Foundations of Machine Learning
African Masters in Machine Intelligence

Gaussian Processes

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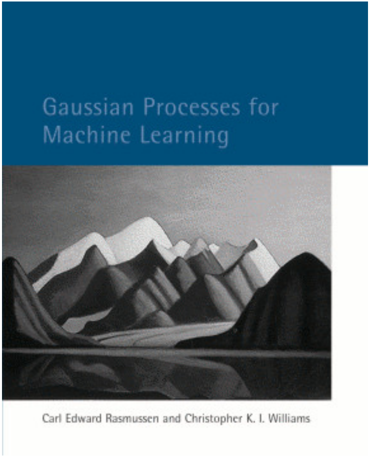
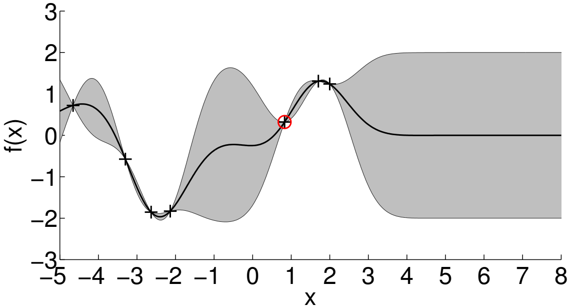
Reference



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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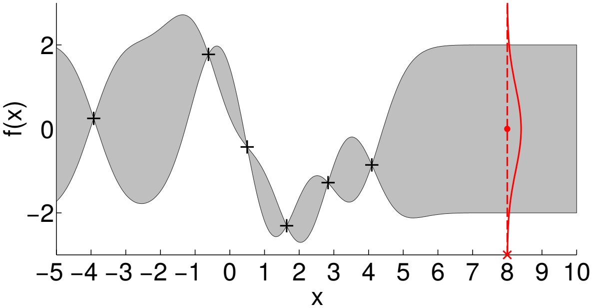

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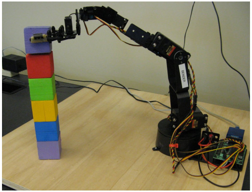
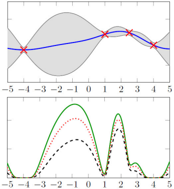
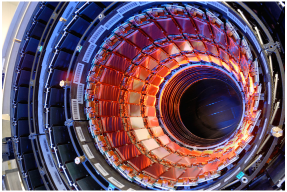
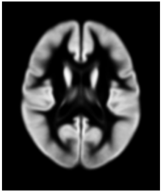
Some Application Areas









- Reinforcement learning and robotics
- Bayesian optimization (experimental design)
- Geostatistics
- Sensor networks
- Time-series modeling and forecasting
- High-energy physics
- Medical applications

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 $f = [f_1, f_2, f_3, ...]$
- A Gaussian process is a generalization of a multivariate Gaussian distribution to infinitely many variables.

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Definition (Rasmussen & Williams, 2006)

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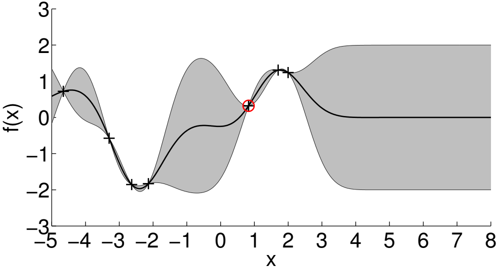
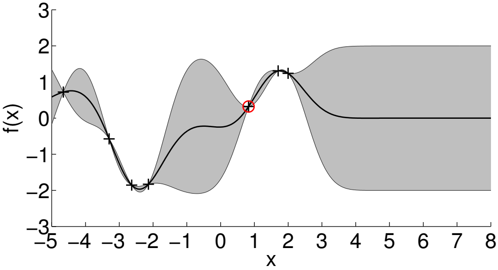
- A Gaussian distribution is specified by a mean vector $\boldsymbol{\mu}$ and a covariance matrix $\boldsymbol{\Sigma}$
- A Gaussian process is specified by a mean function $m(\cdot)$ and a covariance function (kernel) $k(\cdot, \cdot)$

Mean Function



- The "average" function of the distribution over functions
- Allows us to bias the model (can make sense in application-specific settings)
- "Agnostic" mean function in the absence of data or prior knowledge: $m(\cdot) \equiv 0$ everywhere (for symmetry reasons)

Covariance Function



- The covariance function (kernel) is symmetric and positive semi-definite
- It allows us to compute covariances/correlations 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

For a set of observations $y_i = f(\boldsymbol{x}_i) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$, find a (posterior) distribution over functions $p(f|\boldsymbol{X}, \boldsymbol{y})$ that explains the data. Here: $\boldsymbol{X}$ training inputs, $\boldsymbol{y}$ training targets

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

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

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

GP Prior

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

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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

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

GP Prior (2)

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

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

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

▶▶ Computing the joint distribution of an arbitrary number of training and test inputs boils down to manipulating (finite-dimensional) Gaussian distributions

GP Regression as a Bayesian Inference Problem (ctd.)

