Gaussian Processes

Marc Deisenroth
Centre for Artificial Intelligence
Department of Computer Science
University College London

@mpd37
`m.deisenroth@ucl.ac.uk`
`https://deisenroth.cc`

AIMS Rwanda and AIMS Ghana

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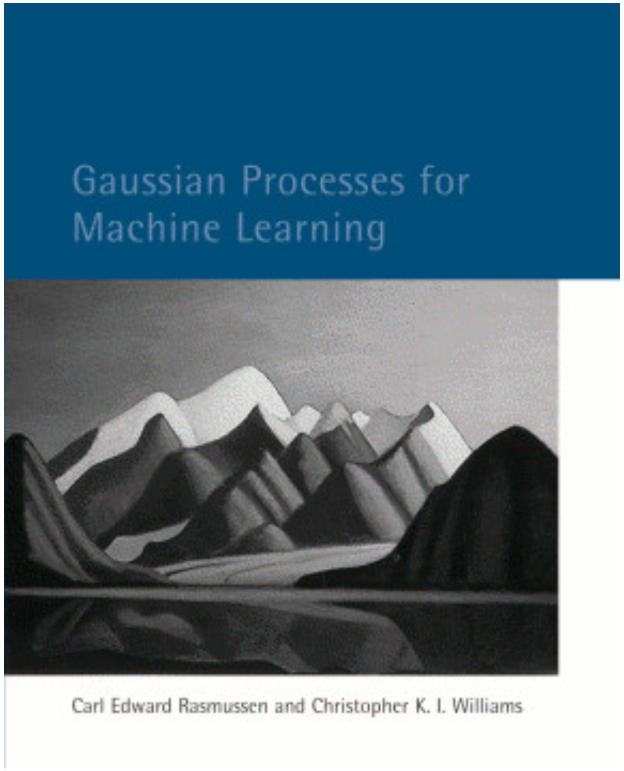
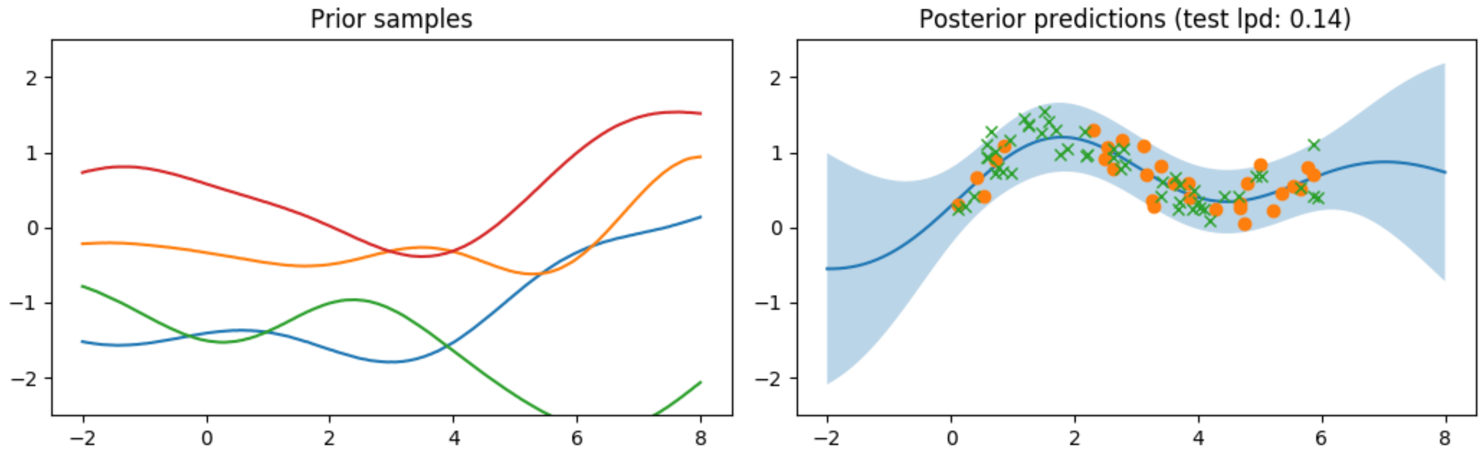
Reference


Gaussian Processes for Machine Learning
Carl Edward Rasmussen and Christopher K. I. Williams

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

Model Selection

Influence of Prior on Posterior



- Generalization error measured by log-predictive density (lpd)

$$\text{lpd} = \log p(y_* | \boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}, \ell)$$

for different length-scales ℓ and different datasets

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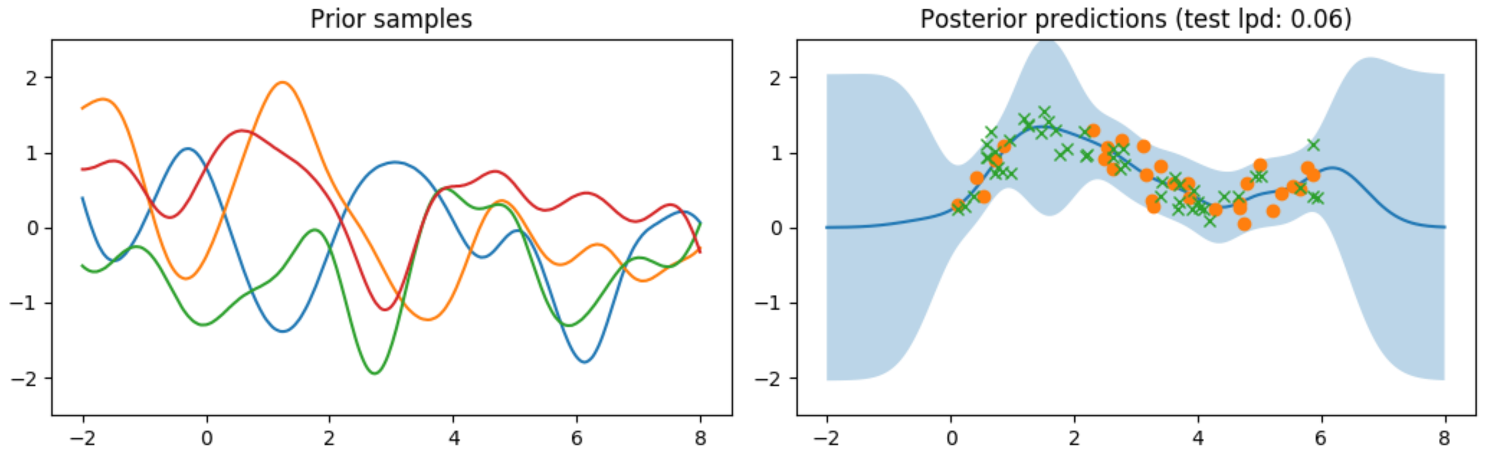

