Gaussian Processes

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Creative Machine Learning

Sargent Centre Summer School

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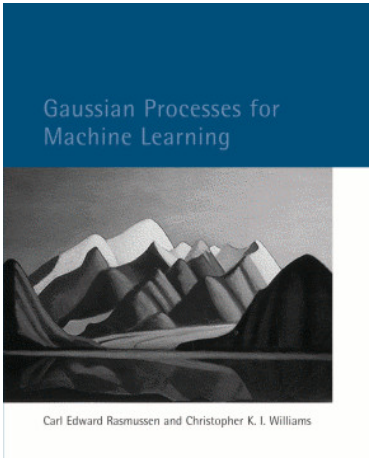
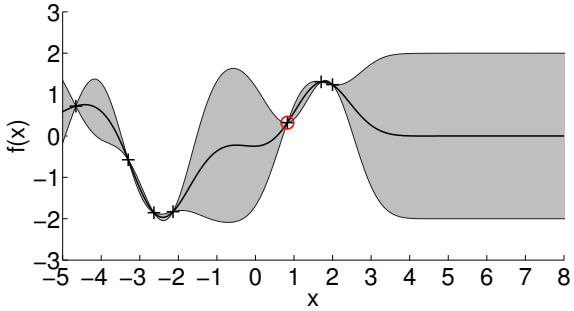
Reference



http://www.gaussianprocess.org/

Problem Setting



Objective

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

⏩ Probabilistic regression problem

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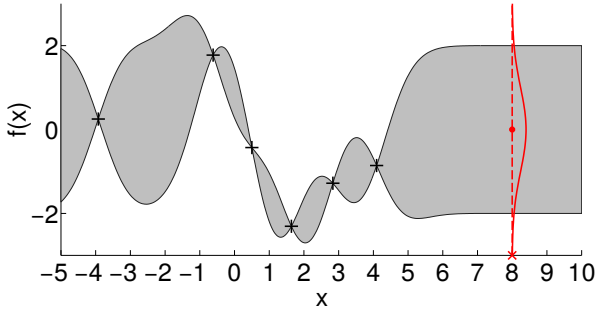

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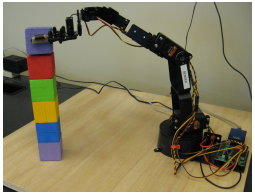
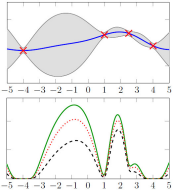
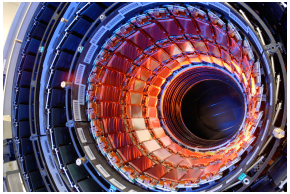
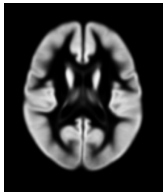
Some Application Areas



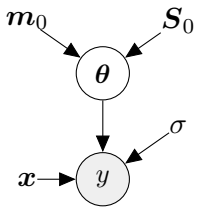






- Reinforcement learning and robotics
- Bayesian optimization (experimental design)
- Geostatistics
- Sensor networks
- Time-series modeling and forecasting
- High-energy physics
- Medical applications

Bayesian Linear Regression: Model



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

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

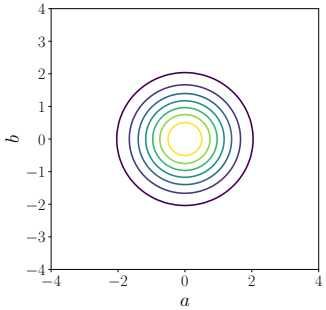
$$\implies y = \boldsymbol{\phi}^\top(\boldsymbol{x})\boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0,\, \sigma^2)$$

- Parameter $\boldsymbol{\theta}$ becomes a latent (random) variable
- Distribution $p(\boldsymbol{\theta})$ induces a distribution over plausible functions
- Choose a conjugate Gaussian prior
  - Closed-form computations
  - Gaussian posterior

Distribution over Functions

Consider a linear regression setting

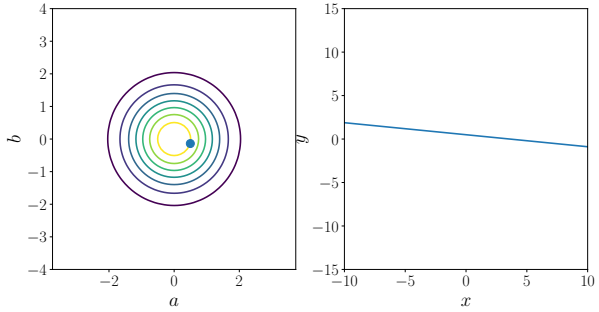
$$y = a + bx + \epsilon\,, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_n^2\big)$$
$$p(a, b) = \mathcal{N}\big(\mathbf{0},\, \boldsymbol{I}\big)$$



Sampling from the Prior over Functions

Consider a linear regression setting

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



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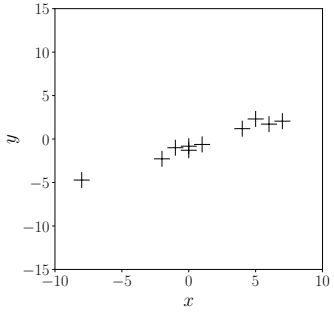
$$\boldsymbol{X} = [x_1, \ldots, x_N],\ \boldsymbol{y} = [y_1, \ldots, y_N] \qquad \text{Training data}$$



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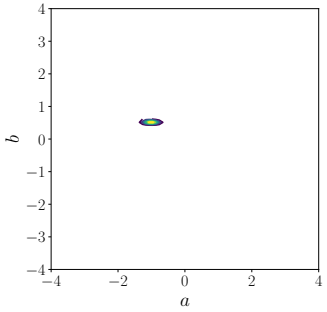
$$p(a, b|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}\big(\boldsymbol{m}_N,\, \boldsymbol{S}_N\big) \qquad \text{Posterior}$$



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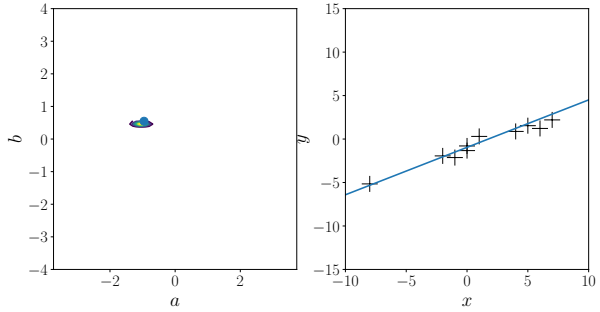
$$[a_i, b_i] \sim p(a, b|\boldsymbol{X}, \boldsymbol{y})$$
$$f_i = a_i + b_i x$$



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

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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

GP Regression as Bayesian Inference

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

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

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

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

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 $f_i(\cdot) := \boldsymbol{\theta}_i^\top \boldsymbol{\phi}(\cdot)$