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

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

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

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$$= Z \times GP\big(m_{\text{post}}(\cdot), k_{post}(\cdot,\cdot)\big)$$

$$m_{\text{post}}(\cdot) = m(\cdot) + k(\cdot,\boldsymbol{X})(\boldsymbol{K}+\sigma_n^2\boldsymbol{I})^{-1}(\boldsymbol{y}-m(\boldsymbol{X}))$$

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Marginal likelihood:

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

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Prediction at $\boldsymbol{x}_*$: $p(f(x_*)|\boldsymbol{X},\boldsymbol{y},\boldsymbol{x}_*) = \mathcal{N}\big(m_{\text{post}}(\boldsymbol{x}_*),\, k_{\text{post}}(\boldsymbol{x}_*,\boldsymbol{x}_*)\big)$

GP Predictions (alternative derivation)

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

- **Objective:** Find $p(f(\boldsymbol{X}_*)|\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*)$ for training data $\boldsymbol{X}, \boldsymbol{y}$ and test inputs $\boldsymbol{X}_*$.
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- With $f \sim GP$ it follows that $\boldsymbol{f}, \boldsymbol{f}_*$ are jointly Gaussian distributed:

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

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

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

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

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Posterior predictive distribution $p(\boldsymbol{f}_*|\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*)$ at test inputs $\boldsymbol{X}_*$ obtained by Gaussian conditioning:

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

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

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

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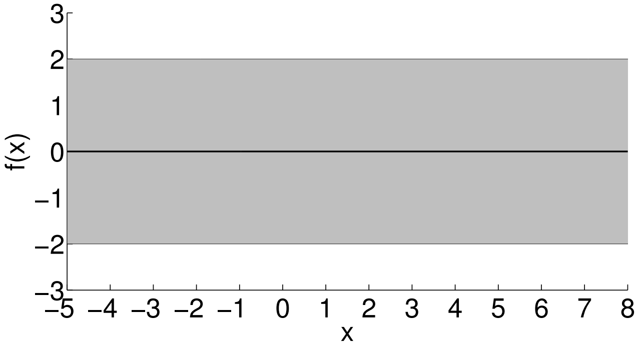
From now: Set prior mean function $m \equiv 0$

Illustration: Inference with Gaussian Processes



Prior belief about the function

Predictive (marginal) mean and variance:

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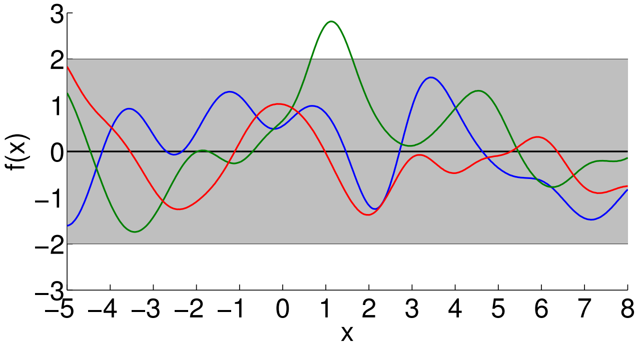

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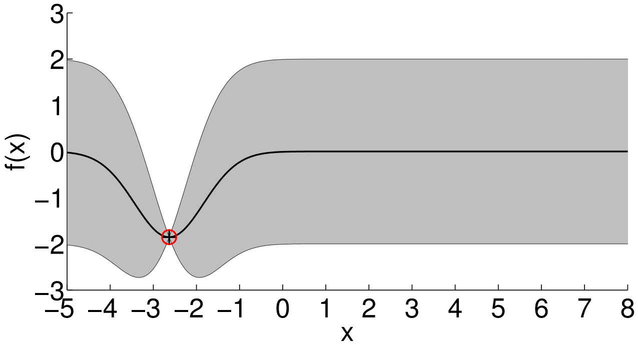

Posterior belief about the function

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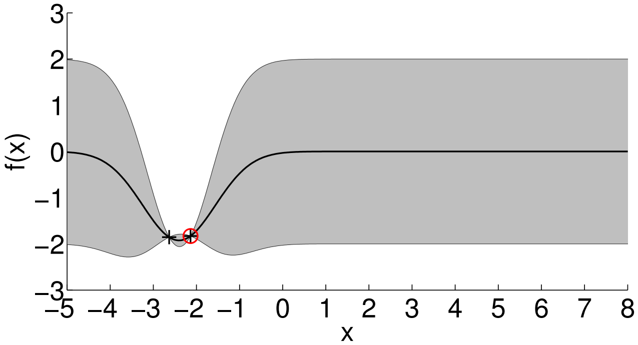

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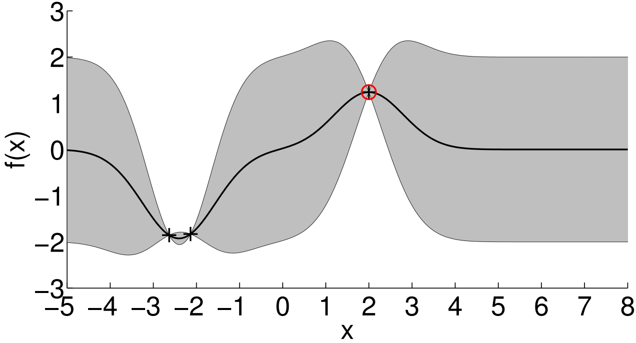

