Gaussian Processes

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AIMS Rwanda and AIMS Ghana

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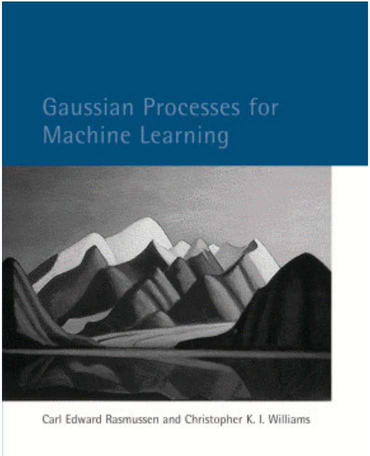
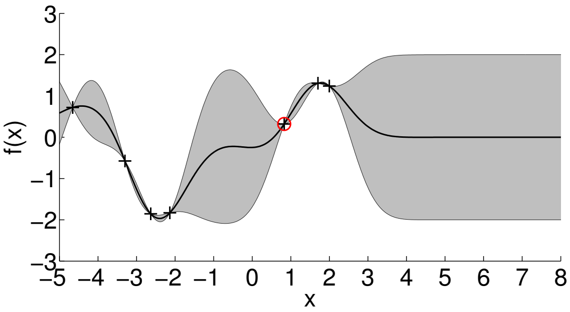
Reference



`http://www.gaussianprocess.org/`

Problem Setting



Objective

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

▶▶ Probabilistic regression problem

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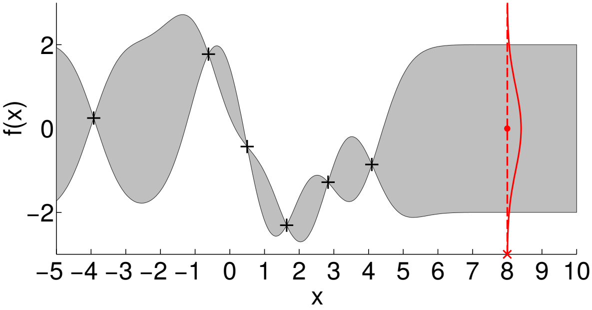

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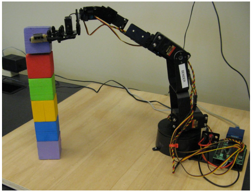
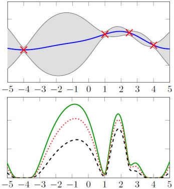
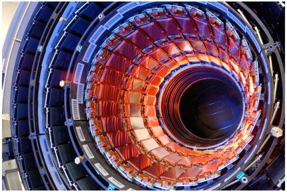
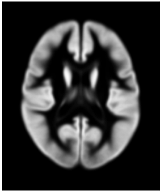






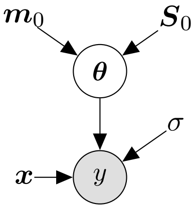


- Reinforcement learning and robotics
- Bayesian optimization (experimental design)
- Geostatistics
- Sensor networks
- Time-series modeling and forecasting
- High-energy physics
- Medical applications

Prior $p(\boldsymbol{\theta}) = \mathcal{N}\big(\boldsymbol{m}_0,\, \boldsymbol{S}_0\big)$

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

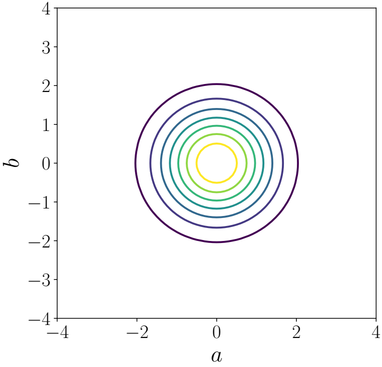
$$\implies y = \boldsymbol{\phi}^\top(\boldsymbol{x})\boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_n^2\big)$$



- Parameter $\boldsymbol{\theta}$ becomes a latent (random) variable
- Distribution $p(\boldsymbol{\theta})$ induces a distribution over plausible functions
- Choose a conjugate Gaussian prior
  - Gaussian posterior $p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}\big(\boldsymbol{\theta} \,|\, \boldsymbol{m}_N,\, \boldsymbol{S}_N\big)$
  - Closed-form computations (e.g., predictions, marginal likelihood)

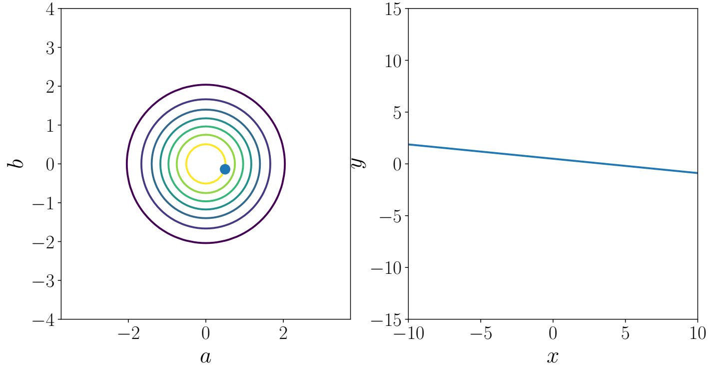
Consider a linear regression setting

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



Consider a linear regression setting

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



Sampling from the Posterior over Functions

Consider a linear regression setting

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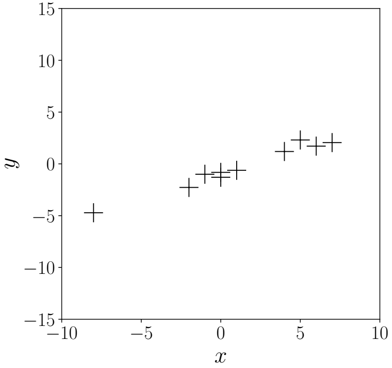
$$p(a,b) = \mathcal{N}\big(\mathbf{0},\, \boldsymbol{I}\big)$$

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



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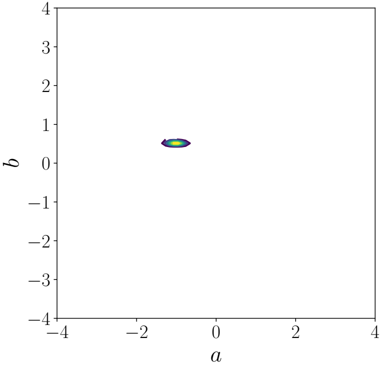
$$p(a, b) = \mathcal{N}\big(\mathbf{0},\, \boldsymbol{I}\big)$$
$$p(a, b|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}\big(\boldsymbol{m}_N,\, \boldsymbol{S}_N\big)$$

Posterior



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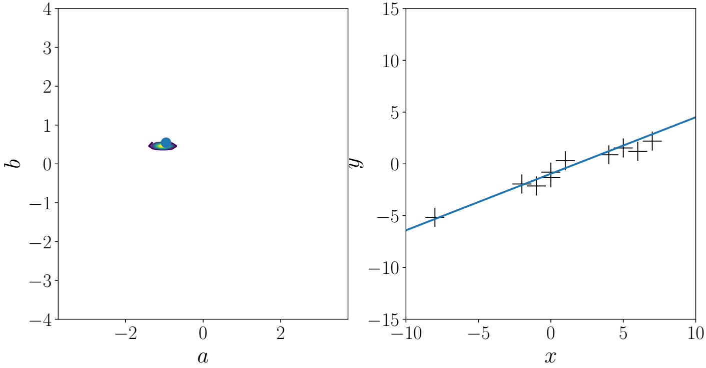
$$[a_i, b_i] \sim p(a, b|\boldsymbol{X}, \boldsymbol{y})$$

$$f_i = a_i + b_i x$$



Approach

- Instead of sampling parameters, which induce a distribution over functions, sample functions directly
  - Place a prior on functions
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▶▶ **Gaussian process**

Overview

1. Gaussian Process: Definition
2. Regression as Inference
   - GP Prior
   - Likelihood
   - Marginal Likelihood
   - Posterior
   - Predictions
3. Model Selection
   - GP Training
   - Hyper-Parameters
   - Inspection of the Marginal Likelihood
   - Covariance Function
4. Limitations and Guidelines
5. Application Areas

Gaussian Process: Definition

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.