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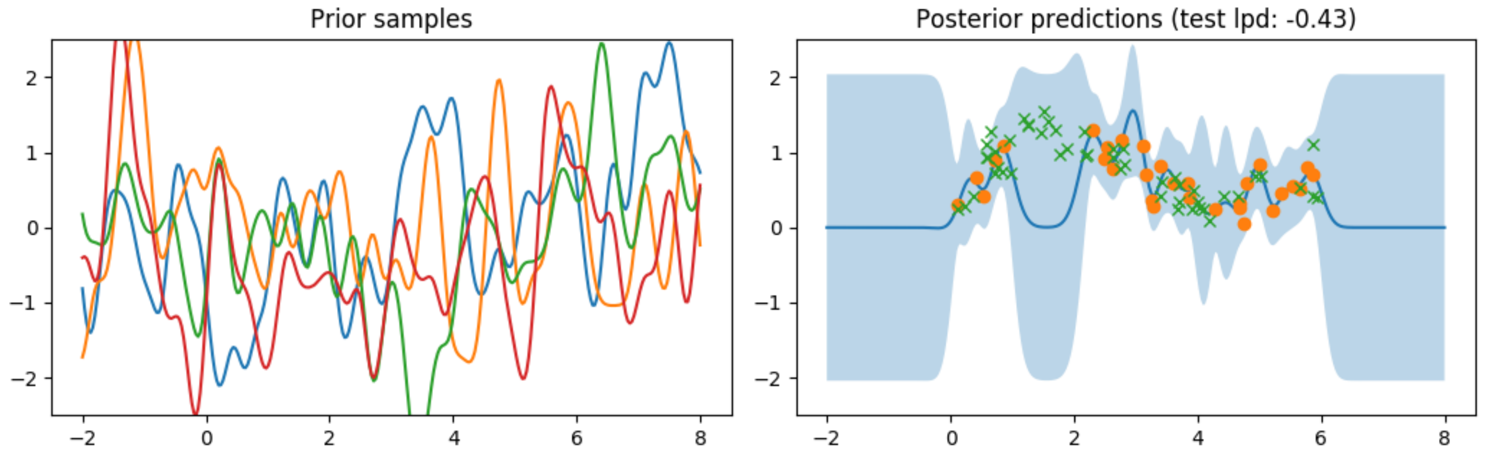

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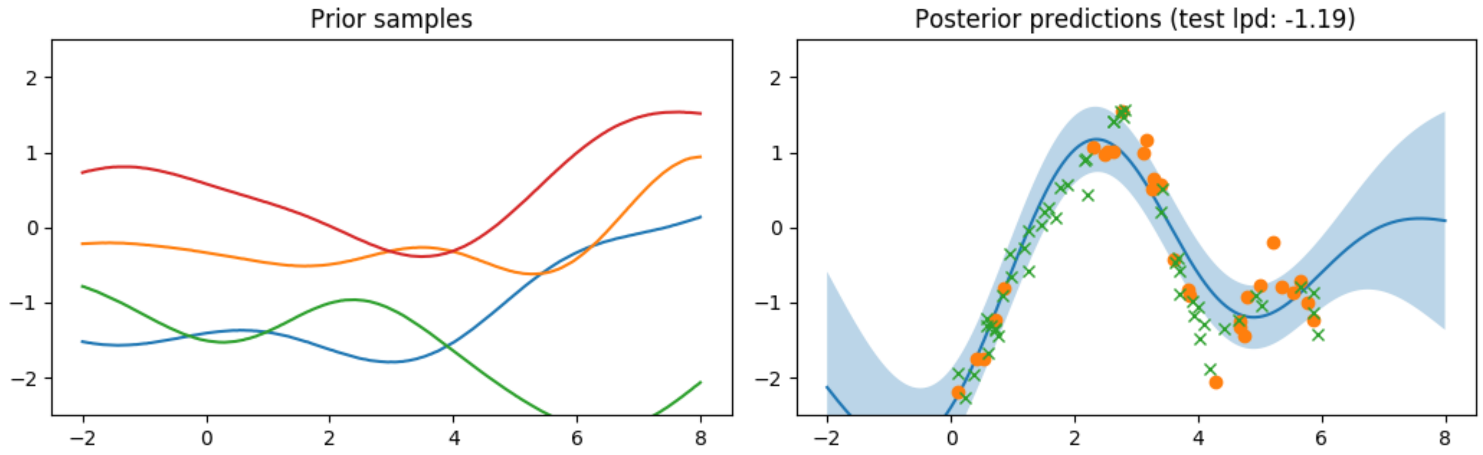

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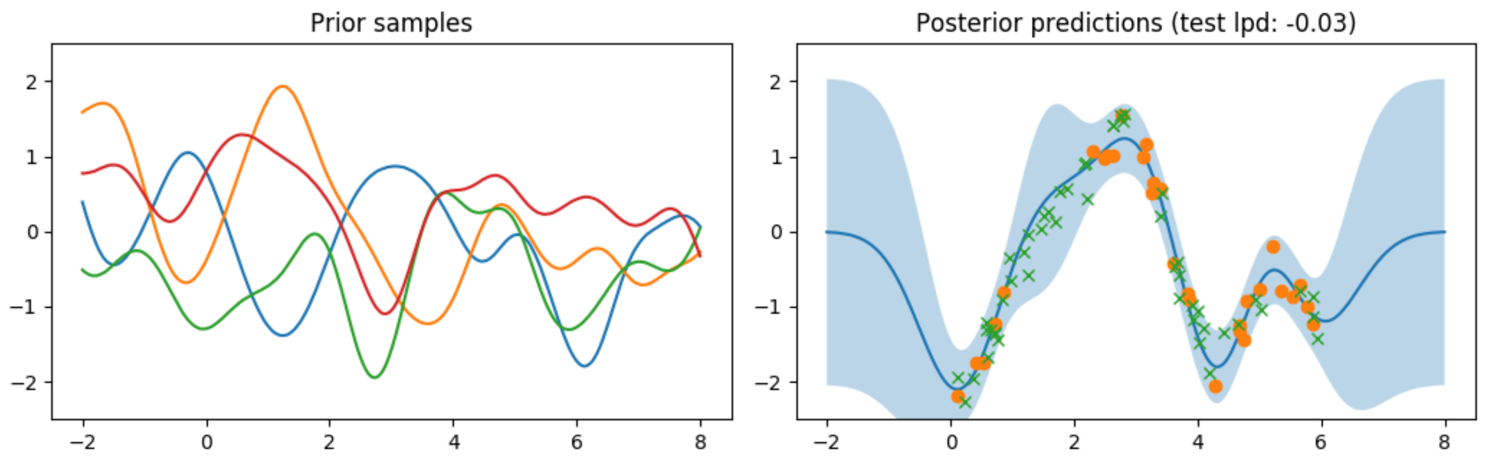