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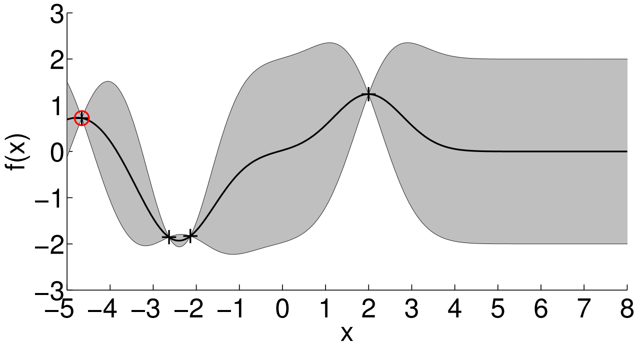

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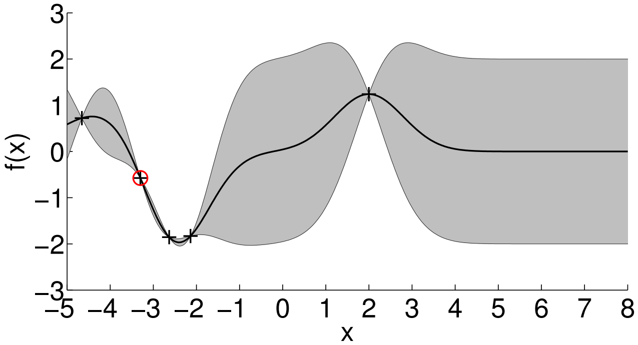

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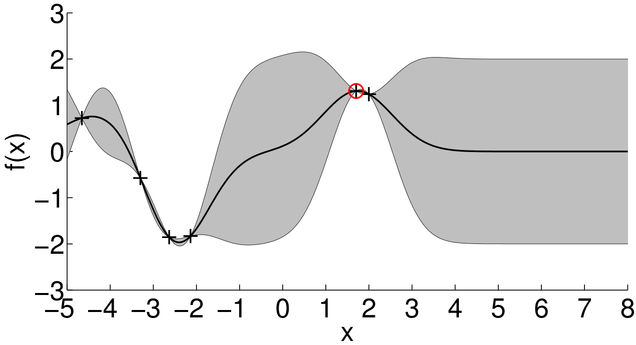

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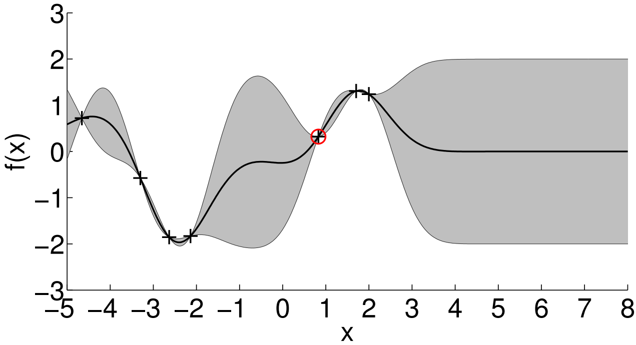

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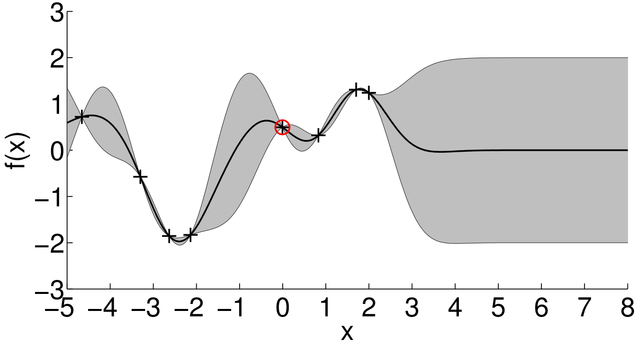

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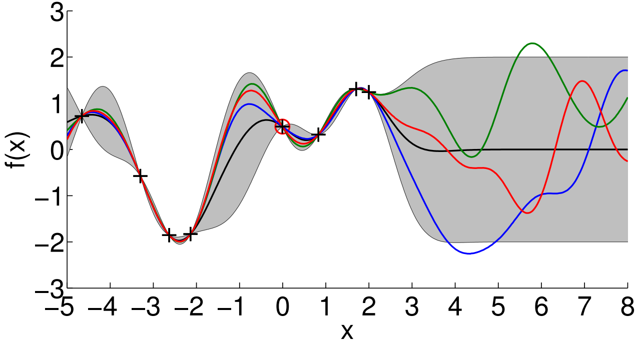

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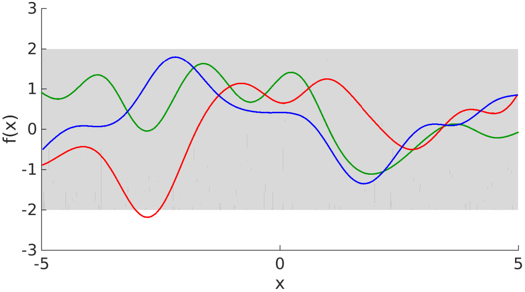
Covariance Function

- 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

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

- σ_f: Amplitude of the latent function



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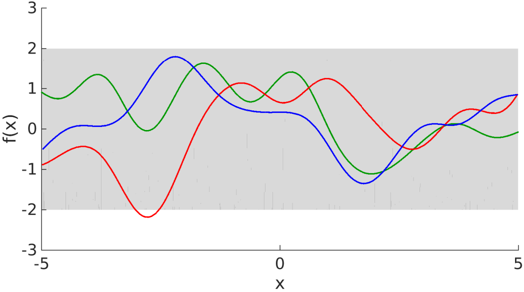
- ℓ: Length-scale. How far do we have to move in input space before the function value changes significantly, i.e., when do function values become uncorrelated?