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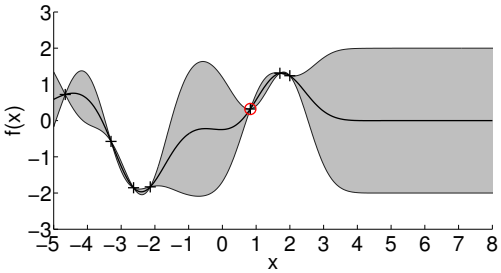
- What characterizes the function we want to model?
  - Mean function
  - Covariance function

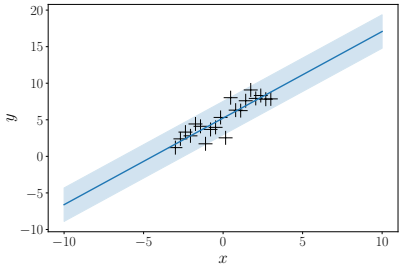
Mean Function

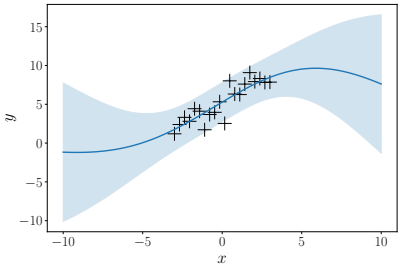


$$m(\boldsymbol{x}) = \mathbb{E}_f[f(\boldsymbol{x})], \quad f \sim GP$$

- 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 or neural network. Example: $m_{\boldsymbol{\theta}}(\boldsymbol{x}) = \boldsymbol{\theta}^\top \boldsymbol{\phi}(\boldsymbol{x})$
- Prior mean function $m_{\boldsymbol{\theta}}$ can incorporate problem-specific prior knowledge (e.g., in robotics, natural sciences)
- Often: "Agnostic" mean function in the absence of data or prior knowledge: $m(\cdot) \equiv 0$

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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

Gaussian Covariance Function

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

- Assumption on latent function: Smooth (∞ differentiable)

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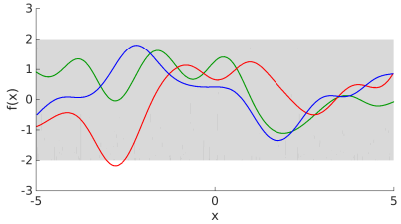
- Assumption on latent function: Smooth (∞ differentiable)
- σ_f: Amplitude of the latent function
- ℓ: Length-scale. How far do we have to move in input space before the function value changes significantly, i.e., when do function values become uncorrelated?
  ⏩ **Smoothness parameter**



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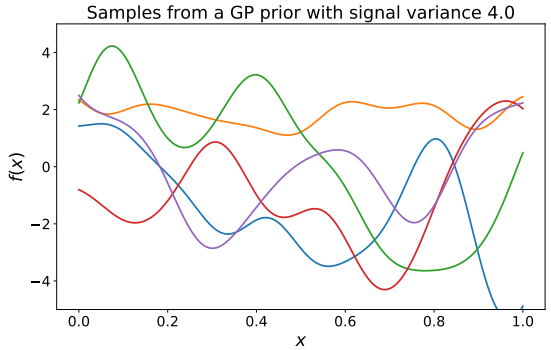

- Controls the amplitude (vertical magnitude) of the function we wish to model

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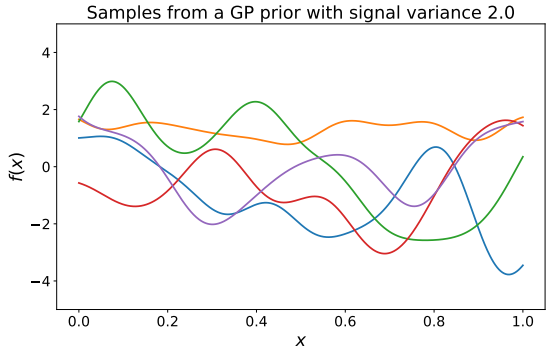

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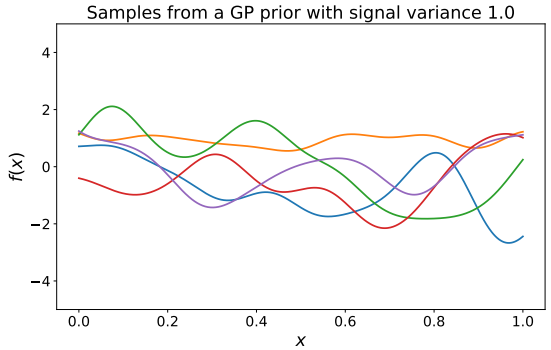

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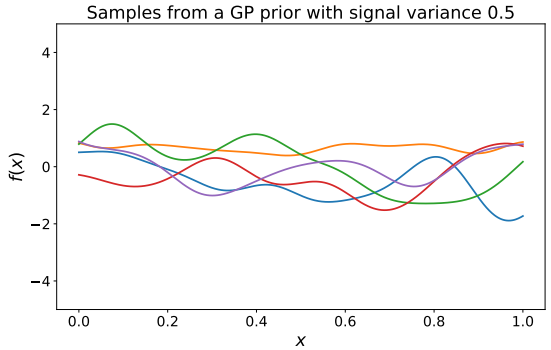

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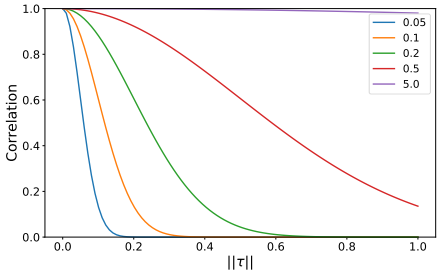
Length-Scale ℓ

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

- 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 $\boldsymbol{x}$ to $\boldsymbol{x}'$ to make $f(\boldsymbol{x})$ and $f(\boldsymbol{x}')$ uncorrelated?

Length-Scale ℓ (2)

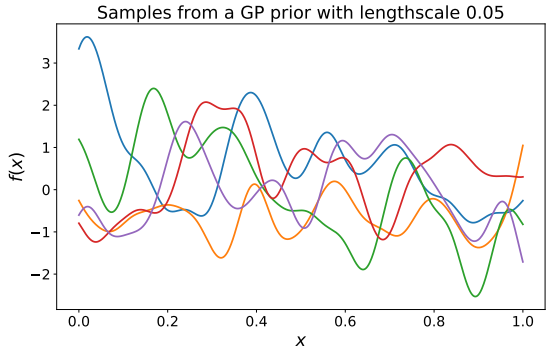
$$k_{Gauss}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sigma_f^2 \exp\left(-(\boldsymbol{x}_i - \boldsymbol{x}_j)^\top (\boldsymbol{x}_i - \boldsymbol{x}_j)/\ell^2\right)$$



- 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)