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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) $k(\cdot, \cdot)$ ▶▶ More on this later

Regression as Inference

GP Regression as Bayesian Inference

Objective

For a set of observations $y_i = f(\boldsymbol{x}_i) + \epsilon, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_n^2\big)$, find a (posterior) distribution over functions $p(f(\cdot)|\boldsymbol{X}, \boldsymbol{y})$ 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

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

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Prior: $p(f(\cdot)) = GP(m, k)$ ▶▶ Specify mean m function and kernel k.

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

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Bayesian linear regression:

- Prior $p(\boldsymbol{\theta})$ on the parameters $\boldsymbol{\theta}$ allows us to encode some properties of the parameters (e.g., range, reasonable values, ...)
- Every sample $\boldsymbol{\theta}_i \sim p(\boldsymbol{\theta})$ induces a function $f_i(\cdot) := \boldsymbol{\theta}_i^\top \boldsymbol{\phi}(\cdot)$

GP Prior

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Gaussian process:

- GP prior: $p(f(\cdot))$
- Function plays the role of the parameters
  - ▶▶ Every sample $f_i(\cdot) \sim GP$ is a function

GP Prior (2)

- Bayesian prior specifies assumptions on the quantity of interest
- What assumptions could we make on the underlying function?
- What characterizes the function we want to model?

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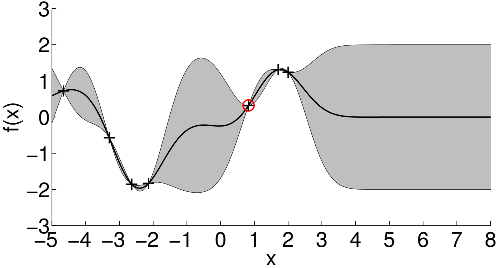
- What characterizes the function we want to model?
  - Mean function
  - Covariance function

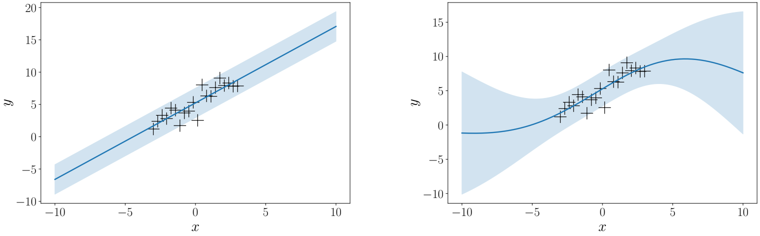
Mean Function



$$m(\boldsymbol{x}) = \mathbb{E}_f[f(\boldsymbol{x})], \quad f \sim GP$$

- The average function of the distribution over functions
- Allows us to bias the model (can make sense in application-specific settings)

Mean Function (2)



- Can be a parametrized function, e.g., linear, exponential, or neural network. Example: $m_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{\theta}^\top \boldsymbol{\phi}(\boldsymbol{x})$

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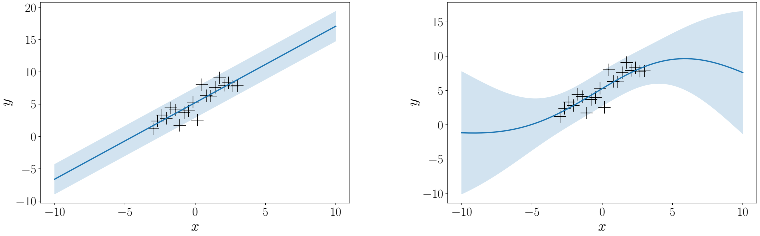

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- Can simplify the learning problem

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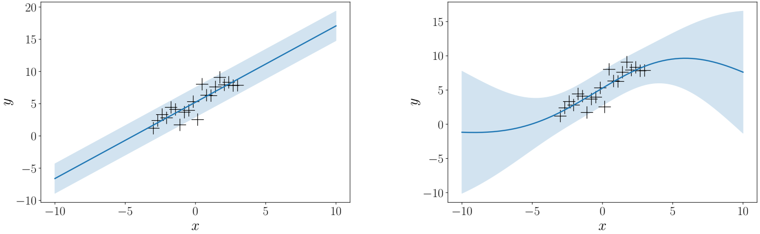

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- Can simplify the learning problem
- Often: “Agnostic” mean function in the absence of data or prior knowledge: $m(\cdot) \equiv 0$ everywhere (for symmetry reasons)

Covariance Function

- Covariance function (kernel) is symmetric and positive semi-definite

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- Compute covariances/correlations between (unknown) function values by just looking at the corresponding inputs:

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

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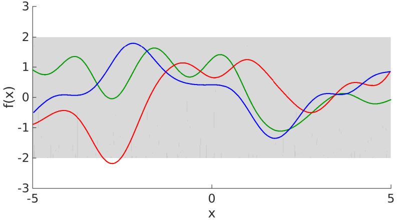
  ▸▸ Kernel trick (Schölkopf & Smola, 2002)
- Encodes high-level structural assumptions (e.g., smoothness, periodicity) of the function we want to model

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

- Assumption on latent function: Smooth (∞ differentiable)



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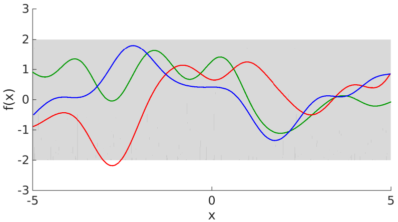

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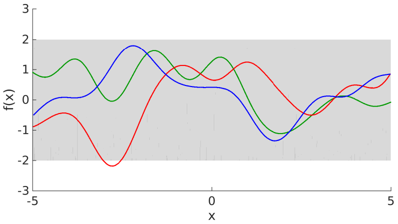
- Assumption on latent function: Smooth (∞ differentiable)
- σ_f: Amplitude of the latent function
- ℓ: Length-scale. How far do we have to move in input space before the function value changes significantly, i.e., when do function values become uncorrelated?

  ▶▶ **Smoothness parameter**



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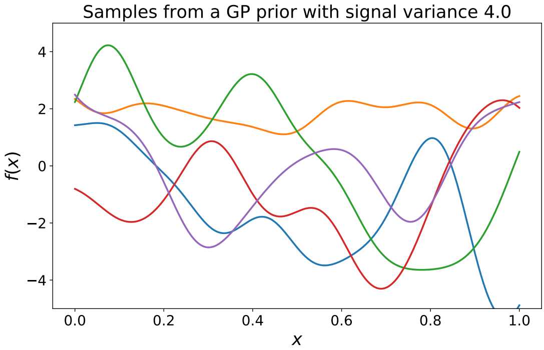

- Controls the amplitude (vertical magnitude) of the function we wish to model

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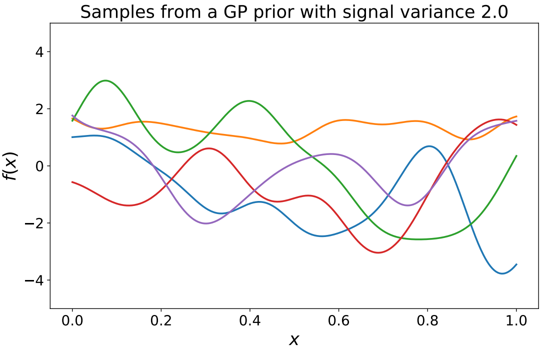