  Smoothness parameter



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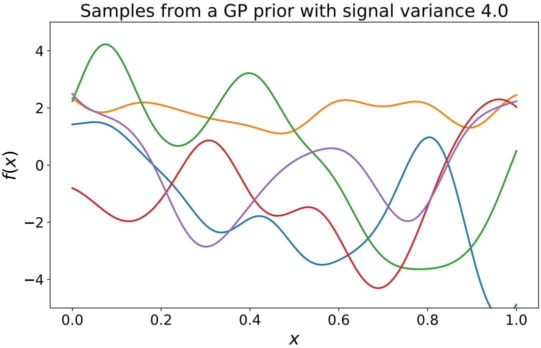

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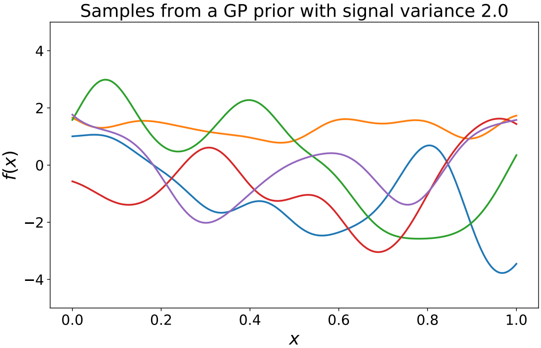

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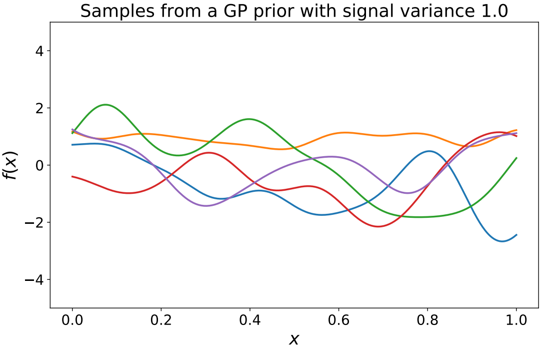

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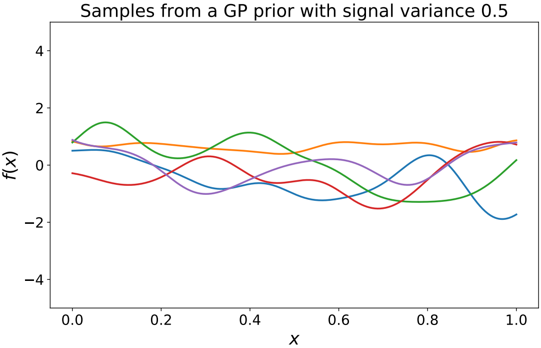

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Length-Scale ℓ

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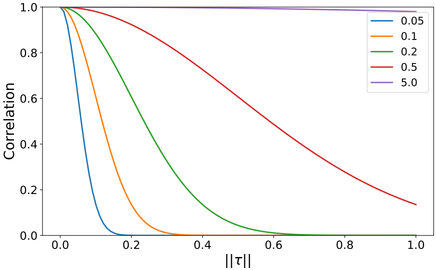
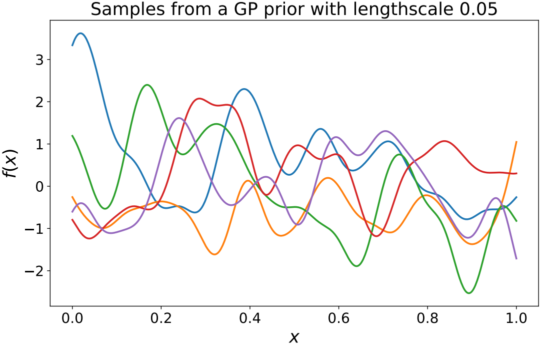


- How "wiggly" is the function?
- How much information we can transfer to other function values?
- How far do we have to move in input space from $\boldsymbol{x}$ to $\boldsymbol{x}'$ to make $f(\boldsymbol{x})$ and $f(\boldsymbol{x}')$ uncorrelated?

Length-Scale ℓ (2)

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



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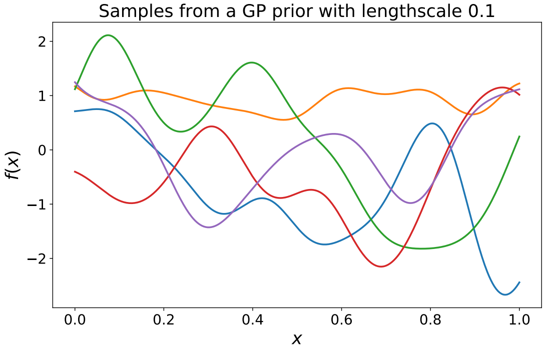