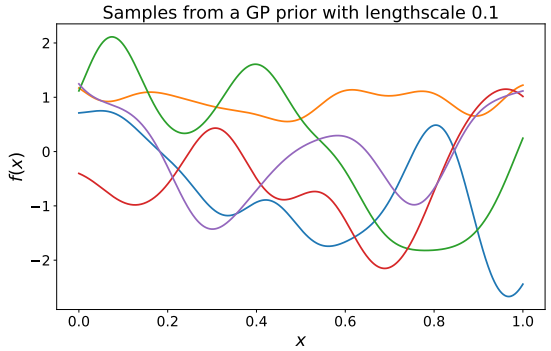
$$k_{Gauss}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sigma_f^2 \exp\left(-(\boldsymbol{x}_i - \boldsymbol{x}_j)^\top (\boldsymbol{x}_i - \boldsymbol{x}_j)/\ell^2\right)$$



⏩ Explore interactive diagrams at https://tinyurl.com/guide2gp

Length-Scale ℓ (3)

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



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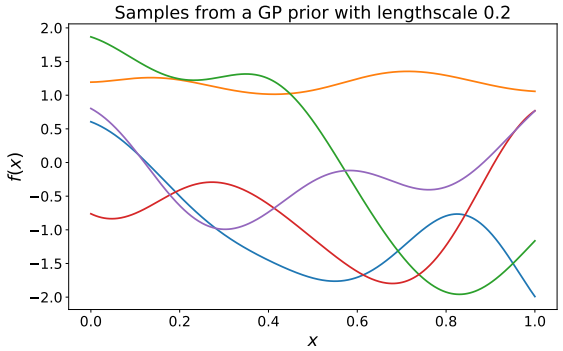

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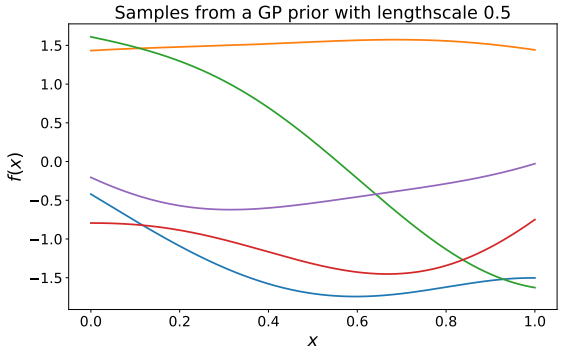

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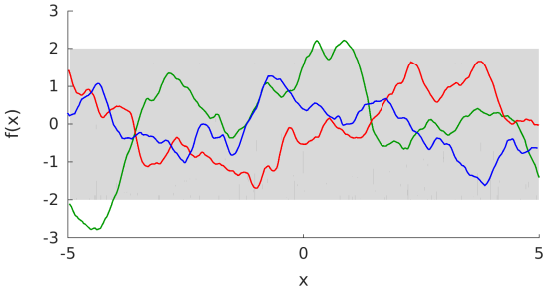
Matérn Covariance Function

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

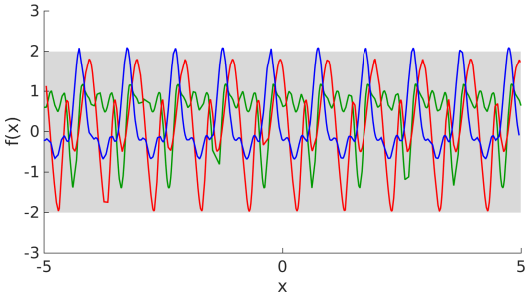
- Assumption on latent function: 1-times differentiable
- σ_f: Amplitude of the latent function
- ℓ: Length-scale. How far do we have to move in input space before the function value changes significantly?



Periodic Covariance Function

$$k_{per}(x_i, x_j) = \sigma_f^2 \exp\Big(- \frac{2 \sin^2\big(\frac{\kappa(x_i - x_j)}{2\pi}\big)}{\ell^2} \Big) = k_{Gauss}(\boldsymbol{u}(x_i), \boldsymbol{u}(x_j)), \quad \boldsymbol{u}(x) = \begin{bmatrix} \cos(\kappa x) \\ \sin(\kappa x) \end{bmatrix}$$

- 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:

$$p(y|\boldsymbol{x}, f(\cdot)) = \mathcal{N}\left(y \,|\, f(\boldsymbol{x}),\, \sigma^2\right)$$

- Parameters are the function f itself

Marginal Likelihood

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

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Gaussian process marginal likelihood

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$$

$$
K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j), \quad i, j = 1, \ldots, N
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Posterior over functions (with training data $\boldsymbol{X}, \boldsymbol{y}$):

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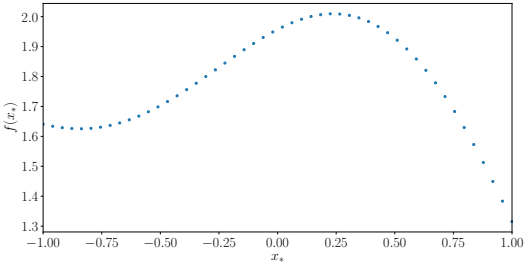

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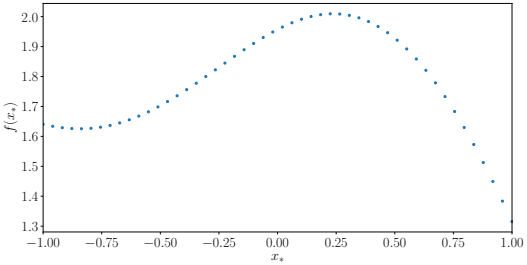
- In practice, we cannot sample functions directly
- Instead: function = collection of function values
- Determine function values at a finite set of input locations $\boldsymbol{X}_* = [\boldsymbol{x}_1^{(1)}, \ldots, \boldsymbol{x}_*^{(K)}]$



Sampling from a GP (2)

- Goal: Generate random functions f_k, so that

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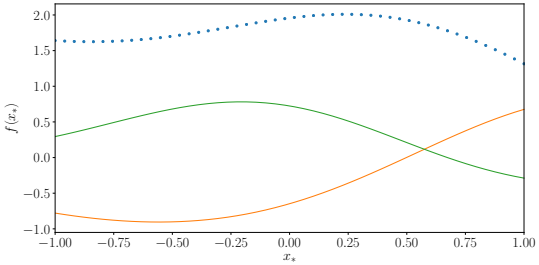

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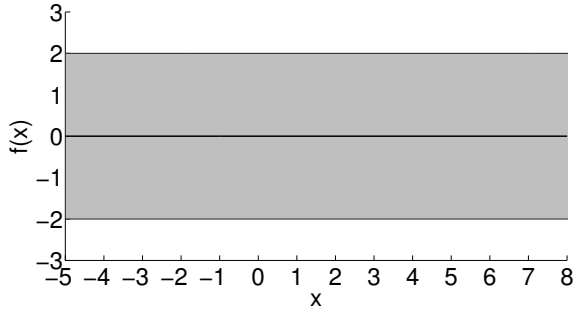
⏩ Sample from a multivariate Gaussian

Illustration: Inference with Gaussian Processes



Prior belief about the function

Predictive (marginal) mean and variance:

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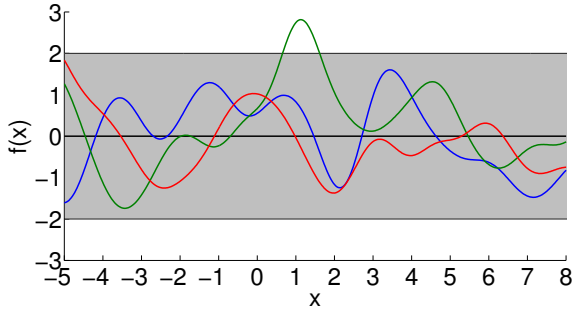

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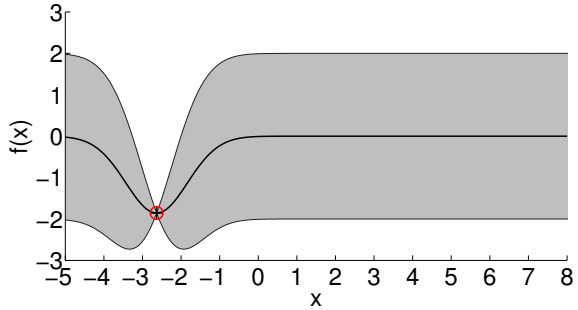

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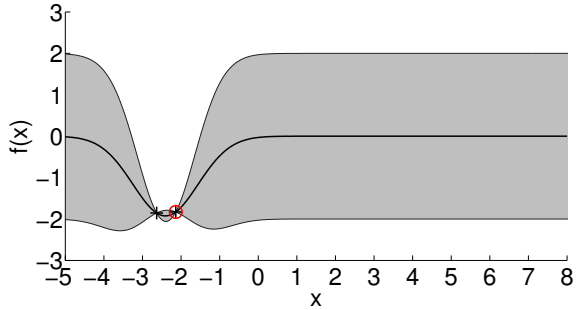

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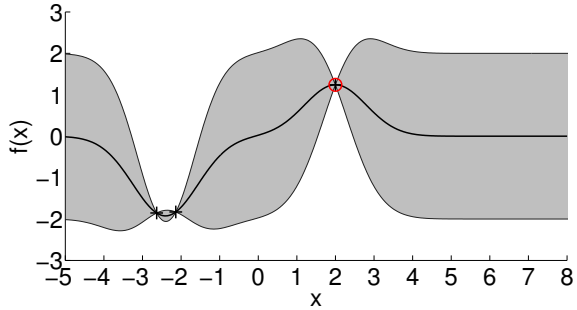

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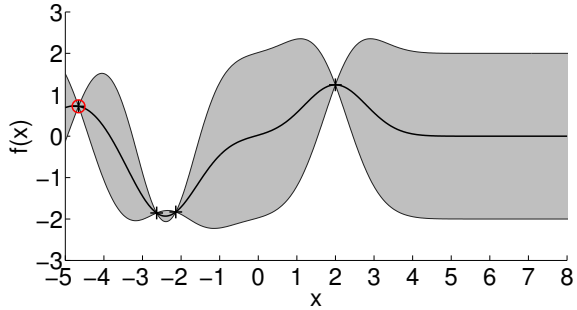

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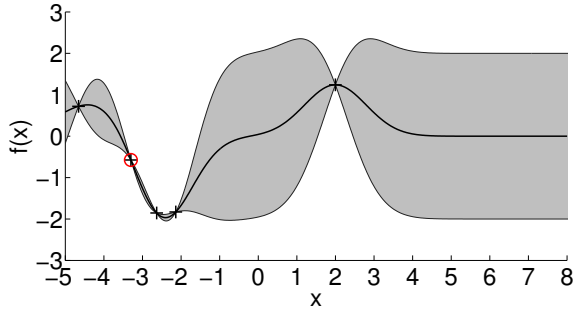

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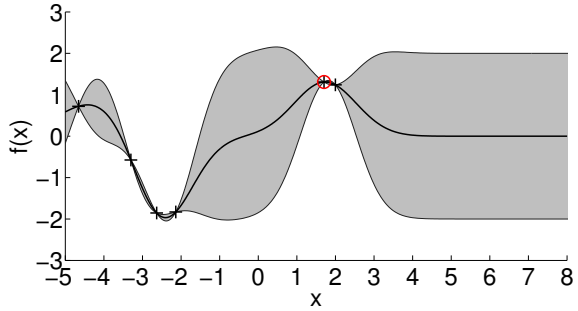

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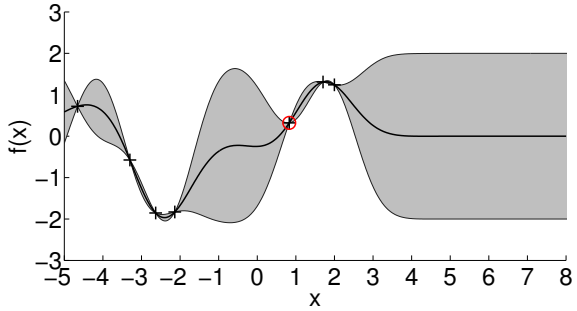

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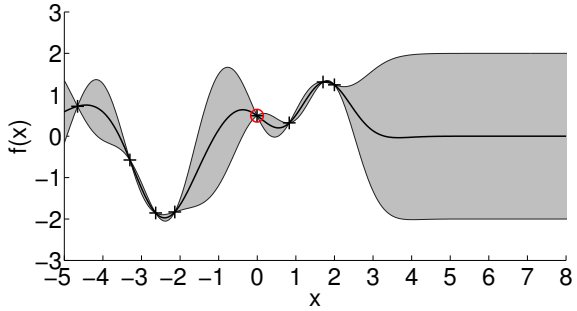
Illustration: Inference with Gaussian Processes



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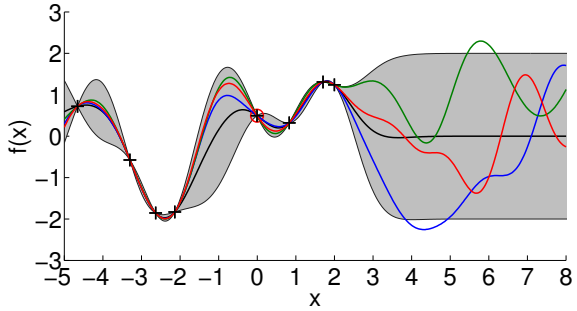

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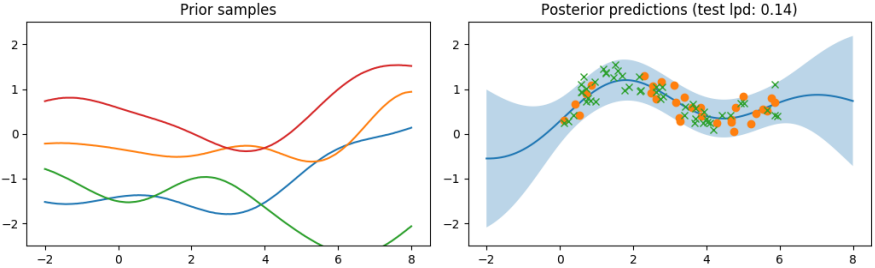

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for different length-scales ℓ and different datasets