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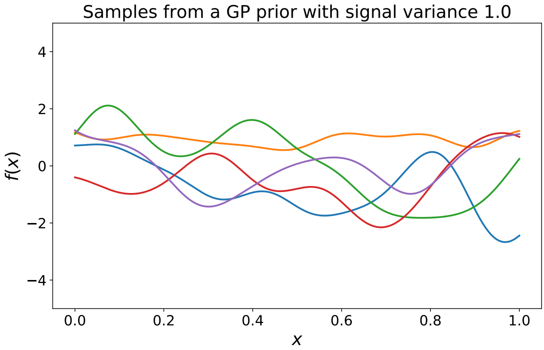

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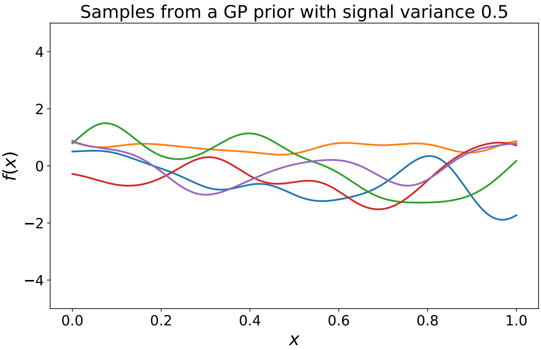

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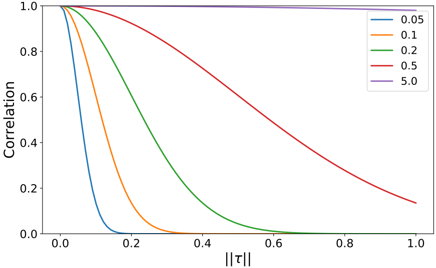
Length-Scale ℓ

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

- How “wiggly” is the function?
- How much information we can transfer to other function values?
  - ▸▸ Correlation between function values
- How far do we have to move in input space from x to x' to make $f(x)$ and $f(x')$ uncorrelated?

Length-Scale ℓ (2)

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



- Correlation between function values $f(\boldsymbol{x})$ and $f(\boldsymbol{x}')$ depends on the (scaled) distance $\|\tau\|/\ell = \|\boldsymbol{x} - \boldsymbol{x}'\|/\ell$ of the corresponding inputs.
- What does a short/long length-scale ℓ imply?

Length-Scale ℓ (3)

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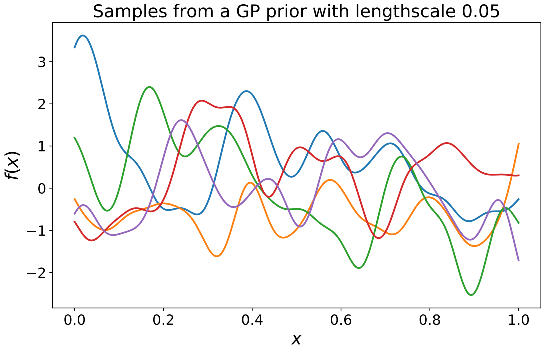

▶▶ Explore interactive diagrams at **https://drafts.distill.pub/gp/**

Length-Scale ℓ (3)

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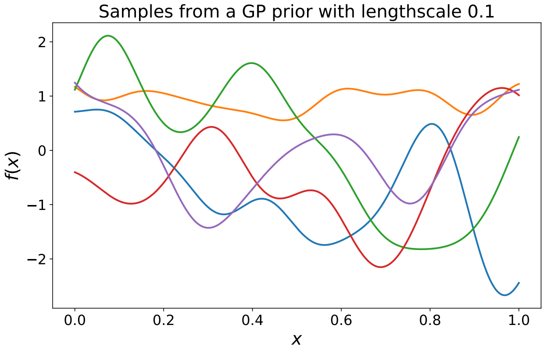

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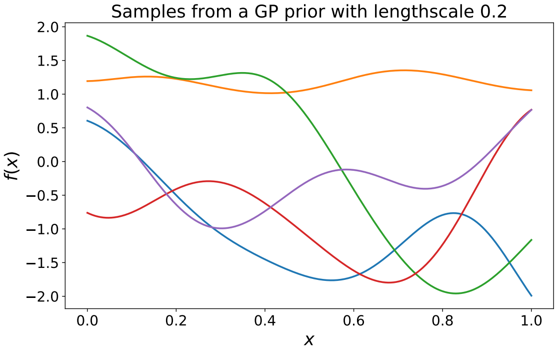

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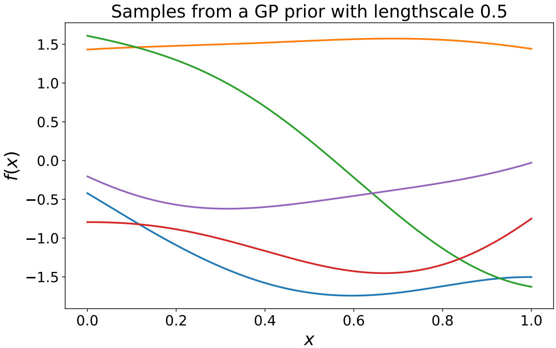

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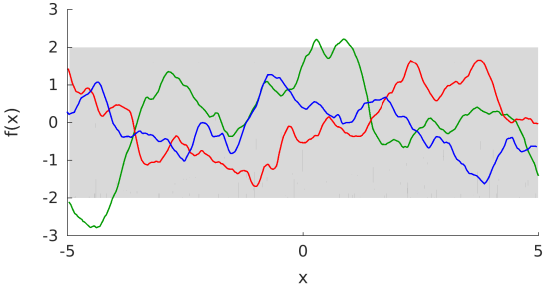
Matérn Covariance Function

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

- Assumption on latent function: 1-times differentiable
- 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?

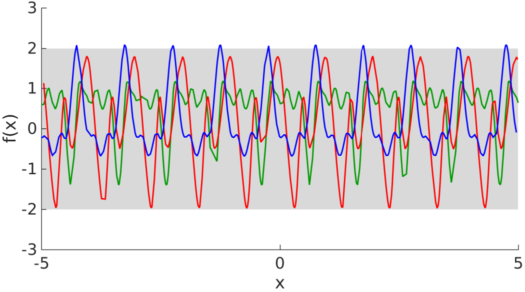


Periodic Covariance Function

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

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

- Assumption on latent function: periodic
- Periodicity parameter κ



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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Gaussian likelihood in Gaussian processes:

$$p(y|f(\boldsymbol{x})) = \mathcal{N}\big(y \,|\, f(\boldsymbol{x}),\, \sigma_n^2\big)$$

- Intuition: Parameters are the function f itself

Marginal Likelihood

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

Bayesian linear regression with a Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{0},\, \boldsymbol{I})$:

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- Expected likelihood (under the parameter prior)
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Marginal Likelihood (2)

Gaussian process marginal likelihood

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$$\log p(\boldsymbol{y}|\boldsymbol{X}) = -\frac{1}{2}\boldsymbol{y}^\top(\boldsymbol{K} + \sigma_n^2\boldsymbol{I})^{-1}\boldsymbol{y} - \frac{1}{2}\log|\boldsymbol{K} + \sigma_n^2\boldsymbol{I}| - \frac{N}{2}\log(2\pi)$$

$$K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j), \quad i, j = 1, \ldots, N$$

GP Posterior

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

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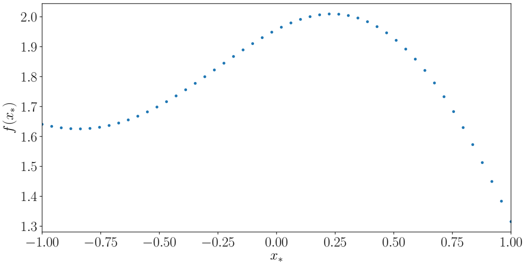