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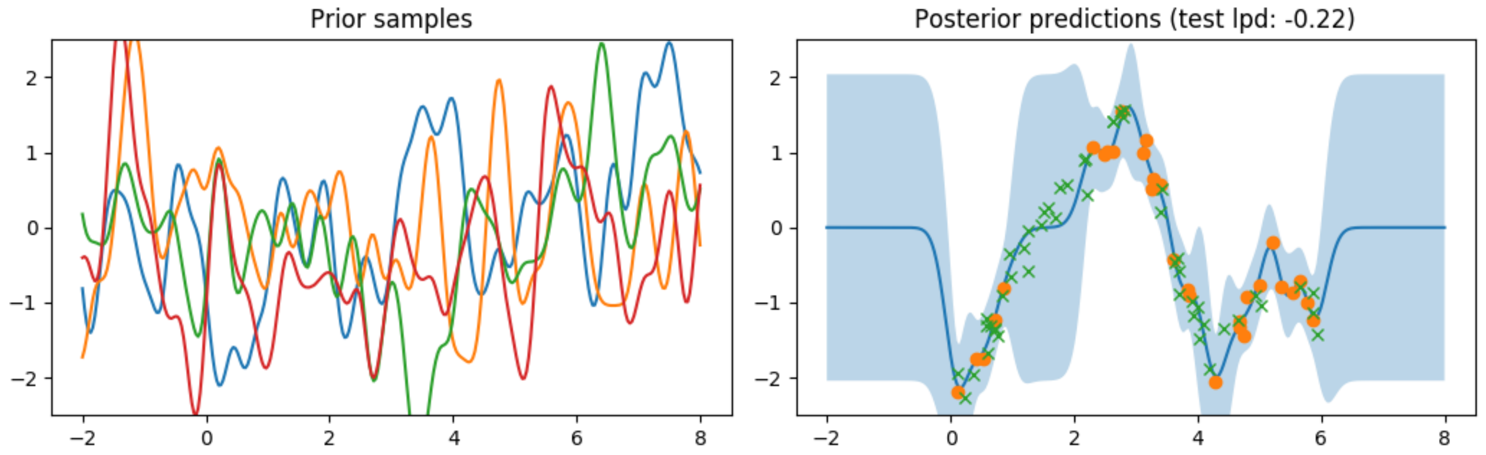

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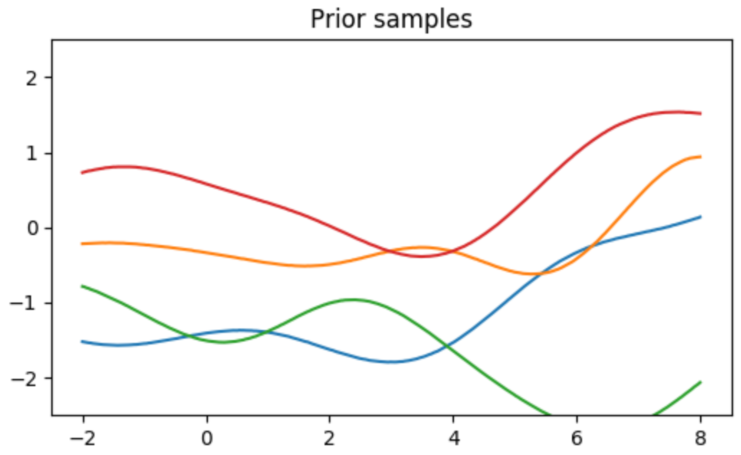