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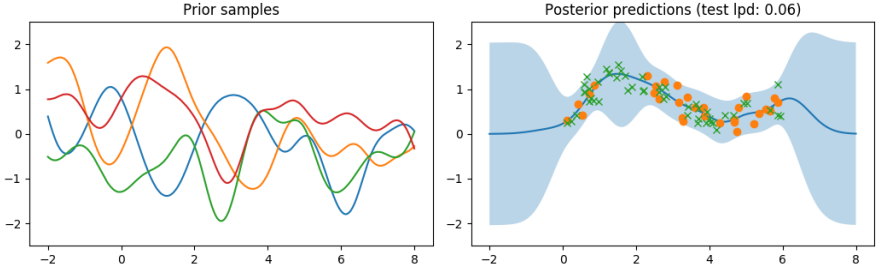

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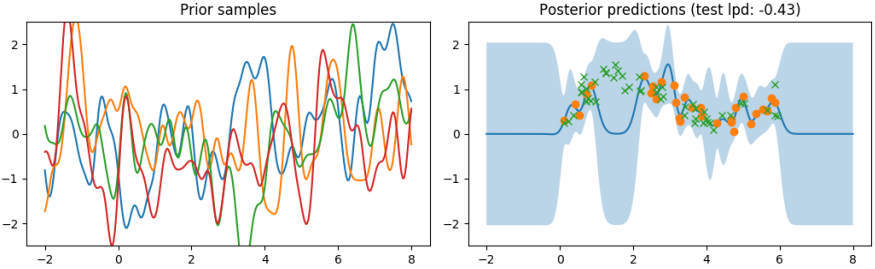

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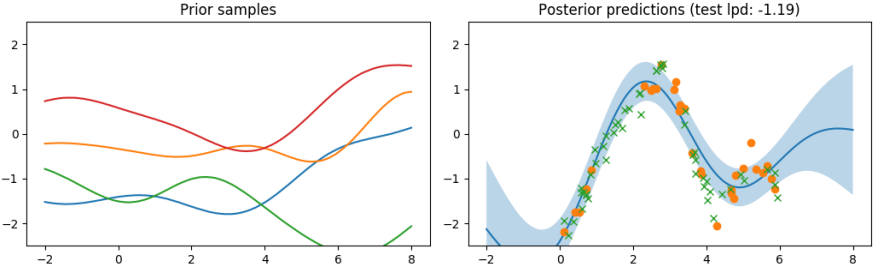

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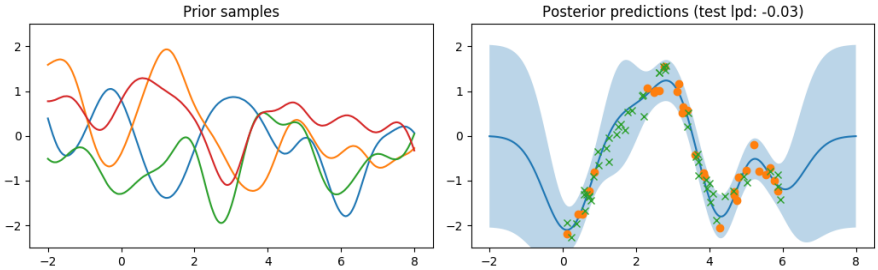

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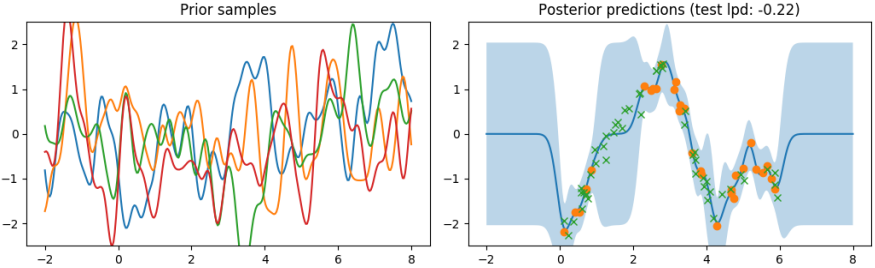

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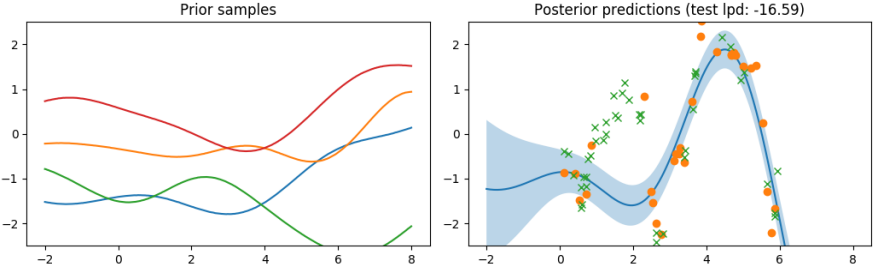

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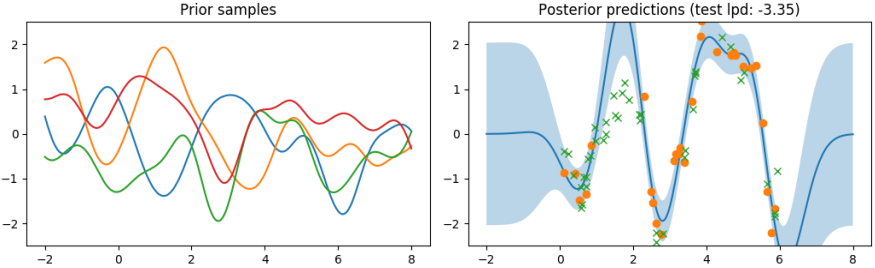

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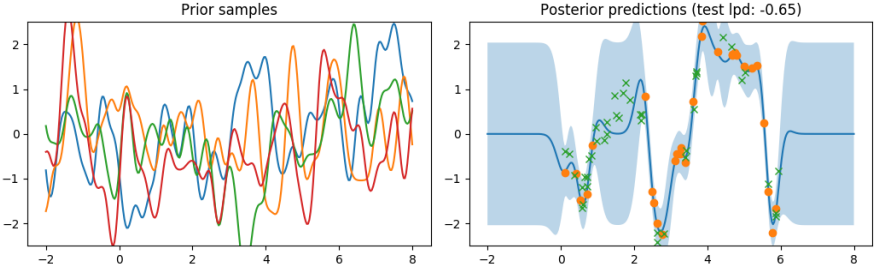

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- Shorter length-scale ⏩ More flexible model ⏩ Faster increase in uncertainty away from data ⏩ Bad generalization

Model Selection

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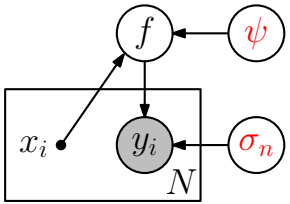
⏩ Higher-level model selection to find good mean and covariance functions
(can also be automated: Automatic Statistician (Lloyd et al., 2014))

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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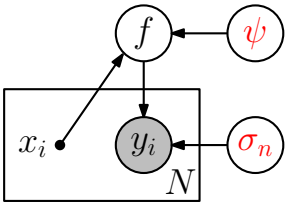