Sampling from the GP Prior

- GP is a distribution over functions
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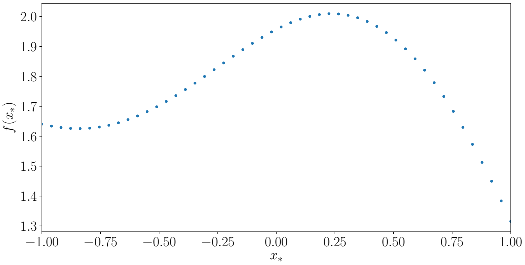
- In practice, we cannot sample functions directly
- Instead: function = collection of function values
- Determine function values at a finite set of input locations $\boldsymbol{X}_* = [\boldsymbol{x}_*^{(1)}, \ldots, \boldsymbol{x}_*^{(K)}]$



Sampling from the GP Prior (2)

- Without any training data, the predictive distribution at test points $\boldsymbol{X}_*$ is

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- Exploited: Definition of GP that all function values are jointly Gaussian distributed
- Generate "function draws" (samples from the GP prior)

$$
f_k(\boldsymbol{X}_*) \sim \mathcal{N}\big(m_{\text{prior}}(\boldsymbol{X}_*),\ k_{\text{prior}}(\boldsymbol{X}_*, \boldsymbol{X}_*)\big)
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- Goal: Generate random functions f_k, so that

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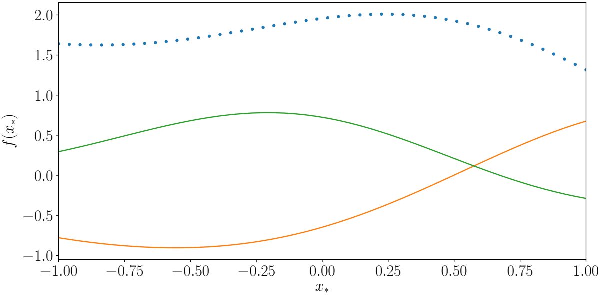

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- Define $\boldsymbol{m}_* := m_{\text{prior}}(\boldsymbol{X}_*)$ and $\boldsymbol{K}_{**} := k_{\text{prior}}(\boldsymbol{X}_*, \boldsymbol{X}_*)$. Then

$$f_k(\boldsymbol{X}_*) \sim \mathcal{N}\big(\boldsymbol{m}_*,\, \boldsymbol{K}_{**}\big)$$

▶▶ Sample from a multivariate Gaussian

GP Predictions (Posterior)

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

- **Objective:** Find $p(f(\boldsymbol{X}_*)|\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*)$ for training data $\boldsymbol{X}, \boldsymbol{y}$ and test inputs $\boldsymbol{X}_*$.
- GP prior at training inputs: $p(f|\boldsymbol{X}) = \mathcal{N}\big(m(\boldsymbol{X}),\, \boldsymbol{K}\big)$
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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 Posterior Predictions

Prior evaluated at $\boldsymbol{X}, \boldsymbol{X}_*$:

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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:

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

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

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Sanity Check

- GP posterior (from earlier):

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

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

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

- GP posterior predictions at $\boldsymbol{X}_*$:

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

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Sanity Check

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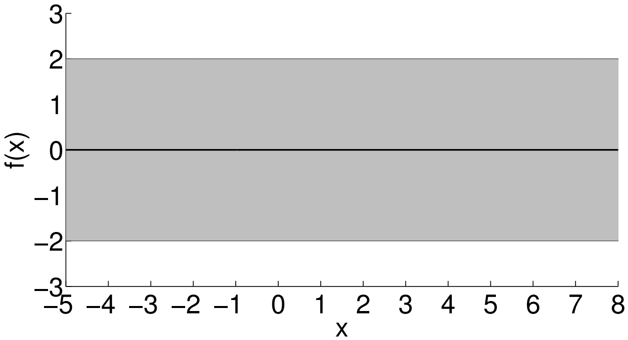
Predictions

Make predictions by evaluating the GP posterior mean and covariance function at a finite number of inputs $\boldsymbol{X}_*$

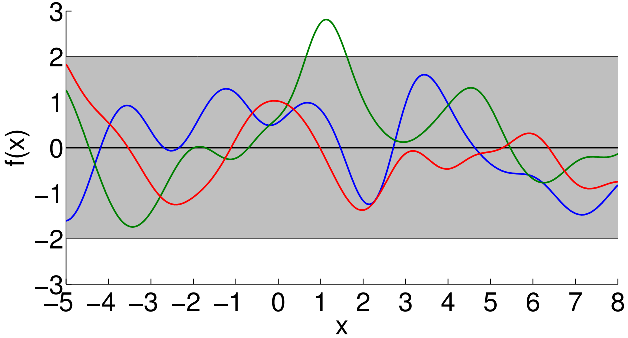


Prior belief about the function

Predictive (marginal) mean and variance:

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

Illustration: Inference with Gaussian Processes



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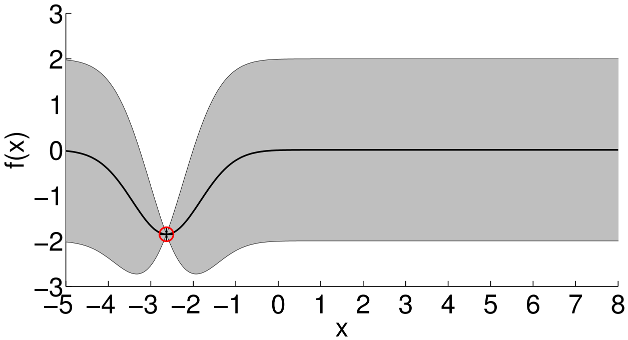

Posterior belief about the function

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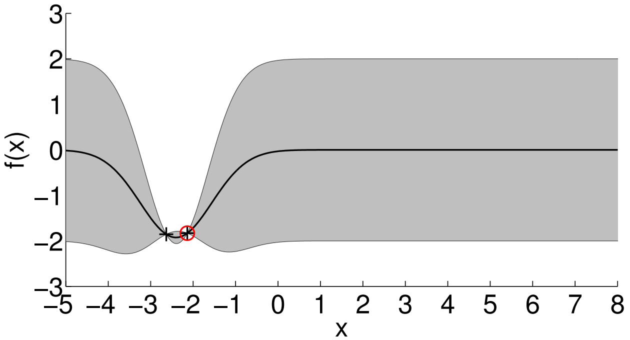

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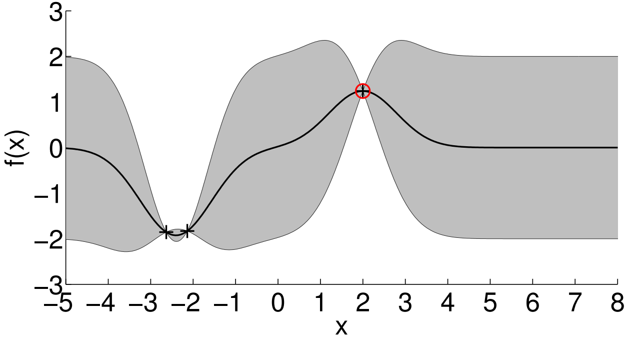

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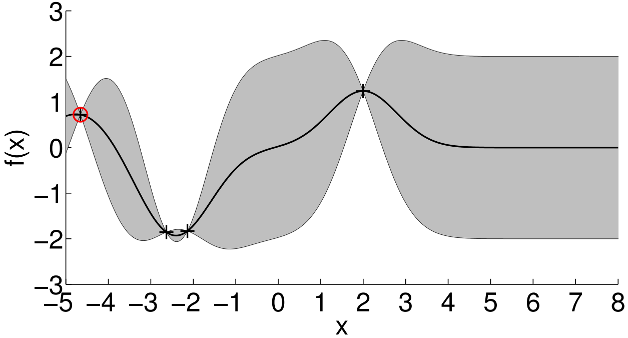