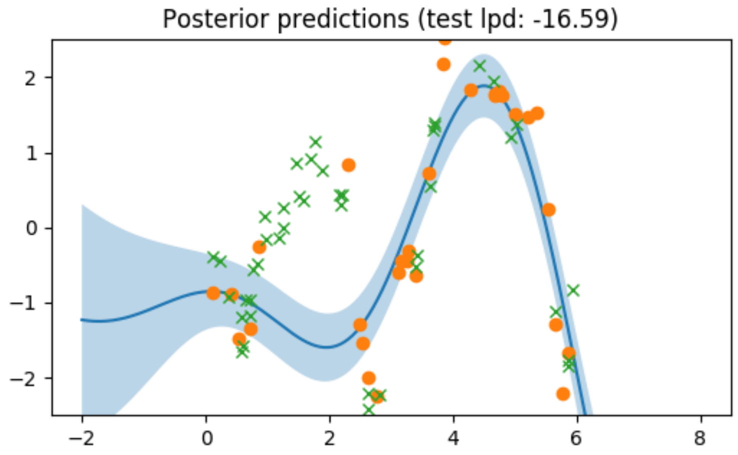

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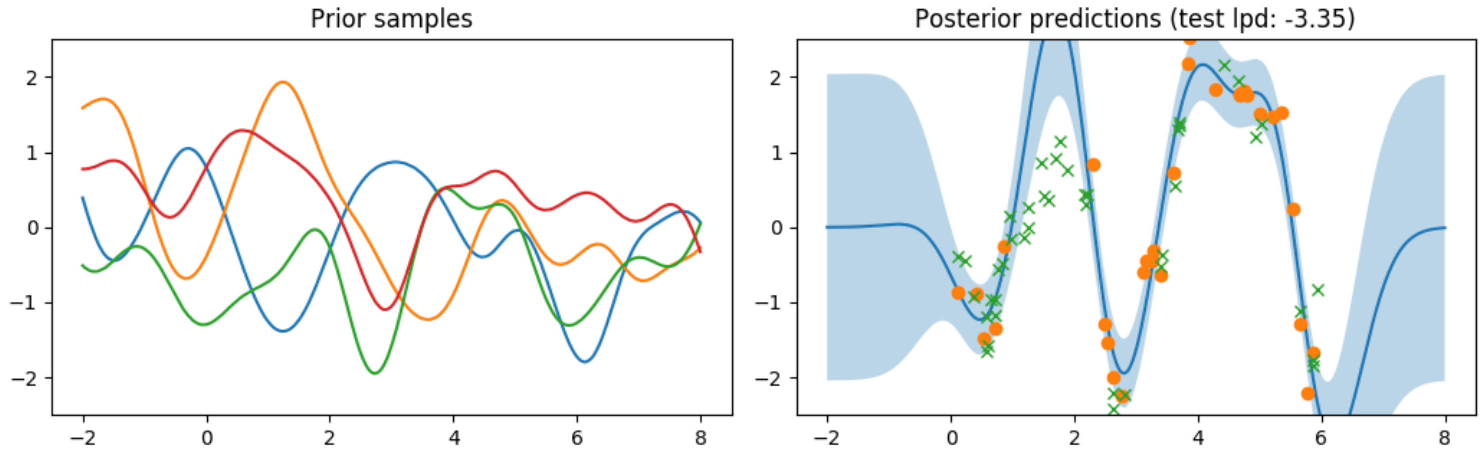

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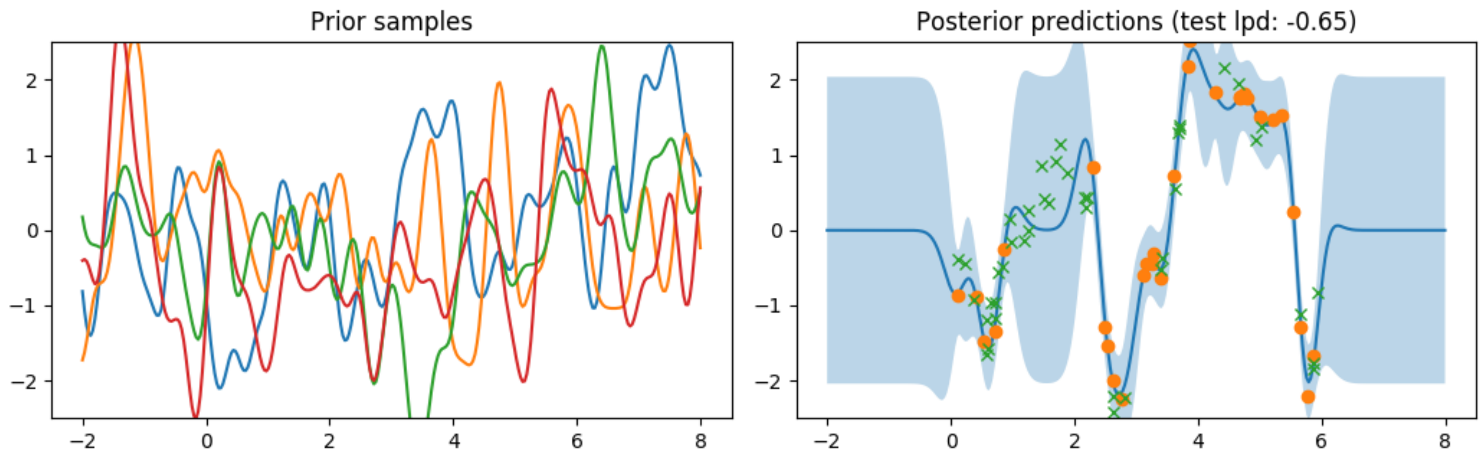

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Model Selection

- Make predictions equipped with uncertainty
- Choice of prior (e.g., length-scale) influences predictions
- Different tasks require different priors

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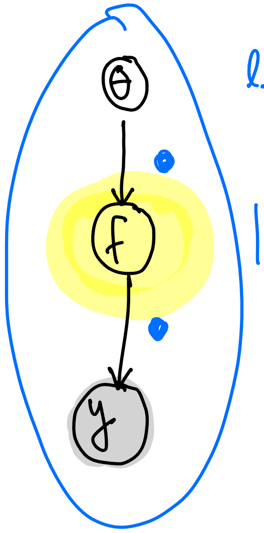
▸▸ Train a GP to find a good set of hyper-parameters

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

GP

$p(a) = \int p(a,b)\,db$ sum rule



level 2 hyper-parameters of the Gaussian process

level 1 unobserved (latent) function

observed function values (noisy)

$$\underset{\theta}{\operatorname{argmax}} \boxed{p(y|\theta)}$$

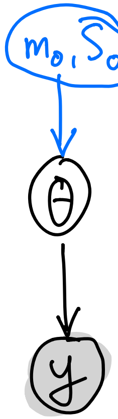
sum rule $\hookrightarrow \int p(\underline{y,f}|\theta)\,df$

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

likelihood GP prior

This is the marginal likelihood (Maximum likelihood Type 2)

Linear Regression



level 1

param. of the model

- Maximum likelihood
- MAP

$\underset{\theta}{\operatorname{argmax}}\ p(y|\theta)$

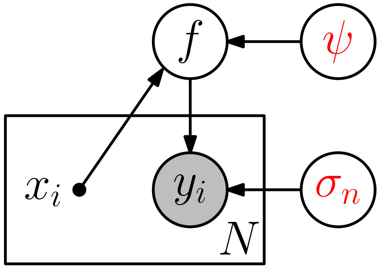
$\underset{\theta}{\operatorname{argmax}}\ p(\theta|y)$

Prior on θ + Bayes' theorem

Gaussian Process Training: Hyper-Parameters

GP Training

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



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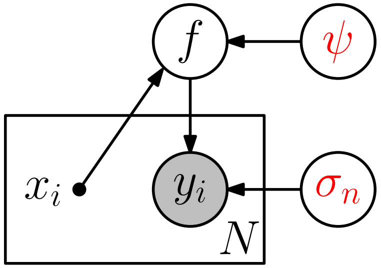