- Place a prior $p(\boldsymbol{\theta})$ on hyper-parameters
- Posterior over hyper-parameters:

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

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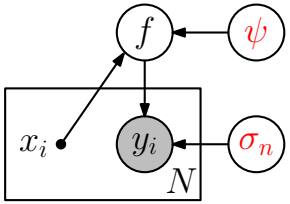

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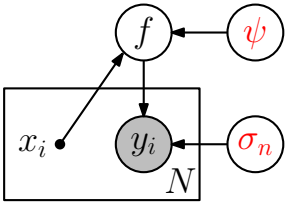

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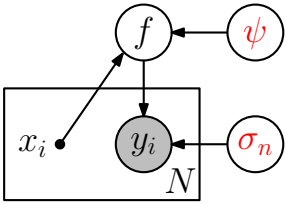

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⏩ Maximize marginal likelihood if $p(\boldsymbol{\theta}) = \mathcal{U}$ (uniform prior)

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

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

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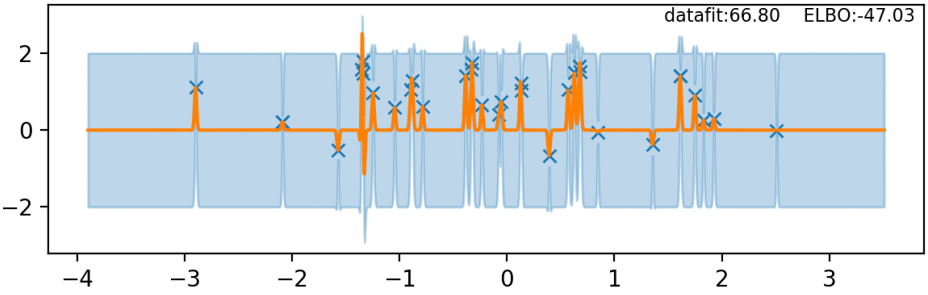
Marginal likelihood

⏩ Automatic trade-off between data fit and model complexity

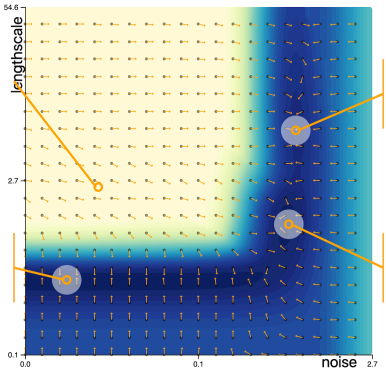
Marginal Likelihood Illustration[1]



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

[1] Credit to Mark van der Wilk

Marginal Likelihood Surface



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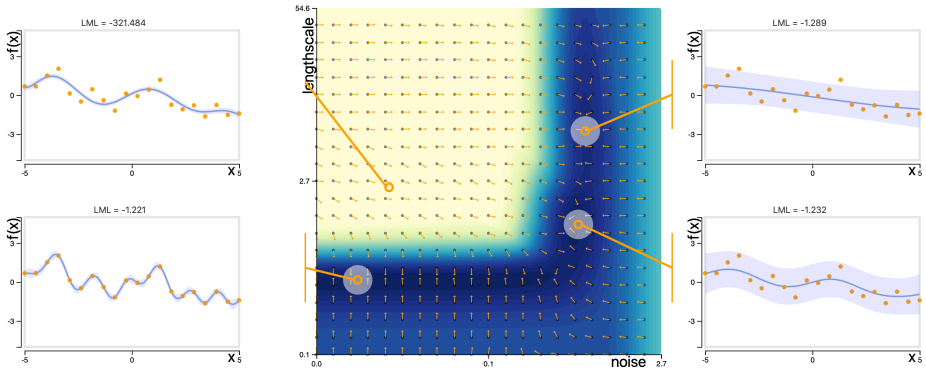

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Demo

https://tinyurl.com/guide2gp/

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

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- Just adding uncertainty does not help either if the model is wrong, but it makes predictions more cautious
- 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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Marginal Likelihood: Incremental Prediction (2)

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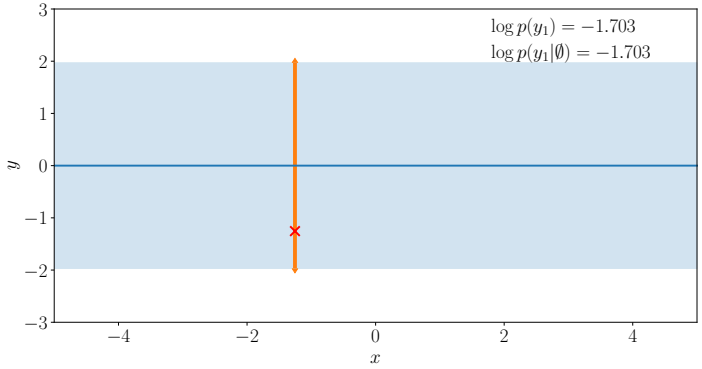
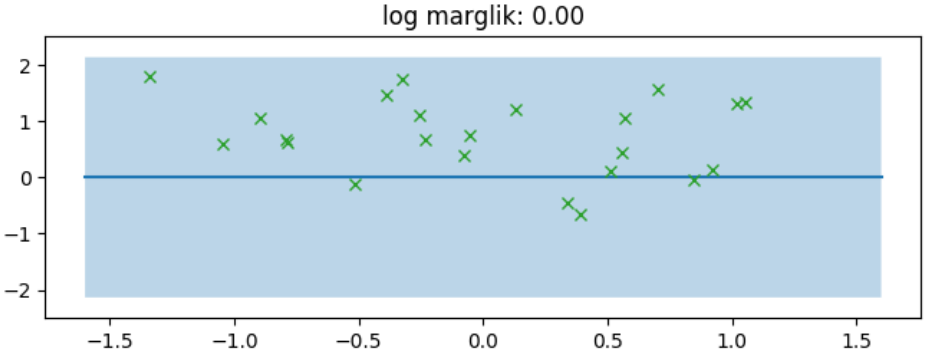
- Intuition: If it continuously predicted well on all N previous points, it probably will do well next time
  ⏩ Proxy for generalization error on unseen test data

Marginal Likelihood: Illustration



$$p(\boldsymbol{y}|\boldsymbol{\theta}) = p(y_1, \ldots, y_N|\boldsymbol{\theta}) = p(y_1|\boldsymbol{\theta}) \prod_{n=2}^{N} p(y_n|y_1, \ldots, y_{n-1}, \boldsymbol{\theta})$$