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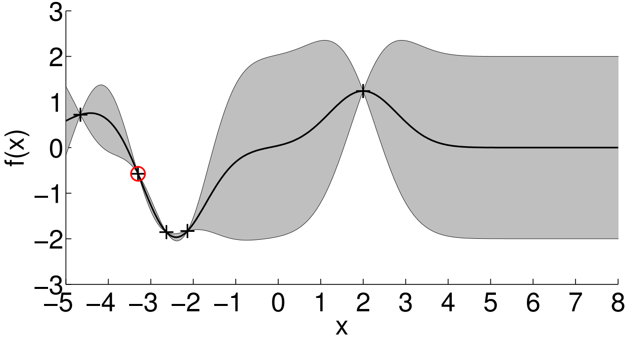

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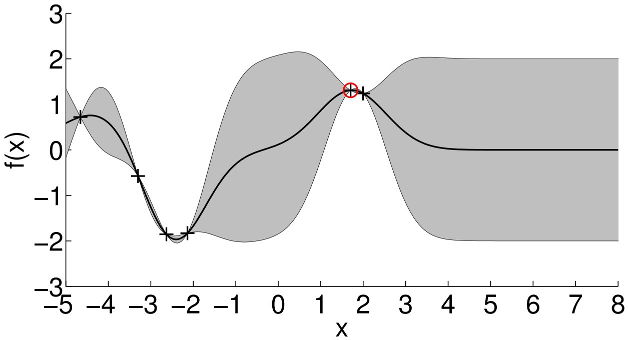

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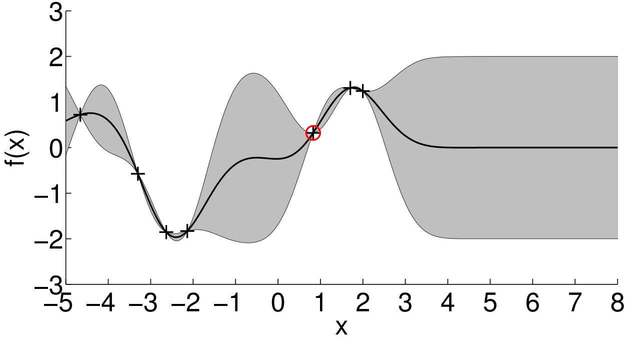

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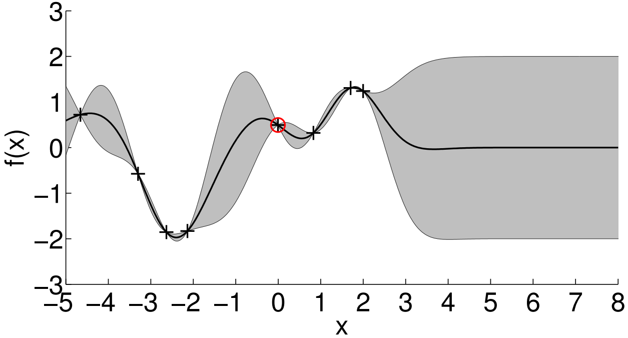

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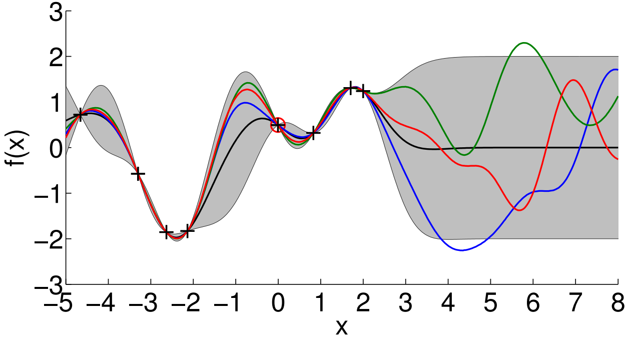

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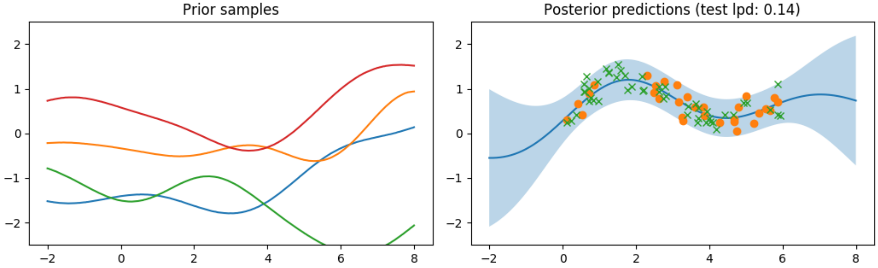
Model Selection

Influence of Prior on Posterior



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for different length-scales ℓ and different datasets

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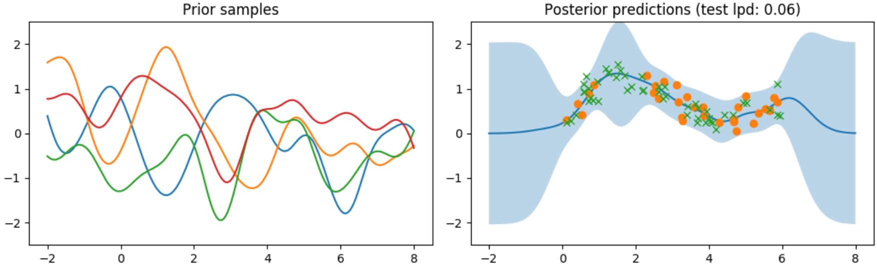

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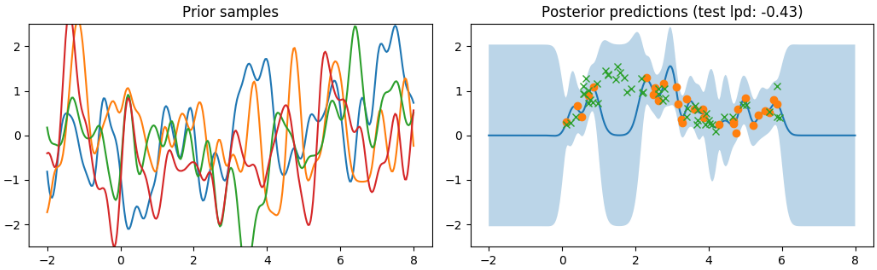

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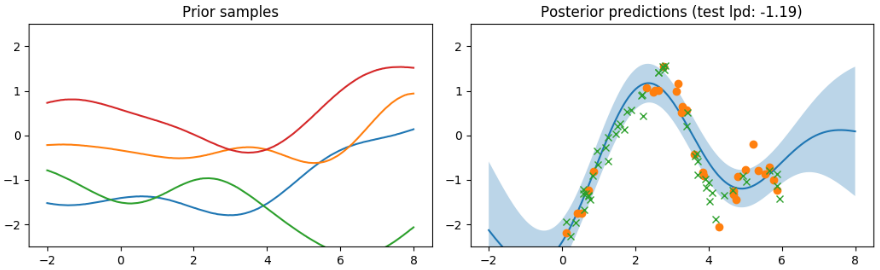

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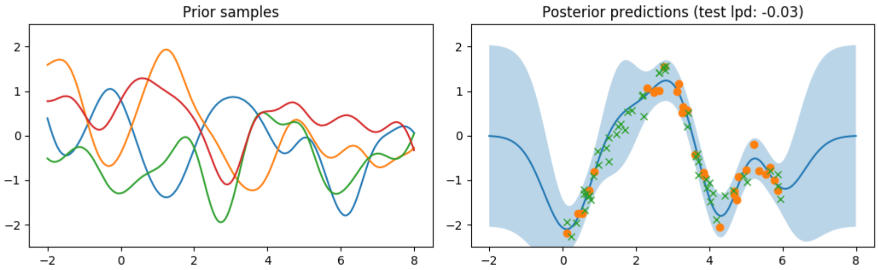