- Place a prior $p(\boldsymbol{\theta})$ on hyper-parameters
- Posterior over hyper-parameters:

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

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

Gaussian Process Training: Hyper-Parameters

marginal likelihood = evidence

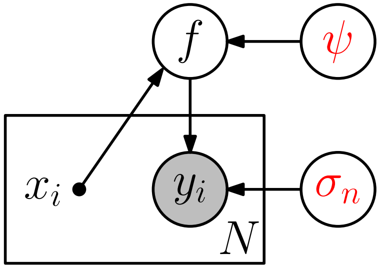
= marginalized likelihood

- Posterior over hyper-parameters: "integrate out"

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

likelihood

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



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

$\longrightarrow$ marginalized marginal likelihood

marginal likelihood

$$= \int \underbrace{\int p(y|f(x))\, p(f(x)|\theta)\, df}_{\text{marginal likelihood = evidence}}\; p(\theta)\, d\theta$$

Gaussian Process Training: Hyper-Parameters

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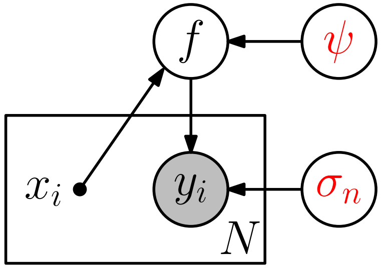

- Choose hyper-parameters $\boldsymbol{\theta}^*$, such that

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

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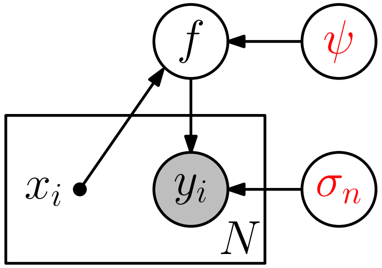

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▸▸ Maximize marginal likelihood if $p(\boldsymbol{\theta}) = \mathcal{U}$ (uniform prior)

Training via Marginal Likelihood Maximization

GP Training

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

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

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\begin{aligned}
p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) &= \int p(\boldsymbol{y}|f(\boldsymbol{X}))\, p(f(\boldsymbol{X})|\boldsymbol{\theta})\, \mathrm{d}f \\
&= \int \mathcal{N}\big(\boldsymbol{y} \,|\, f(\boldsymbol{X}),\, \sigma_n^2 \boldsymbol{I}\big)\, \mathcal{N}\big(f(\boldsymbol{X}) \,|\, \boldsymbol{0},\, \boldsymbol{K}\big)\, \mathrm{d}f \\
&= \mathcal{N}\big(\boldsymbol{y} \,|\, \boldsymbol{0},\, \boldsymbol{K} + \sigma_n^2 \boldsymbol{I}\big)
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Learning the GP hyper-parameters:

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

Gradient-based Optimization

- Log-marginal likelihood:

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

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

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

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

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

Log-marginal likelihood:

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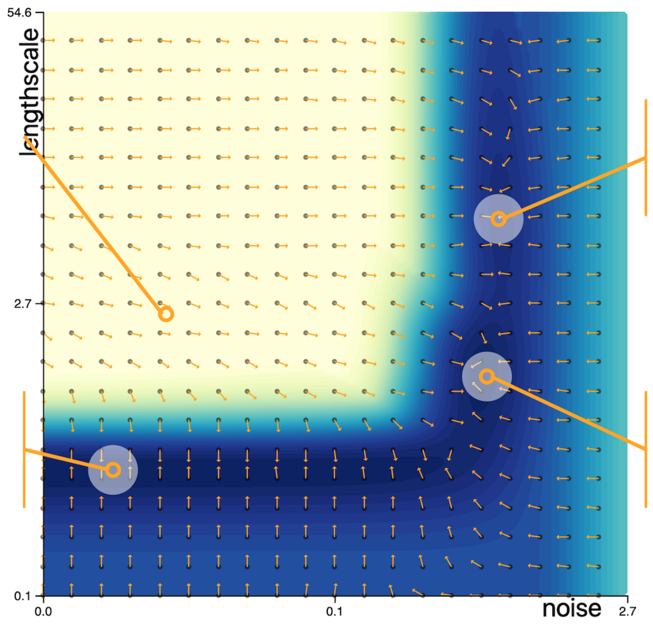
Marginal likelihood

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

Marginal Likelihood Surface



- Several plausible hyper-parameters (local optima)
- What do you expect to happen in each local optimum?

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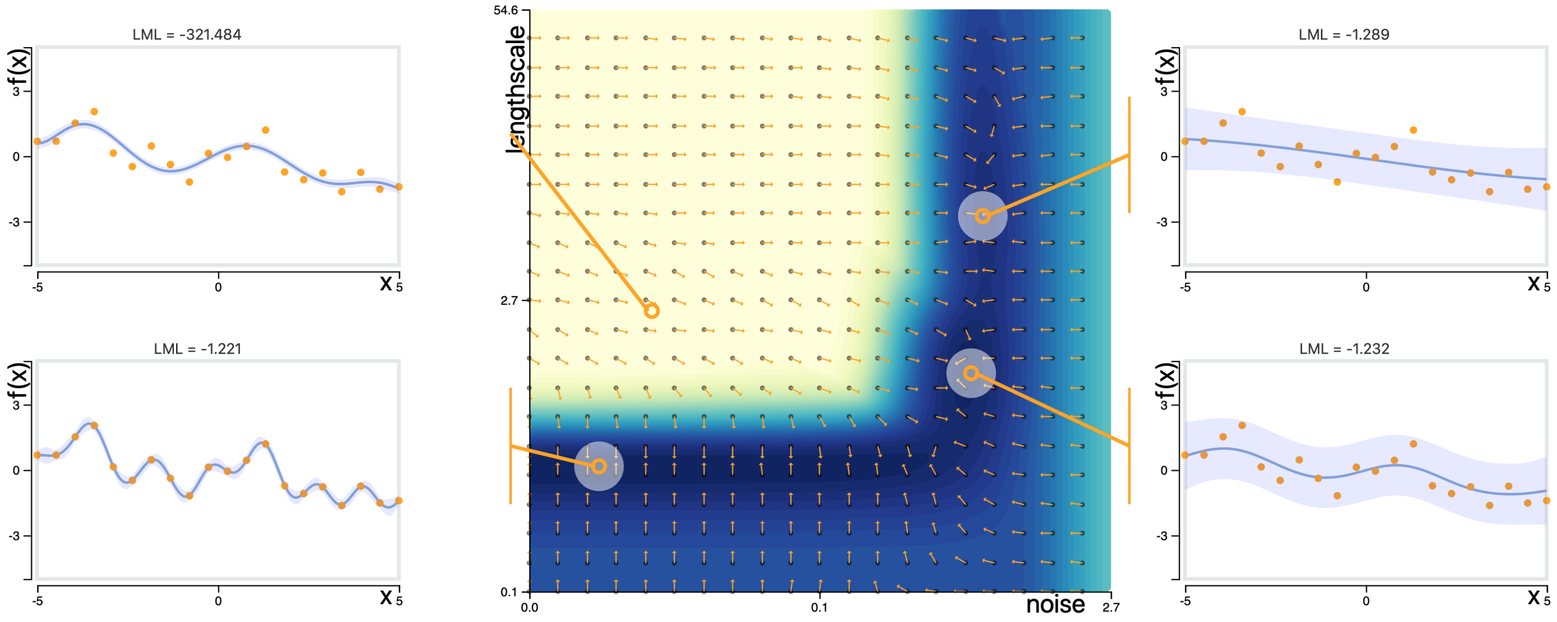