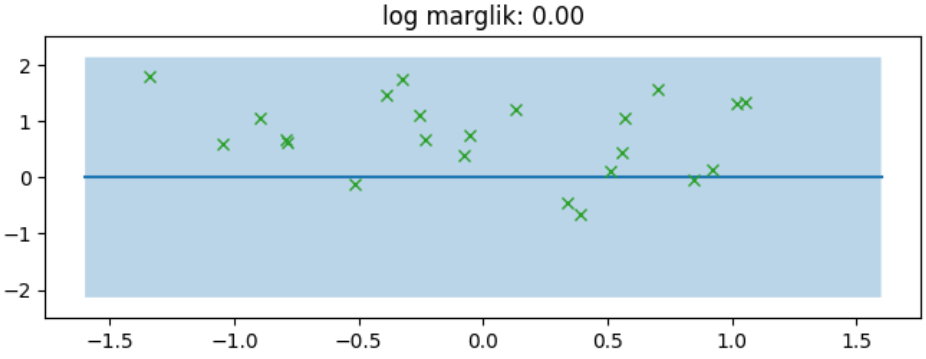
Marginal Likelihood Computation in Action[2]



- Short length-scale

[2] Credit to Mark van der Wilk

Marginal Likelihood Computation in Action[3]



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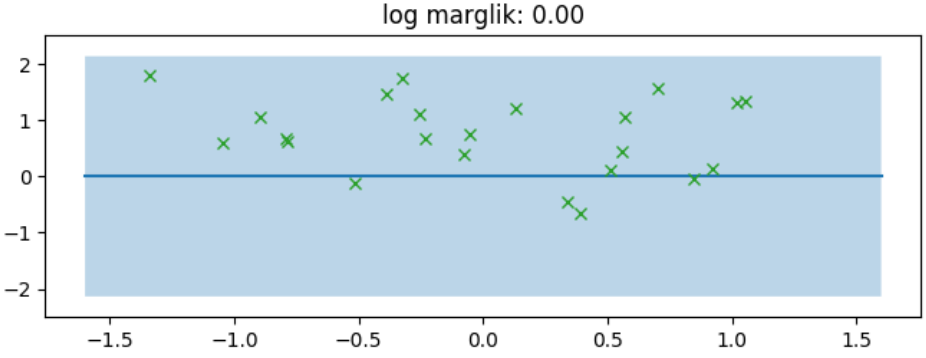
Marginal Likelihood Computation in Action[4]



- Optimal length-scale

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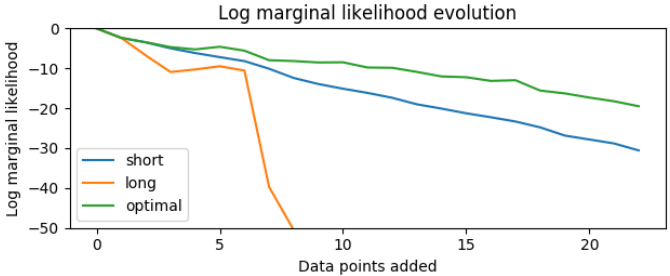
Marginal Likelihood Evolution



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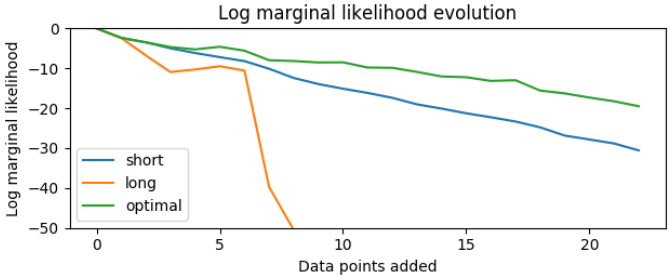
  - ⏩ No high density, even with observations inside the error bars

Marginal Likelihood Evolution



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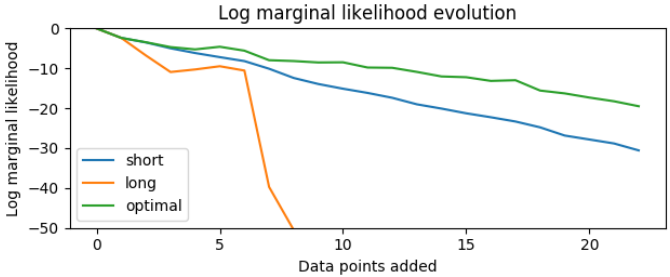

- Short lengthscale: consistently overestimates variance
  - ⏩ No high density, even with observations inside the error bars
- Long lengthscale: consistently underestimates variance
  - ⏩ Low density because observations are outside the error bars
- Optimal lengthscale: trades off both behaviors reasonably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

Model Selection—Mean Function and Kernel

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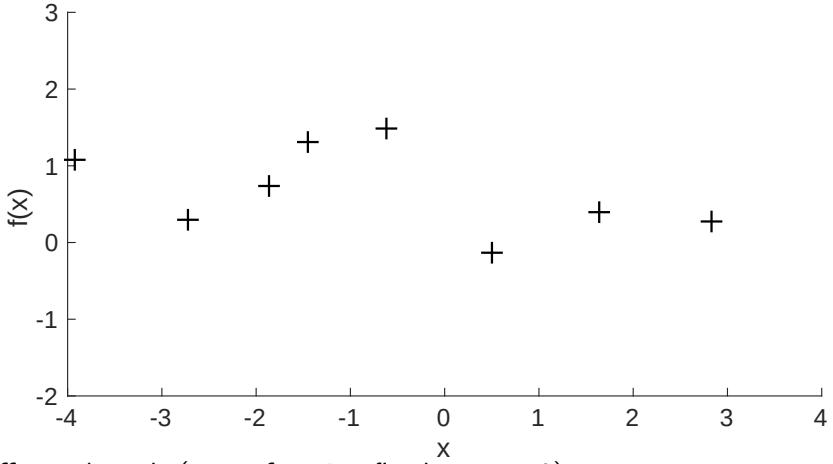
- Assume we have a finite set of models M_i, each one specifying a mean function m_i and a kernel k_i. How do we find the best one?
- Some options:
  - Cross validation
  - Bayesian Information Criterion, Akaike Information Criterion
  - Compare marginal likelihood values (assuming a uniform prior on the set of models)

Example



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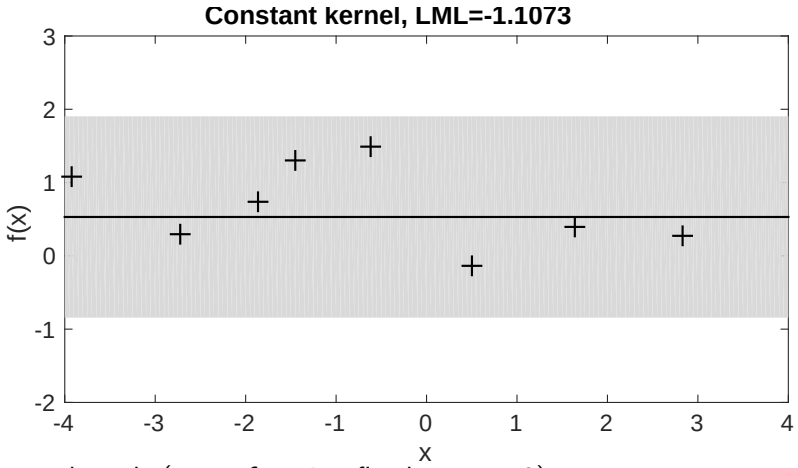