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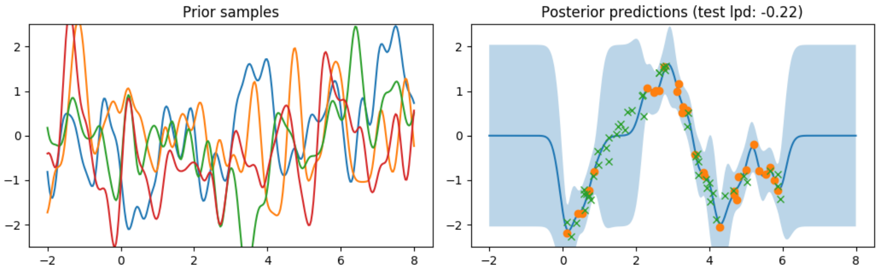

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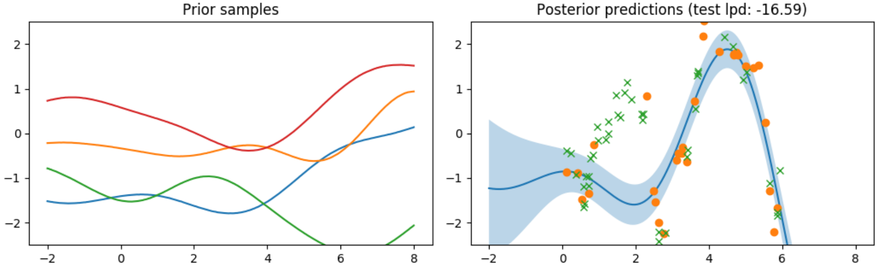

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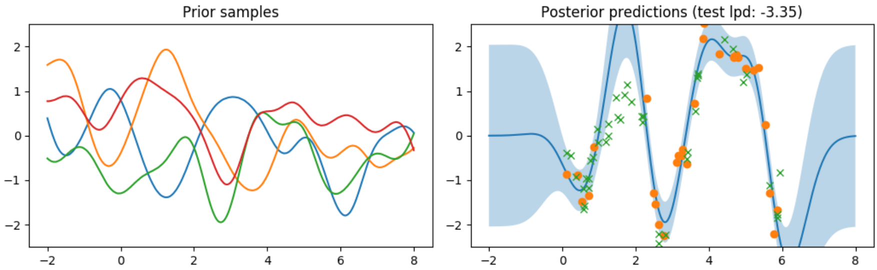

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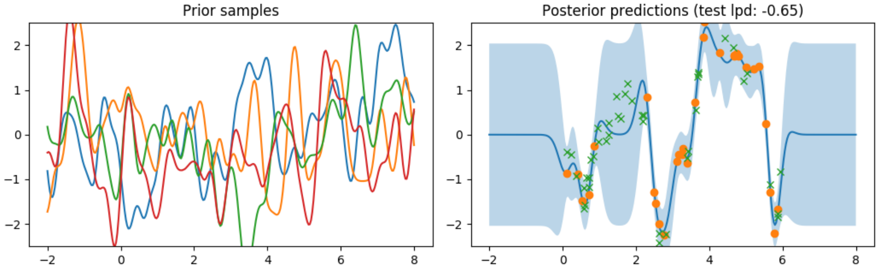

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How do we select a good prior?

Model Selection in GPs

- Choose hyper-parameters of the GP
- Choose good mean function and kernel

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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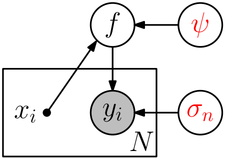
▸▸ Higher-level model selection to find good mean and covariance functions
(can also be automated: Automatic Statistician (Lloyd et al., 2014))

GP Training

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



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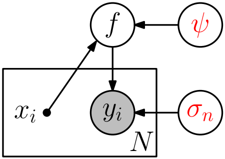

- Place a prior $p(\boldsymbol{\theta})$ on hyper-parameters
- Posterior over hyper-parameters:

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

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

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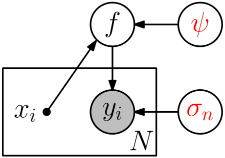

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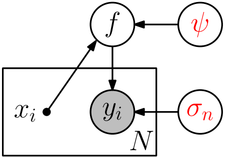

- Choose hyper-parameters $\boldsymbol{\theta}^*$, such that

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Gaussian Process Training: Hyper-Parameters

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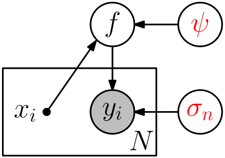

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▶▶ Maximize marginal likelihood if $p(\boldsymbol{\theta}) = \mathcal{U}$ (uniform prior)

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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Learning the GP hyper-parameters:

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\boldsymbol{\theta}^* \in \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})
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- Log-marginal likelihood:

$$\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) = -\tfrac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}_{\boldsymbol{\theta}}^{-1}\boldsymbol{y} - \tfrac{1}{2}\log|\boldsymbol{K}_{\boldsymbol{\theta}}| + \text{const}$$

$$\boldsymbol{K}_{\boldsymbol{\theta}} := \boldsymbol{K} + \sigma_n^2 \boldsymbol{I}$$

Gradient-based Optimization

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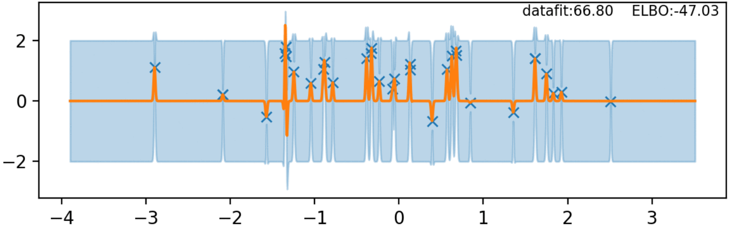
- Gradient-based optimization to get hyper-parameters $\boldsymbol{\theta}^*$:

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

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

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

Marginal Likelihood Illustration[1]



- "ELBO" refers to the log-marginal likelihood
- Data-fit term gets worse, but marginal likelihood increases

[1] Thanks to Mark van der Wilk

Inspecting the Marginal Likelihood

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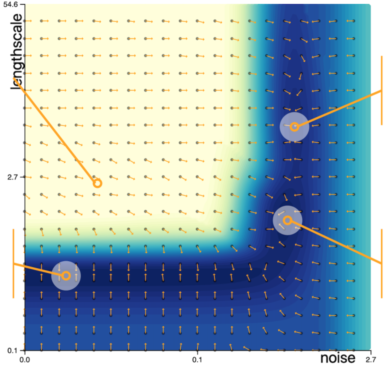
Marginal likelihood

▸▸ Automatic trade-off between data fit and model complexity

Marginal Likelihood Surface



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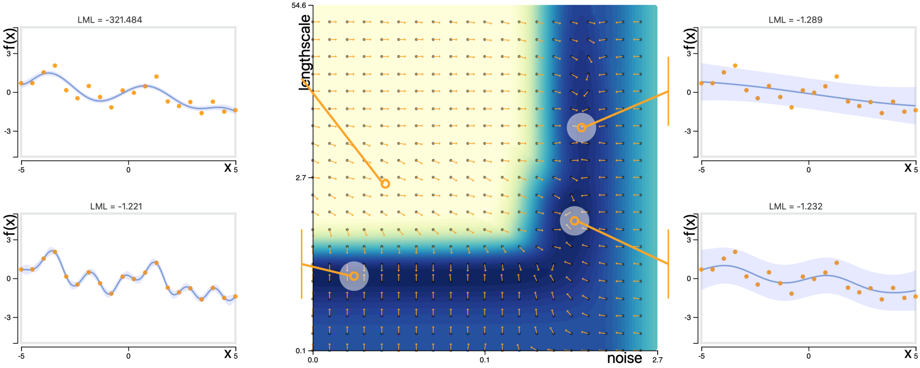

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https://drafts.distill.pub/gp/

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- Ideally, we would integrate the hyper-parameters out
  No closed-form solution ⏩ Markov chain Monte Carlo

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- Marginal likelihood seems to find a good balance between fitting the data and finding a simple model (Occam's razor)

Why does the marginal likelihood lead to models that generalize well?