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Demo

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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- Minimizing training error is not a good idea (e.g., maximum likelihood) ⏩ Overfitting
- 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

$$\underline{p(a,b) = p(a|b)\,p(b)}$$

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

marginal likelihood

$$p(\underline{\boldsymbol{y}}|\boldsymbol{\theta}) = p(\underline{y_1, \ldots, y_N}|\boldsymbol{\theta}) = \underbrace{\underbrace{p(y_1|\theta)\,p(y_2|y_1,\theta)}_{p(y_1,y_2|\theta)}\,p(y_3|y_1,y_2,\theta)}_{p(y_1,y_2,y_3|\theta)}$$

$$\cdots\cdots\; p(y_N|y_1,\ldots,y_{N-1},\theta)$$

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&= p(y_1|\boldsymbol{\theta}) \prod_{n=2}^{N} p(y_n|y_1, \dots, y_{n-1}, \boldsymbol{\theta})
\end{aligned}
$$

Marginal Likelihood: Incremental Prediction (2)

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

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- If we think of this as a sequence model (where data arrives sequentially), the marginal likelihood predicts the nth training observation given all “previous” observations

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  ⏩ Proxy for generalization error on unseen test data

Marginal Likelihood: Illustration

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

Marginal Likelihood Computation in Action[2]

- Short length-scale

[2] Thanks to Mark van der Wilk

Marginal Likelihood Computation in Action[3]

- Long length-scale

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Marginal Likelihood Computation in Action[4]

- Optimal length-scale

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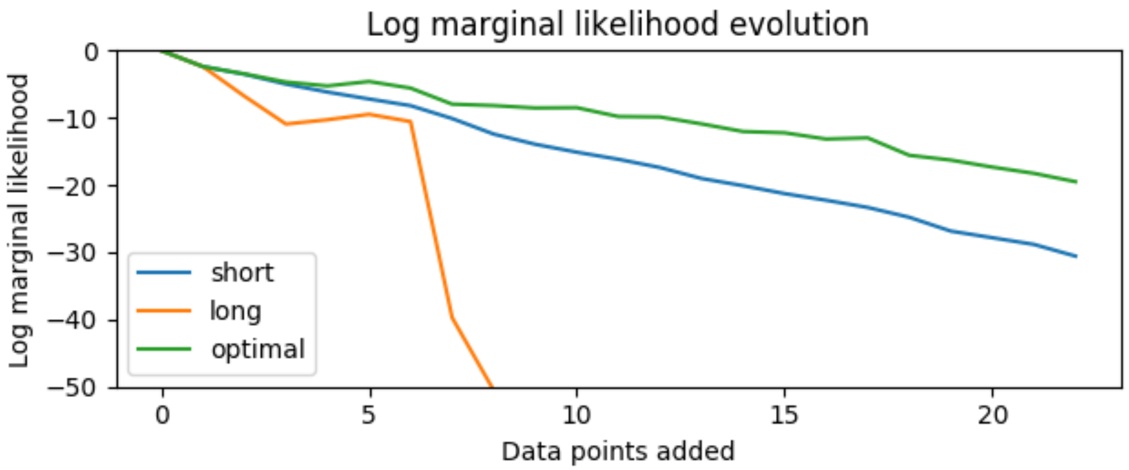
Marginal Likelihood Evolution



- Short lengthscale: consistently overestimates variance
  - No high density, even with observations inside the error bars

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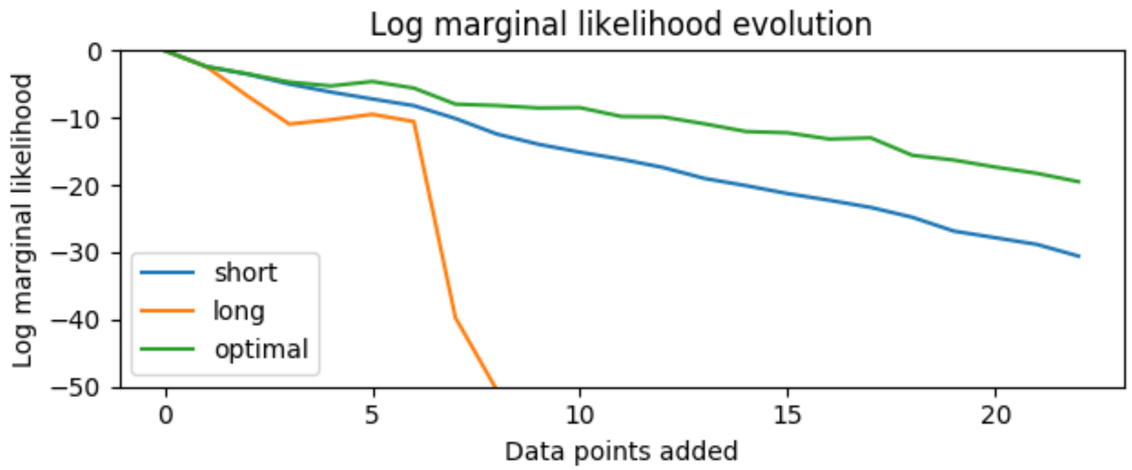