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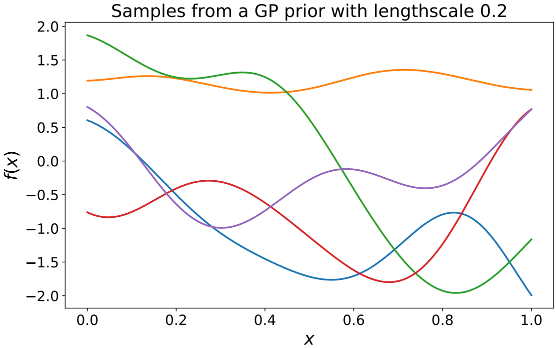

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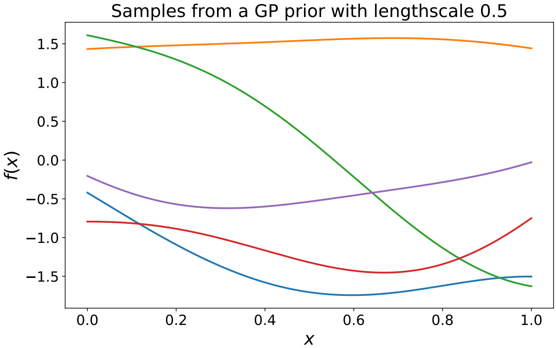

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Matérn Covariance Function

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

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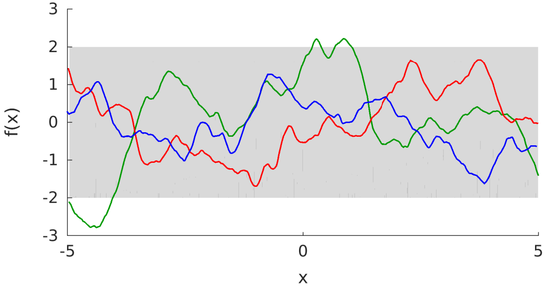


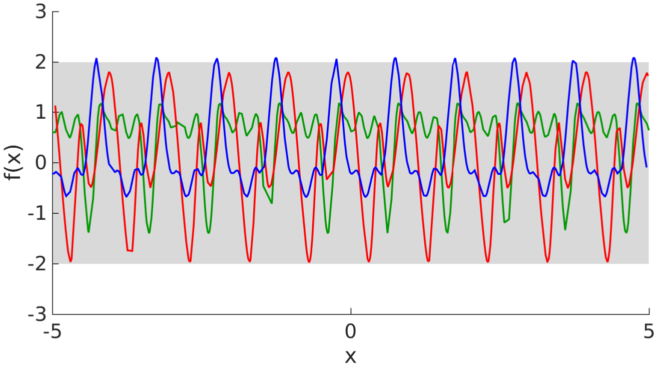
- Assumption on latent function: 1-times differentiable

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



Creating New Covariance Functions

Assume k_1 and k_2 are valid covariance functions and $u(\cdot)$ is a (nonlinear) transformation of the input space. Then

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Hyper-Parameters of a GP

The GP possesses a set of hyper-parameters:

- Parameters of the mean function
- 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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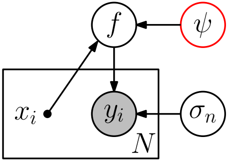
▶▶ Train a GP to find a good set of hyper-parameters

▶▶ 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 hyper-parameters $\boldsymbol{\theta}$ (kernel/mean function parameters $\boldsymbol{\psi}$, noise variance σ_n^2)



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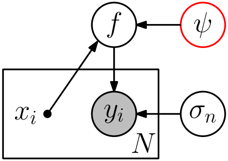

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Find good hyper-parameters $\boldsymbol{\theta}$ (kernel/mean function parameters $\boldsymbol{\psi}$, noise variance σ_n^2)

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- Posterior over hyper-parameters:

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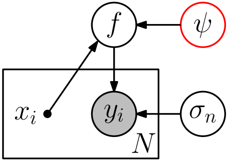

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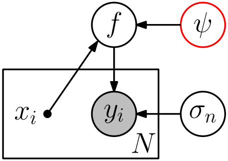

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▸▸ Maximize marginal likelihood if $p(\boldsymbol{\theta}) = \mathcal{U}$ (uniform prior)

Training via Marginal Likelihood Maximization

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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

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Marginal likelihood (with a prior mean function $m(\cdot) \equiv 0$):

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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

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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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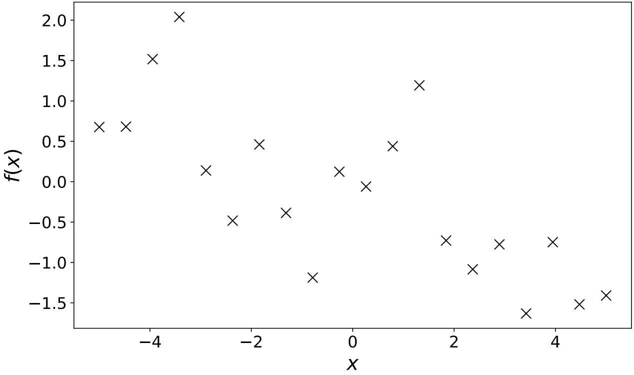
- Gradient-based optimization of hyper-parameters $\boldsymbol{\theta}$:

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

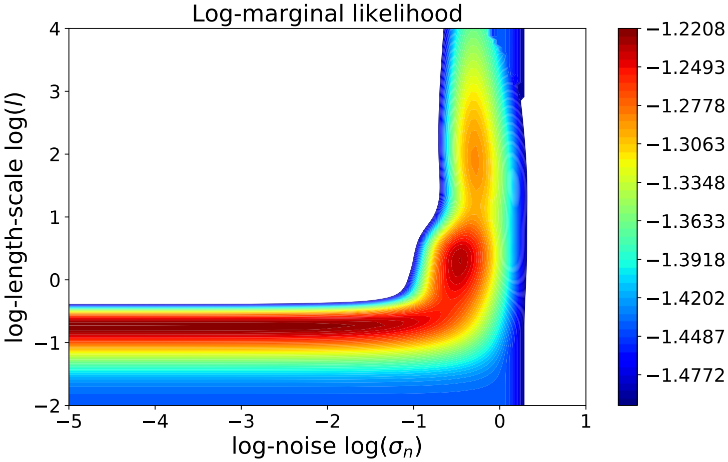
$$= \tfrac{1}{2}\operatorname{tr}\big((\boldsymbol{\alpha}\boldsymbol{\alpha}^\top - \boldsymbol{K}_{\boldsymbol{\theta}}^{-1})\frac{\partial \boldsymbol{K}_{\boldsymbol{\theta}}}{\partial \theta_i}\big)\,,$$

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

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 “hybrid” mode. Other modes are unlikely.
- Ideally, we would integrate the hyper-parameters out
  No closed-form solution ⏩ Markov chain Monte Carlo

Model Selection—Mean Function and Kernel

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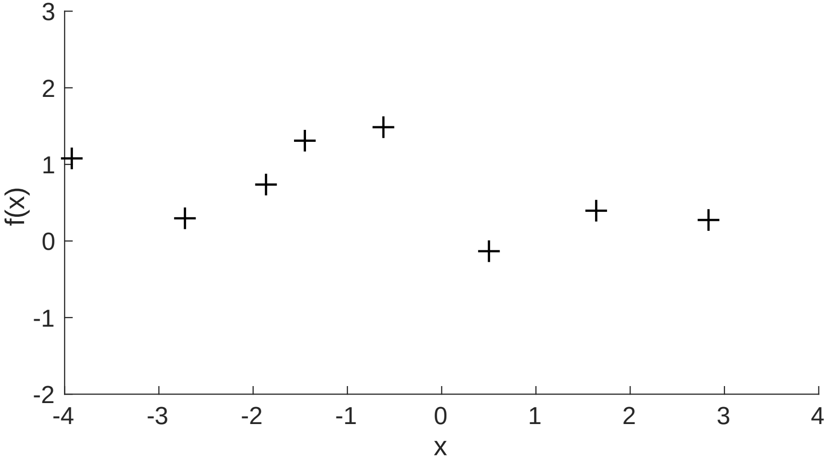
- Some options:
  - Cross validation
  - Bayesian Information Criterion, Akaike Information Criterion
  - Compare marginal likelihood values (assuming a uniform prior on the set of models)

Example



- Four different kernels (mean function fixed to $m \equiv 0$)
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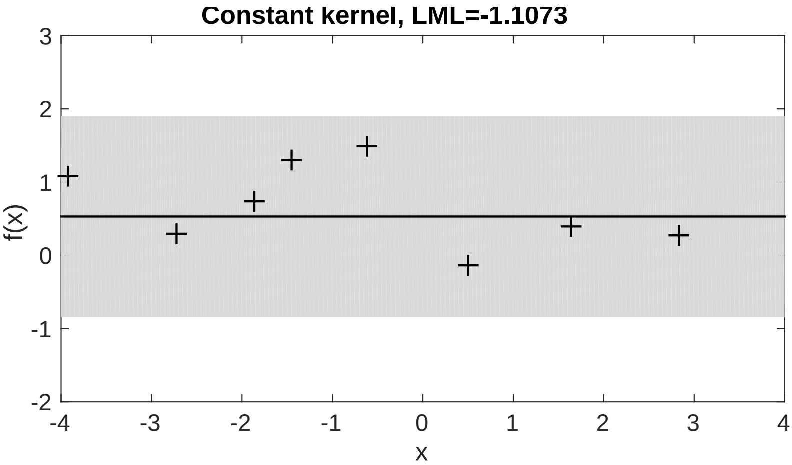

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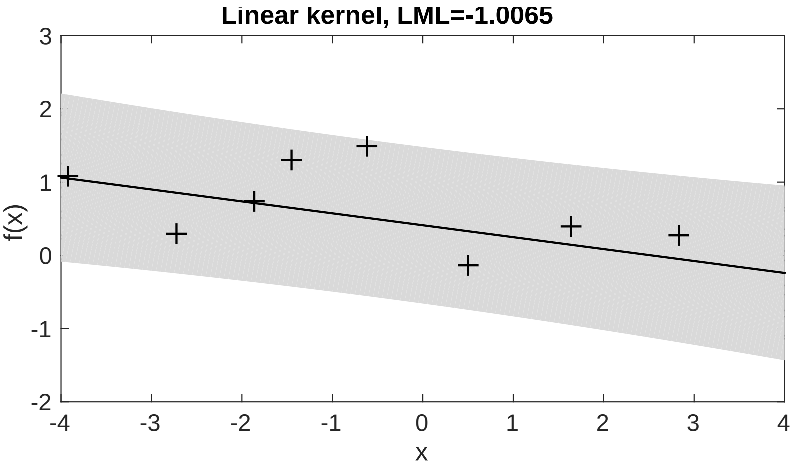