Marginal Likelihood: Incremental Prediction

- "Probability of the training data" given the parameters
- General factorization (ignoring inputs $\boldsymbol{X}$):

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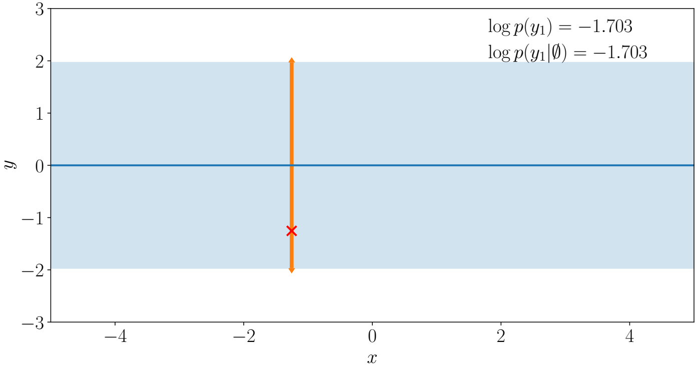
  ▶▶ Proxy for generalization error on unseen test data

Marginal Likelihood: Illustration



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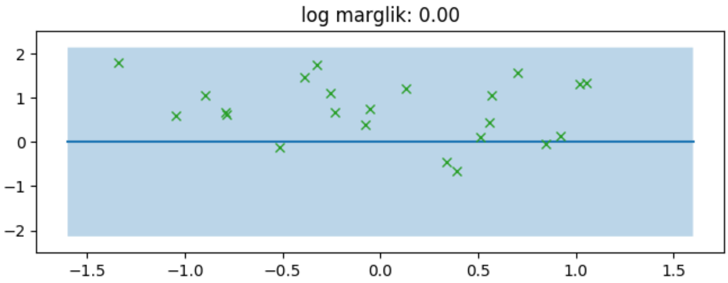
Marginal Likelihood Computation in Action[2]



- Short length-scale

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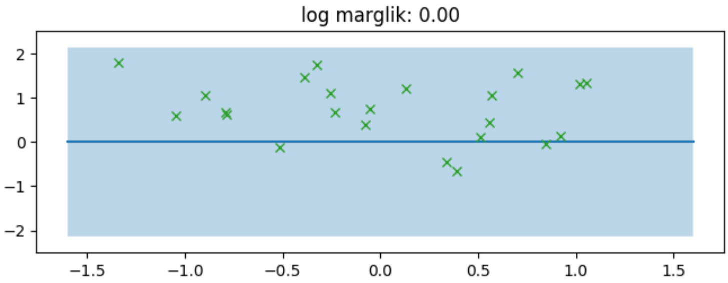
Marginal Likelihood Computation in Action[3]



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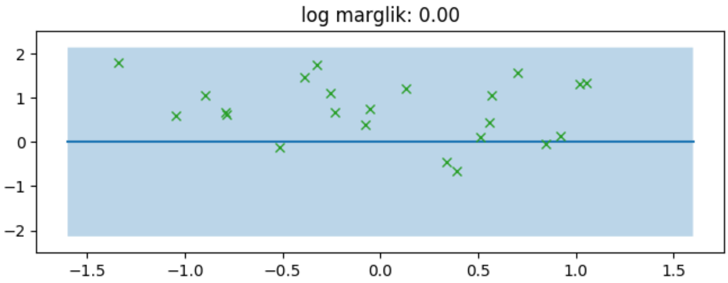

- Optimal length-scale

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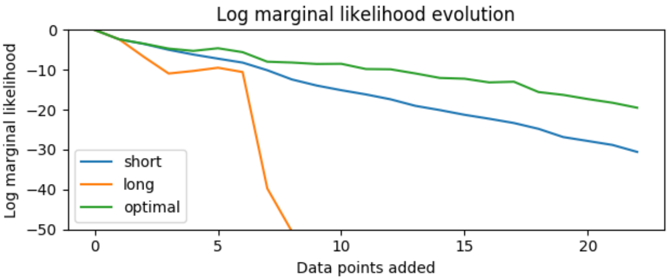
Marginal Likelihood Evolution



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  - No high density, even with observations inside the error bars

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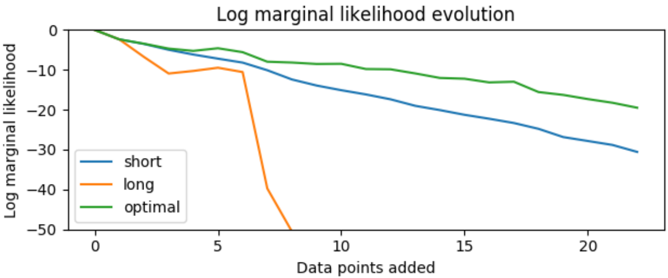

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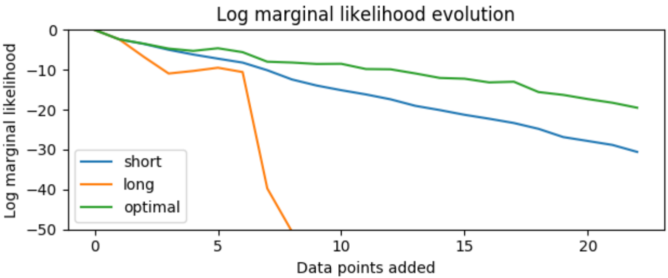


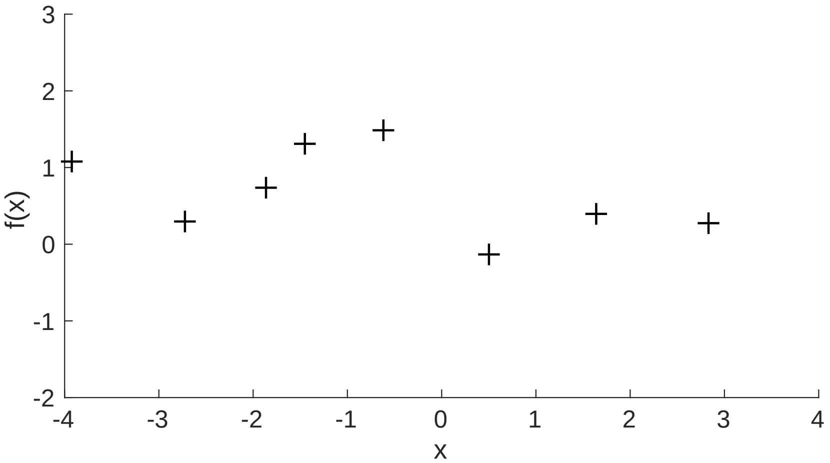
- Short lengthscale: consistently overestimates variance
  - No high density, even with observations inside the error bars
- Long lengthscale: consistently underestimates variance
  - Low density because observations are outside the error bars
- Optimal lengthscale: trades off both behaviors reasonably well

- 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?