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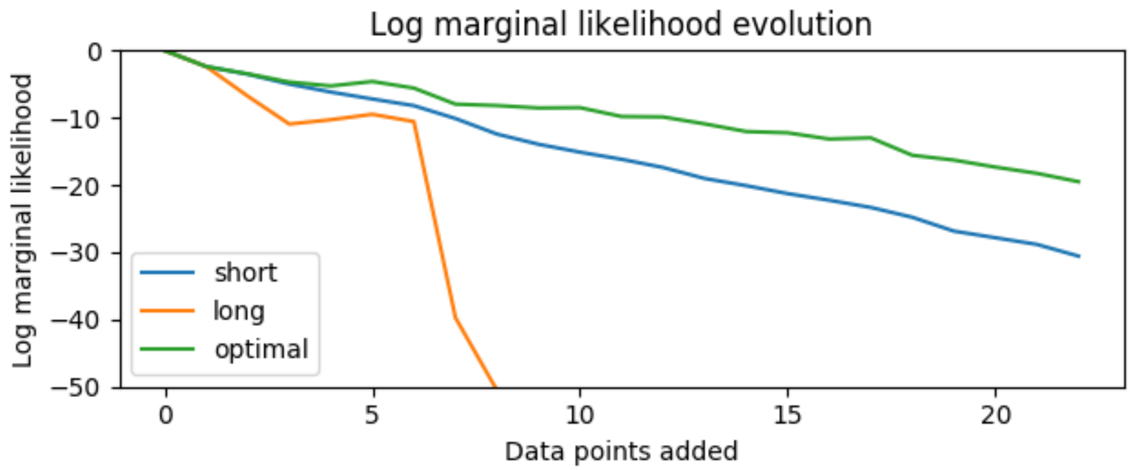

- Short lengthscale: consistently overestimates variance
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- Long lengthscale: consistently underestimates variance
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- Optimal lengthscale: trades off both behaviors reasonably well

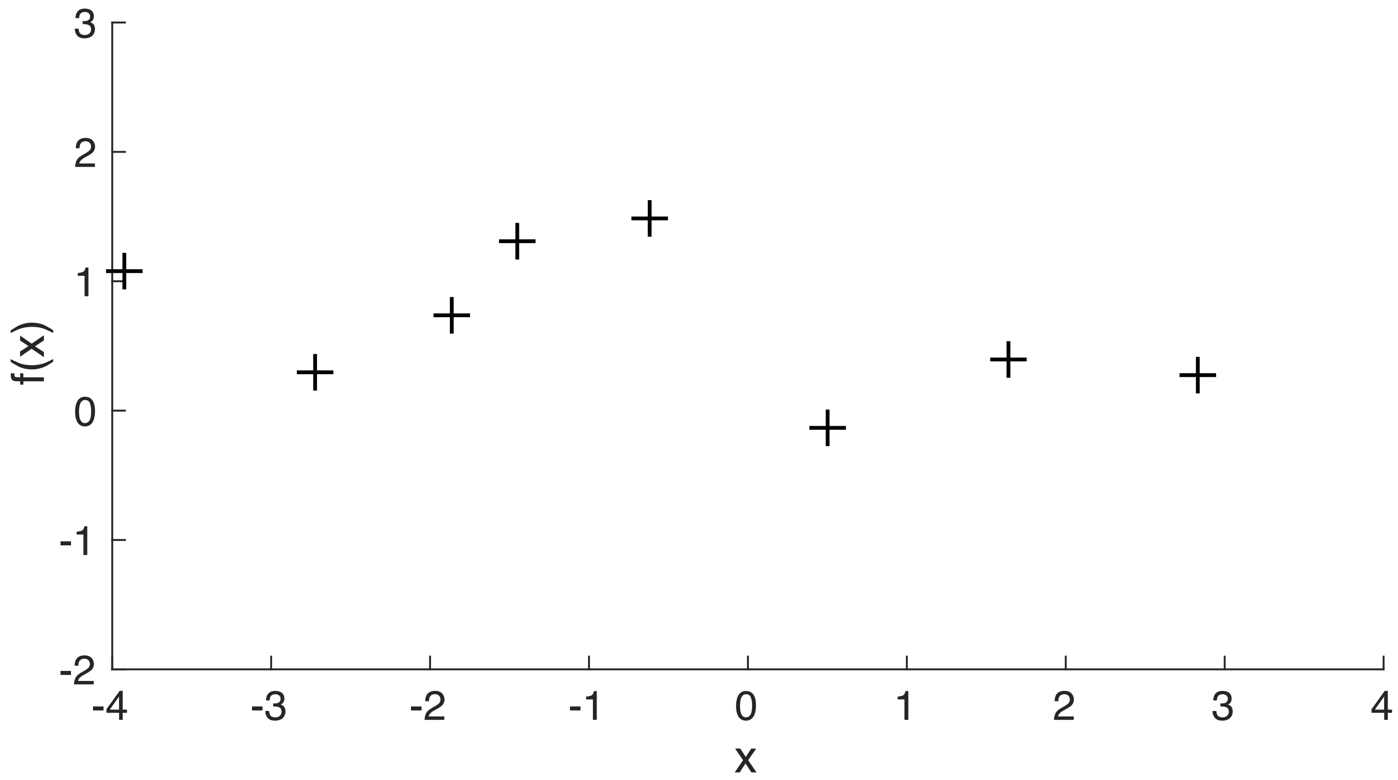
Model Selection—Mean Function and Kernel

- 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?