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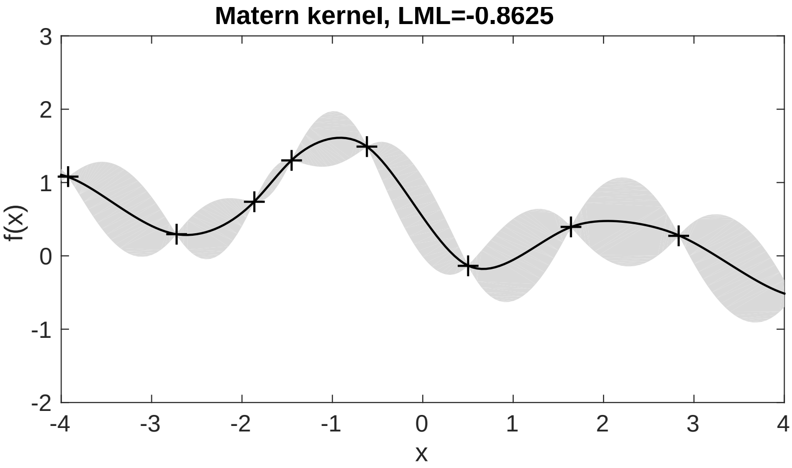

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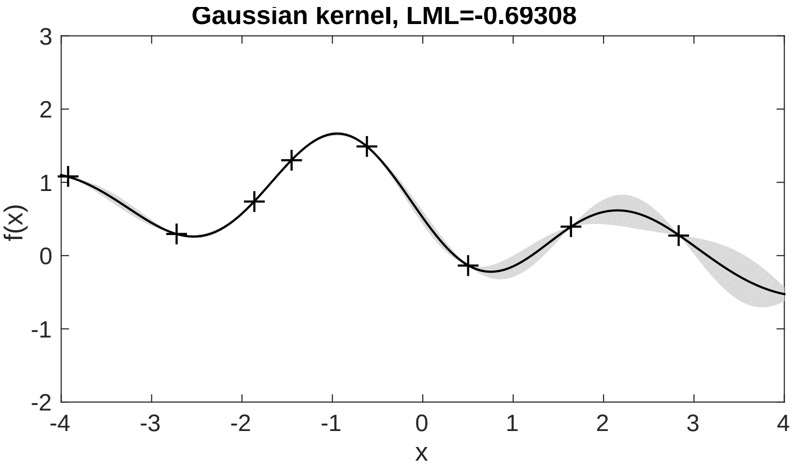

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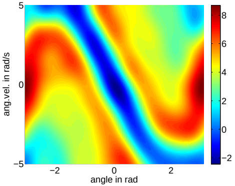
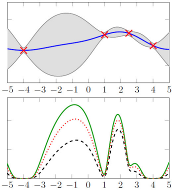
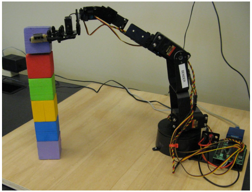
Application Areas







- 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 $\mathcal{O}(N^3)$
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- Memory requirement: $\mathcal{O}(ND + N^2)$

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Some solution approaches:

- Sparse GPs with inducing variables (e.g., Snelson & Ghahramani, 2006; Quiñonero-Candela & Rasmussen, 2005; Titsias 2009; Hensman et al., 2013; Matthews et al., 2016)
- Combination of local GP expert models (e.g., Tresp 2000; Cao & Fleet 2014; Deisenroth & Ng, 2015)

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- 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

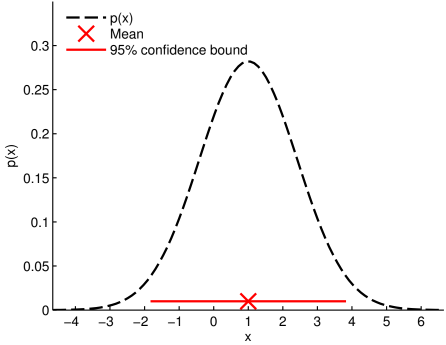
➤➤ `https://drafts.distill.pub/gp`

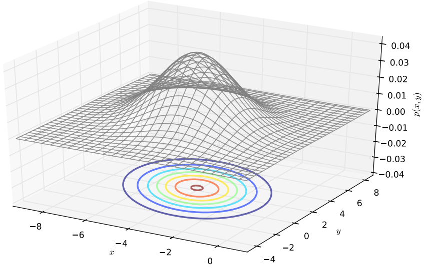
Appendix

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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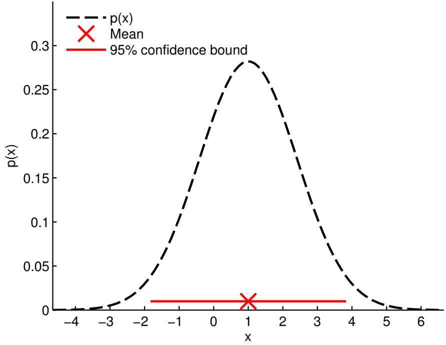