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?
- 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 $m \equiv 0$)
- MAP hyper-parameters for each kernel
- Log-marginal likelihood values for each (optimized) model

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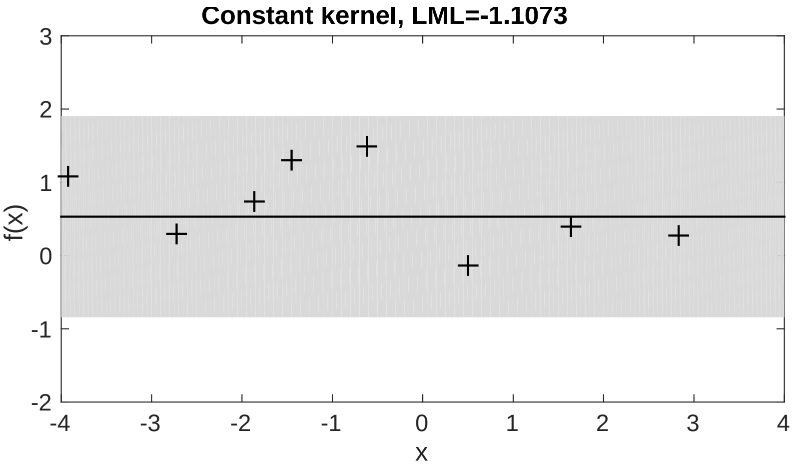

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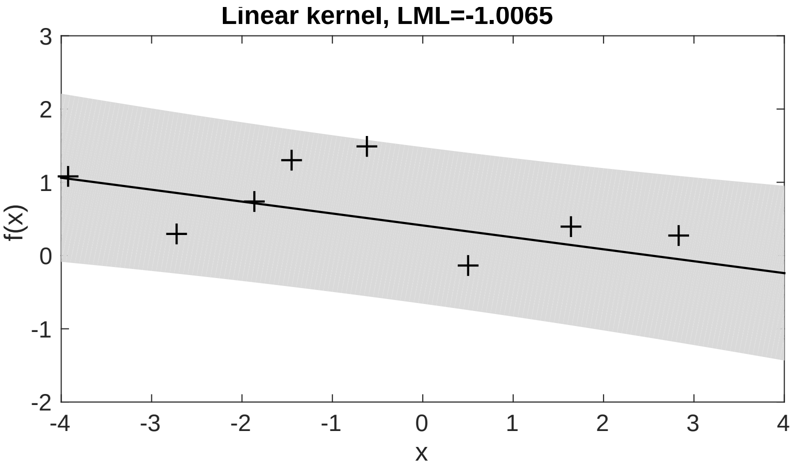

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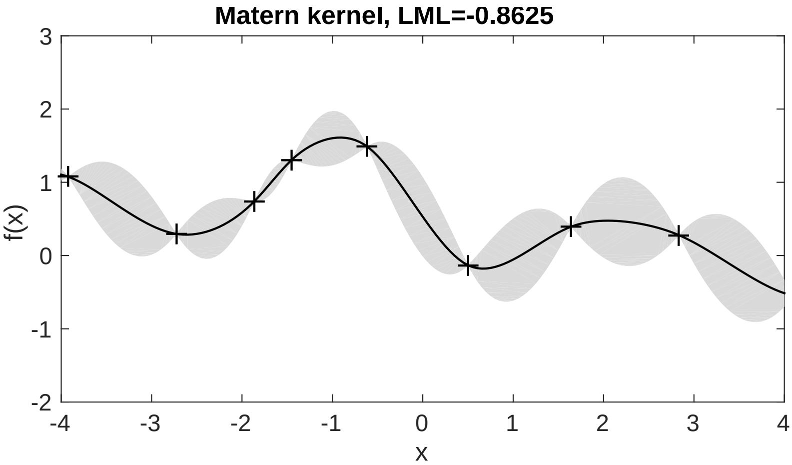

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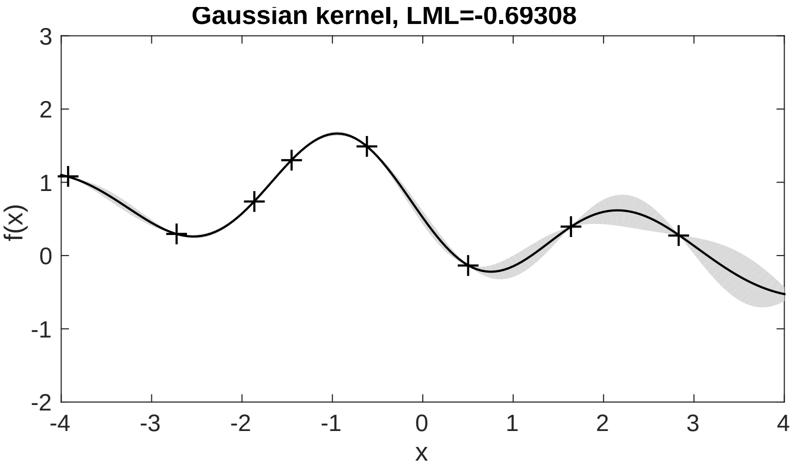

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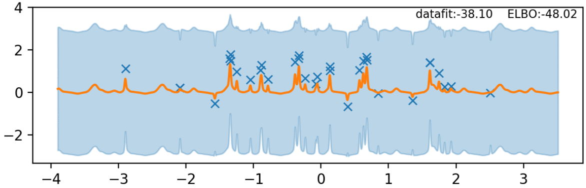
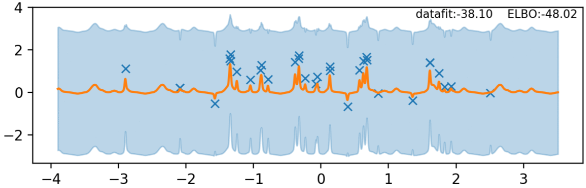


- Prior: $f(\boldsymbol{x}) = \theta_s f_{\text{smooth}}(\boldsymbol{x}) + \theta_p f_{\text{periodic}}(\boldsymbol{x})$, with smooth and periodic GP priors, respectively.

[5] Thanks to Mark van der Wilk

GP Training: Illustration[5]



- Prior: $f(\boldsymbol{x}) = \theta_s f_{\text{smooth}}(\boldsymbol{x}) + \theta_p f_{\text{periodic}}(\boldsymbol{x})$, with smooth and periodic GP priors, respectively.
- Amount of periodicity vs. smoothness is automatically chosen by selecting hyper-parameters θ_s, θ_p.
- Marginal likelihood learns how to generalize, not just to fit the data

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Limitations and Guidelines

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** $N \approx 10,000$

Limitations of Gaussian Processes

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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)
- Variational Fourier features (Hensman et al., 2018)

Tips and Tricks for Practitioners

- To set initial hyper-parameters, use domain knowledge.

⏩ `https://drafts.distill.pub/gp`

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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

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Application Areas

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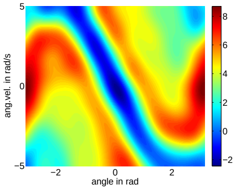
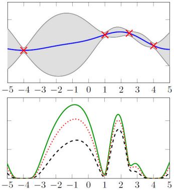
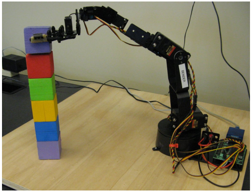
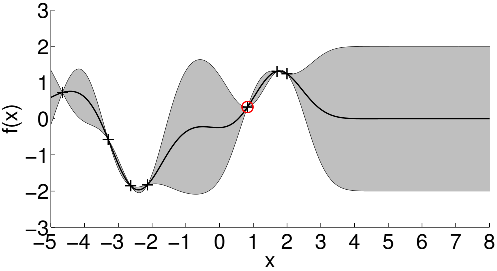
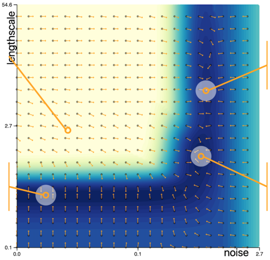






- Reinforcement learning and robotics
  - Model value functions and/or dynamics with GPs
- Bayesian optimization (Experimental Design)
  - Model unknown utility functions with GPs
- Geostatistics
  - Spatial modeling (e.g., landscapes, resources)
- Sensor networks
- Time-series modeling and forecasting





- Gaussian processes are the gold-standard for regression
- Closely related to Bayesian linear regression
- Computations boil down to manipulating multivariate Gaussian distributions
- Marginal likelihood objective automatically trades off data fit and model complexity

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