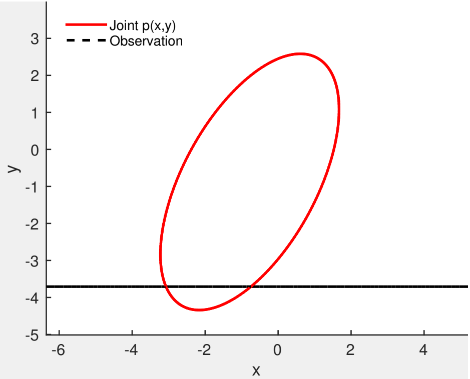

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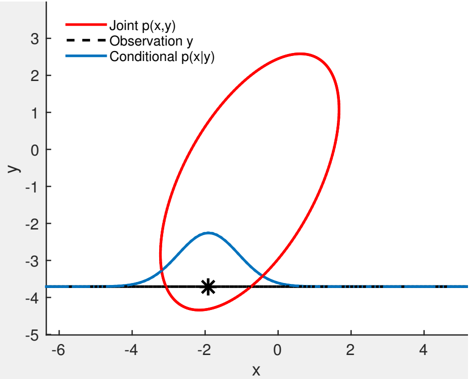

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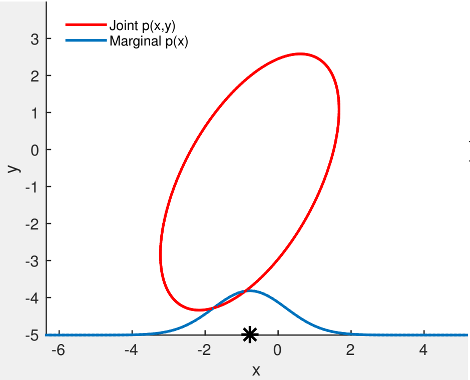
$$\boldsymbol{\mu}_{x|y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y)$$

$$\boldsymbol{\Sigma}_{x|y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx}$$

Conditional $p(\boldsymbol{x}|\boldsymbol{y})$ is also Gaussian

▶▶ Computationally convenient

Marginal



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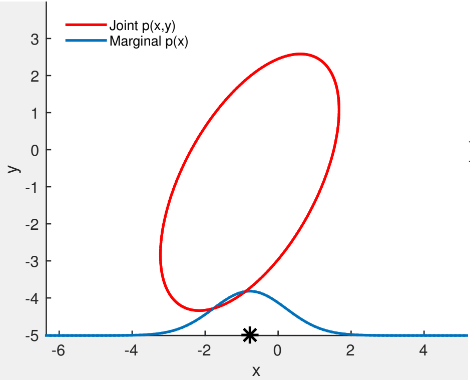

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- The marginal of a joint Gaussian distribution is Gaussian
- Intuitively: Ignore (integrate out) everything you are not interested in

The Gaussian Distribution in the Limit

Consider the joint Gaussian distribution $p(\boldsymbol{x}, \tilde{\boldsymbol{x}})$, where $\boldsymbol{x} \in \mathbb{R}^D$ and $\tilde{\boldsymbol{x}} \in \mathbb{R}^k, k \to \infty$ are random variables.

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where $\boldsymbol{\Sigma}_{\tilde{x}\tilde{x}} \in \mathbb{R}^{k \times k}$ and $\boldsymbol{\Sigma}_{x\tilde{x}} \in \mathbb{R}^{D \times k}, k \to \infty$.

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where $\boldsymbol{\Sigma}_{\tilde{x}\tilde{x}} \in \mathbb{R}^{k\times k}$ and $\boldsymbol{\Sigma}_{x\tilde{x}} \in \mathbb{R}^{D\times k}$, $k \to \infty$.
However, the marginal remains finite

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \tilde{\boldsymbol{x}}) d\tilde{\boldsymbol{x}} = \mathcal{N}(\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx})$$

where we integrate out an infinite number of random variables $\tilde{x}_i$.