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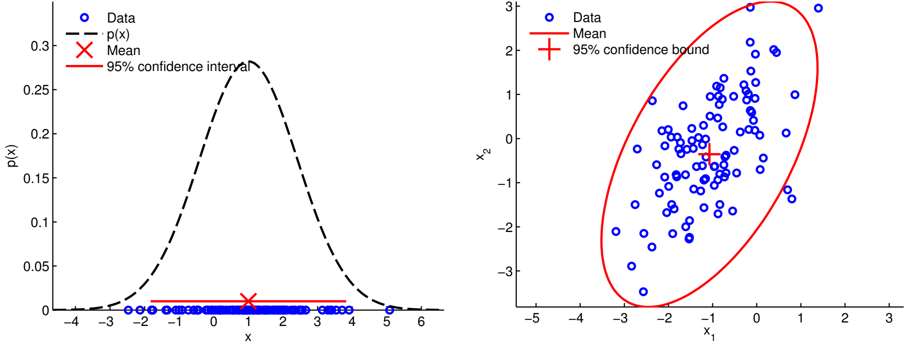
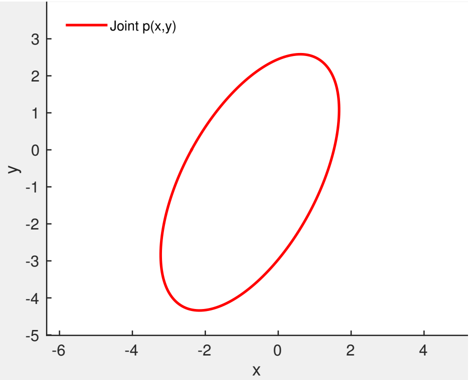


Conditional



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

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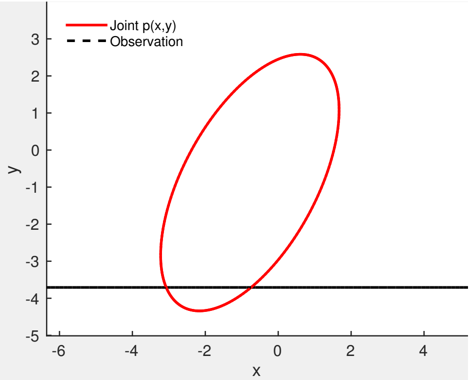

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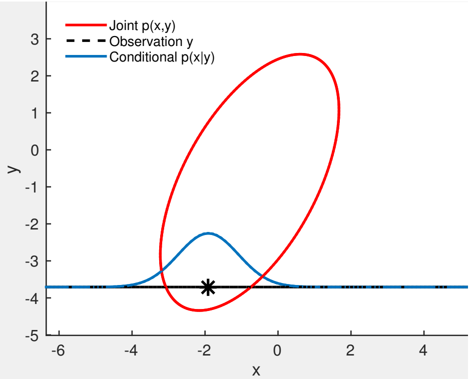

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$$p(\boldsymbol{x}|\boldsymbol{y}) = \mathcal{N}\left(\boldsymbol{\mu}_{x|y}, \boldsymbol{\Sigma}_{x|y}\right)$$

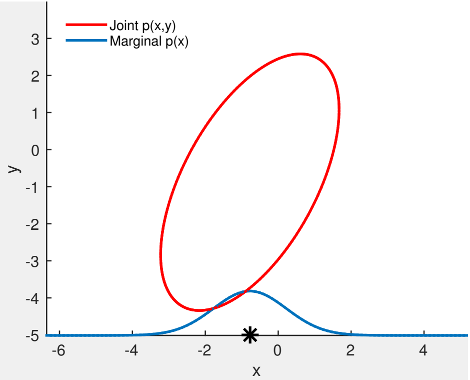
$$\boldsymbol{\mu}_{x|y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y)$$

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

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

▶▶ Computationally convenient

Marginal



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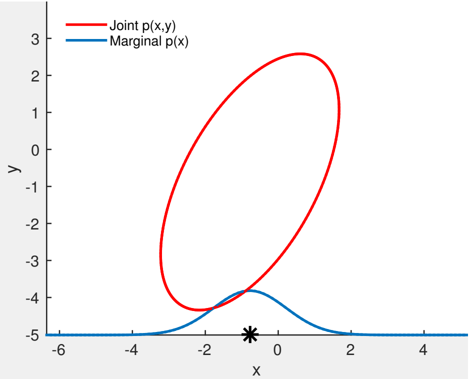

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- The marginal of a joint Gaussian distribution is Gaussian
- Intuitively: Ignore (integrate out) everything you are not interested in

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

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

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

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

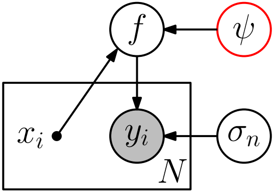
Gaussian Process Training: Hierarchical Inference

$\boldsymbol{\theta}$: Collection of all hyper-parameters

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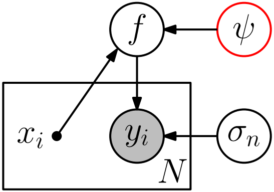
- Level-2 inference (posterior on $\boldsymbol{\theta}$)

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



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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