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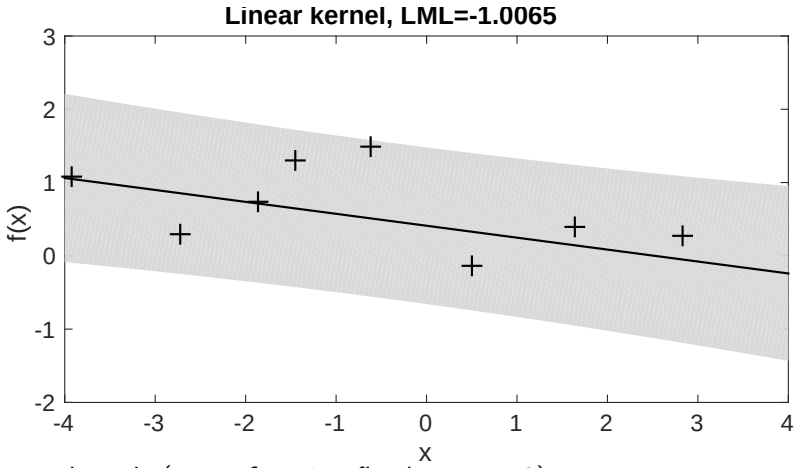

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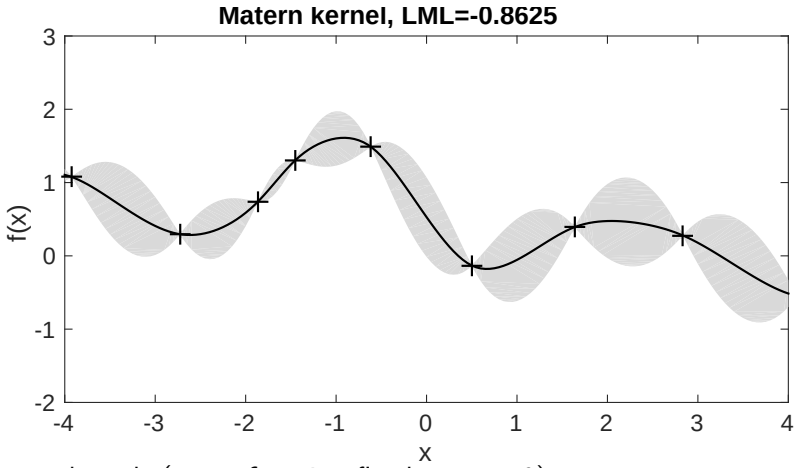

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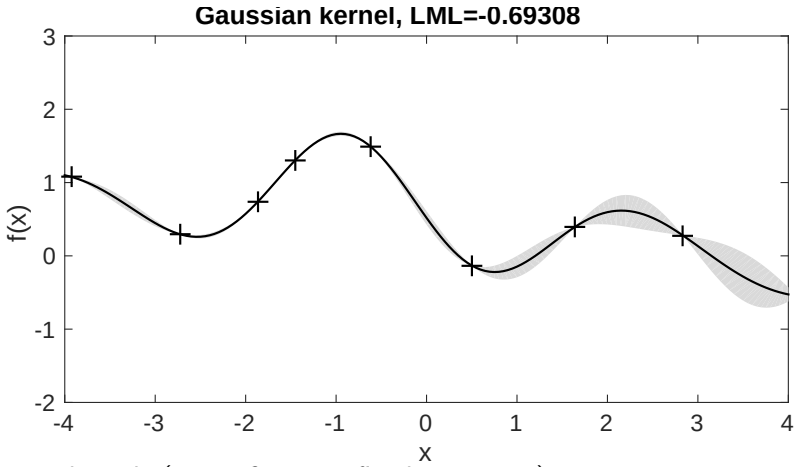

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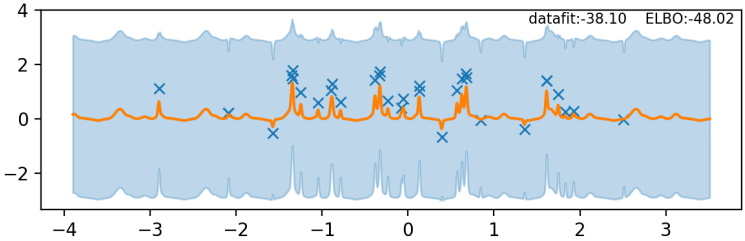
GP Training: Illustration[5]



- 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.

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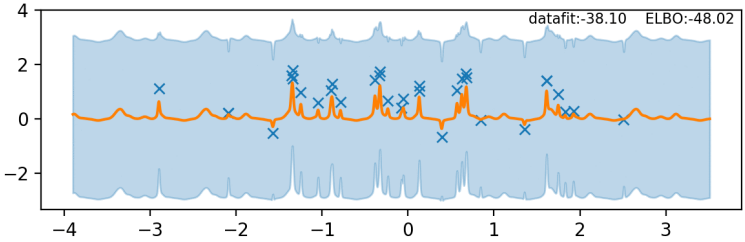

- Prior: $f(\boldsymbol{x}) = \theta_s f_{\text{smooth}}(\boldsymbol{x}) + \theta_p f_{\text{periodic}}(\boldsymbol{x})$, with smooth and periodic GP priors, respectively.
- Amount of periodicity vs. smoothness is automatically chosen by selecting hyper-parameters θ_s, θ_p.
- Marginal likelihood learns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

[5] Credit to Mark van der Wilk

Limitations of Gaussian Processes

Computational and memory complexity

Training set size: N

- Training scales in $\mathcal{O}(N^3)$
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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)

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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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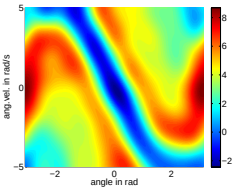
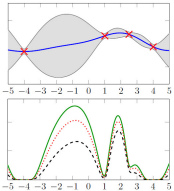
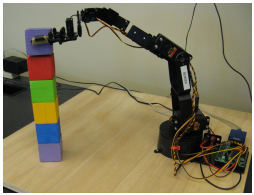
Application Areas

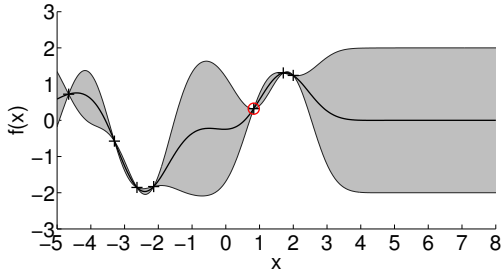


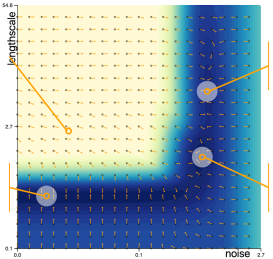




- Reinforcement learning and robotics
  - ⏩ Model value functions and/or dynamics with GPs
- Bayesian optimization (Experimental Design)
  - ⏩ Model unknown utility functions with GPs
- Geostatistics
  - ⏩ Spatial modeling (e.g., landscapes, resources)
- Sensor networks
- Time-series modeling and forecasting

Summary





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

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