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- Then, $\boldsymbol{x} = \{\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}, \boldsymbol{x}_{\text{other}}\}$
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$$p(\boldsymbol{x}) = \mathcal{N}\left(\begin{bmatrix}\boldsymbol{\mu}_{\text{train}} \\ \boldsymbol{\mu}_{\text{test}} \\ \boldsymbol{\mu}_{\text{other}}\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{\text{train}} & \boldsymbol{\Sigma}_{\text{train,test}} & \boldsymbol{\Sigma}_{\text{train,other}} \\ \boldsymbol{\Sigma}_{\text{test,train}} & \boldsymbol{\Sigma}_{\text{test}} & \boldsymbol{\Sigma}_{\text{test,other}} \\ \boldsymbol{\Sigma}_{\text{other,train}} & \boldsymbol{\Sigma}_{\text{other,test}} & \boldsymbol{\Sigma}_{\text{other}}\end{bmatrix}\right)$$

$$p(\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}) = \int p(\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}, \boldsymbol{x}_{\text{other}}) d\boldsymbol{x}_{\text{other}}$$

Marginal and Conditional in the Limit

- In practice, we consider finite training and test data $\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}$
- Then, $\boldsymbol{x} = \{\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}, \boldsymbol{x}_{\text{other}}\}$
  ($\boldsymbol{x}_{\text{other}}$ plays the role of $\tilde{\boldsymbol{x}}$ from previous slide)

$$p(\boldsymbol{x}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_{\text{train}} \\ \boldsymbol{\mu}_{\text{test}} \\ \boldsymbol{\mu}_{\text{other}} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{\text{train}} & \boldsymbol{\Sigma}_{\text{train,test}} & \boldsymbol{\Sigma}_{\text{train,other}} \\ \boldsymbol{\Sigma}_{\text{test,train}} & \boldsymbol{\Sigma}_{\text{test}} & \boldsymbol{\Sigma}_{\text{test,other}} \\ \boldsymbol{\Sigma}_{\text{other,train}} & \boldsymbol{\Sigma}_{\text{other,test}} & \boldsymbol{\Sigma}_{\text{other}} \end{bmatrix}\right)$$

$$p(\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}) = \int p(\boldsymbol{x}_{\text{train}}, \boldsymbol{x}_{\text{test}}, \boldsymbol{x}_{\text{other}}) d\boldsymbol{x}_{\text{other}}$$

$$p(\boldsymbol{x}_{\text{test}}|\boldsymbol{x}_{\text{train}}) = \mathcal{N}(\boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*)$$

$$\boldsymbol{\mu}_* = \boldsymbol{\mu}_{\text{test}} + \boldsymbol{\Sigma}_{\text{test,train}} \boldsymbol{\Sigma}_{\text{train}}^{-1} (\boldsymbol{x}_{\text{train}} - \boldsymbol{\mu}_{\text{train}})$$

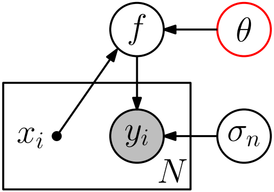
$$\boldsymbol{\Sigma}_* = \boldsymbol{\Sigma}_{\text{test}} - \boldsymbol{\Sigma}_{\text{test,train}} \boldsymbol{\Sigma}_{\text{train}}^{-1} \boldsymbol{\Sigma}_{\text{train,test}}$$

Gaussian Process Training: Hierarchical Inference

- Level-1 inference (posterior on f):

$$p(f|\boldsymbol{X},\boldsymbol{y},\boldsymbol{\theta}) = \frac{p(\boldsymbol{y}|\boldsymbol{X},f)\,p(f|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})}$$

$$p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta}) = \int p(\boldsymbol{y}|f,\boldsymbol{X})\,p(f|\boldsymbol{X},f\boldsymbol{\theta})df$$



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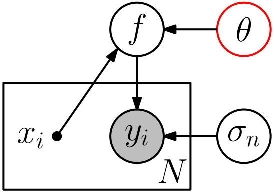
- Level-2 inference (posterior on $\boldsymbol{\theta}$)

$$p(\boldsymbol{\theta}|\boldsymbol{X},\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})\,p(\boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{X})}$$



GP as the Limit of an Infinite RBF Network

Consider the universal function approximator

$$f(x) = \sum_{i \in \mathbb{Z}} \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \gamma_n \exp\left(-\frac{(x - (i + \frac{n}{N}))^2}{\lambda^2}\right), \quad x \in \mathbb{R}, \quad \lambda \in \mathbb{R}^+$$

with $\gamma_n \sim \mathcal{N}(0, 1)$ (random weights)
▶▶ Gaussian-shaped basis functions (with variance $\lambda^2/2$) everywhere on the real axis

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- Mean: $\mathbb{E}[f(x)] = 0$
- Covariance: $\mathrm{Cov}[f(x), f(x')] = \theta_1^2 \exp\left(-\frac{(x-x')^2}{2\lambda^2}\right)$ for suitable $\boldsymbol{\theta}_1^2$

▶▶ GP with mean 0 and Gaussian covariance function

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