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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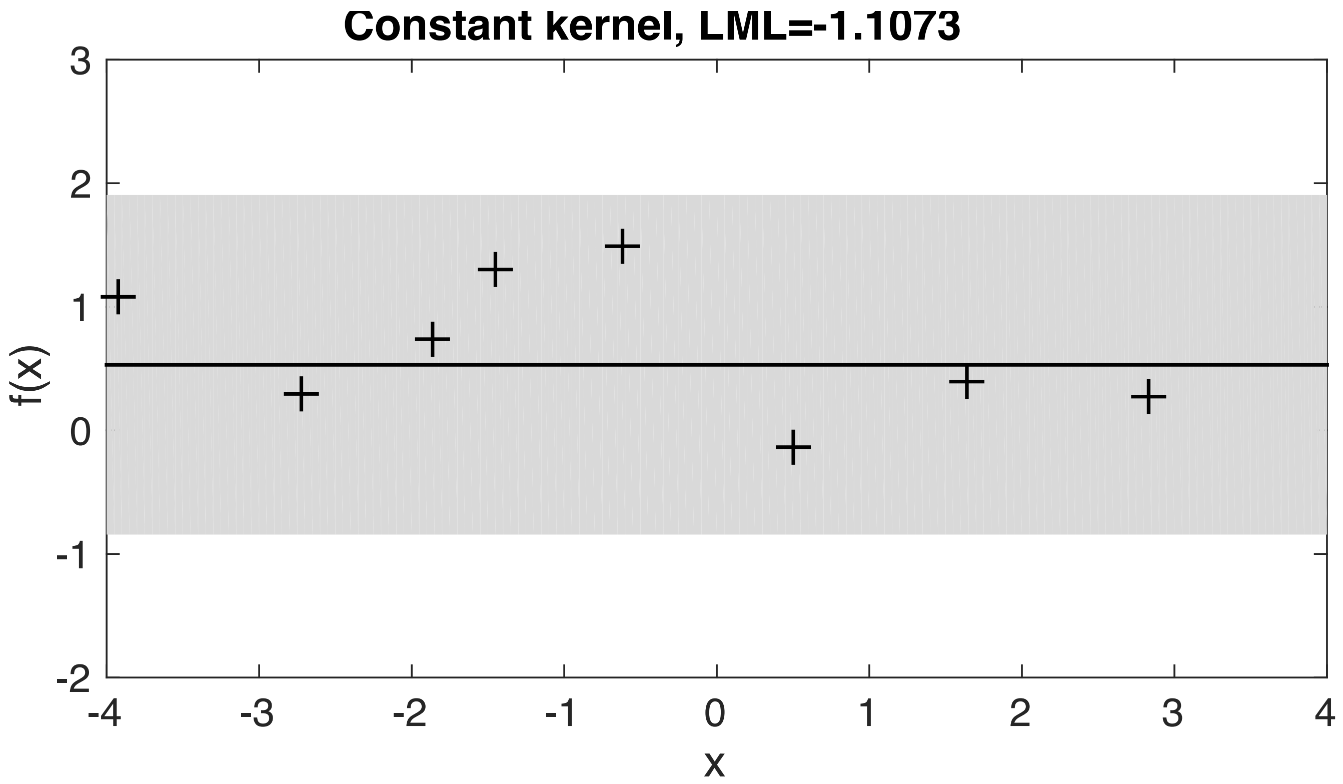

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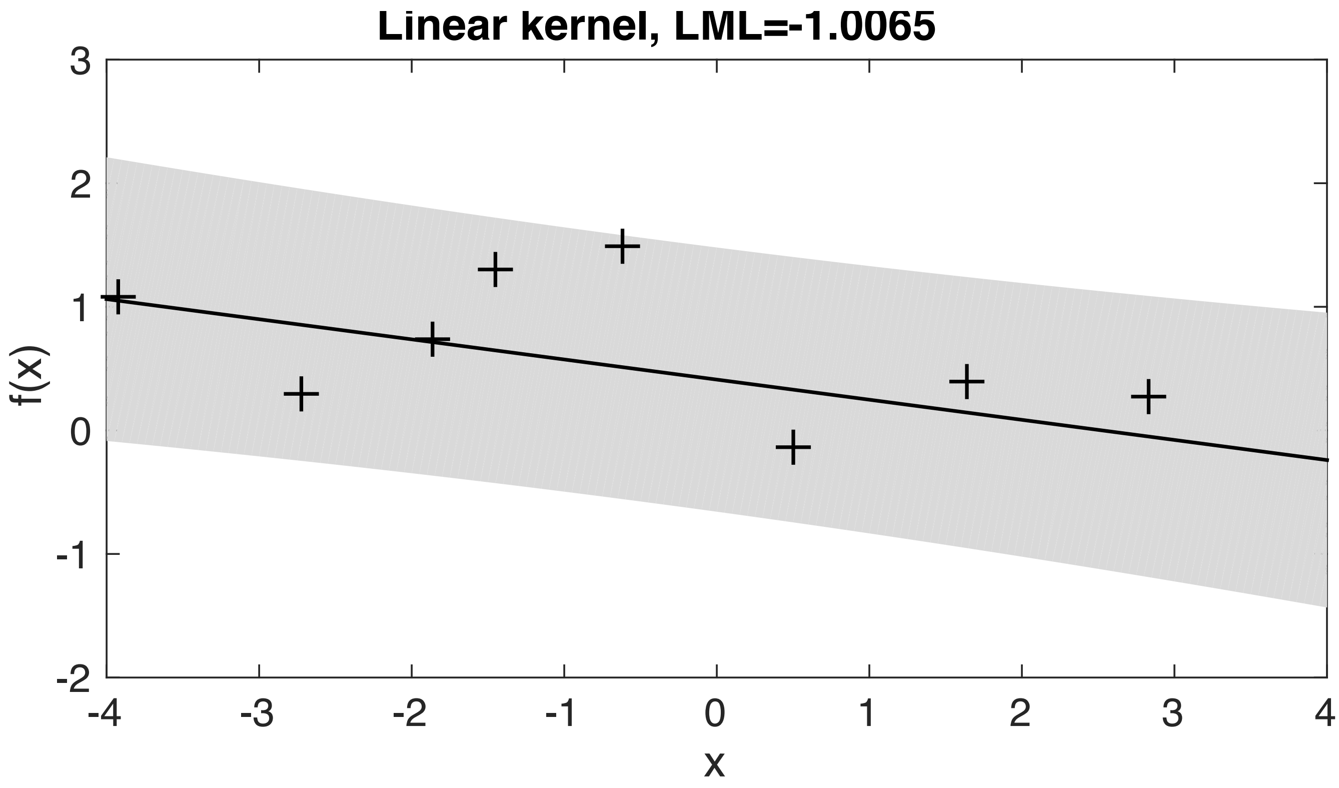

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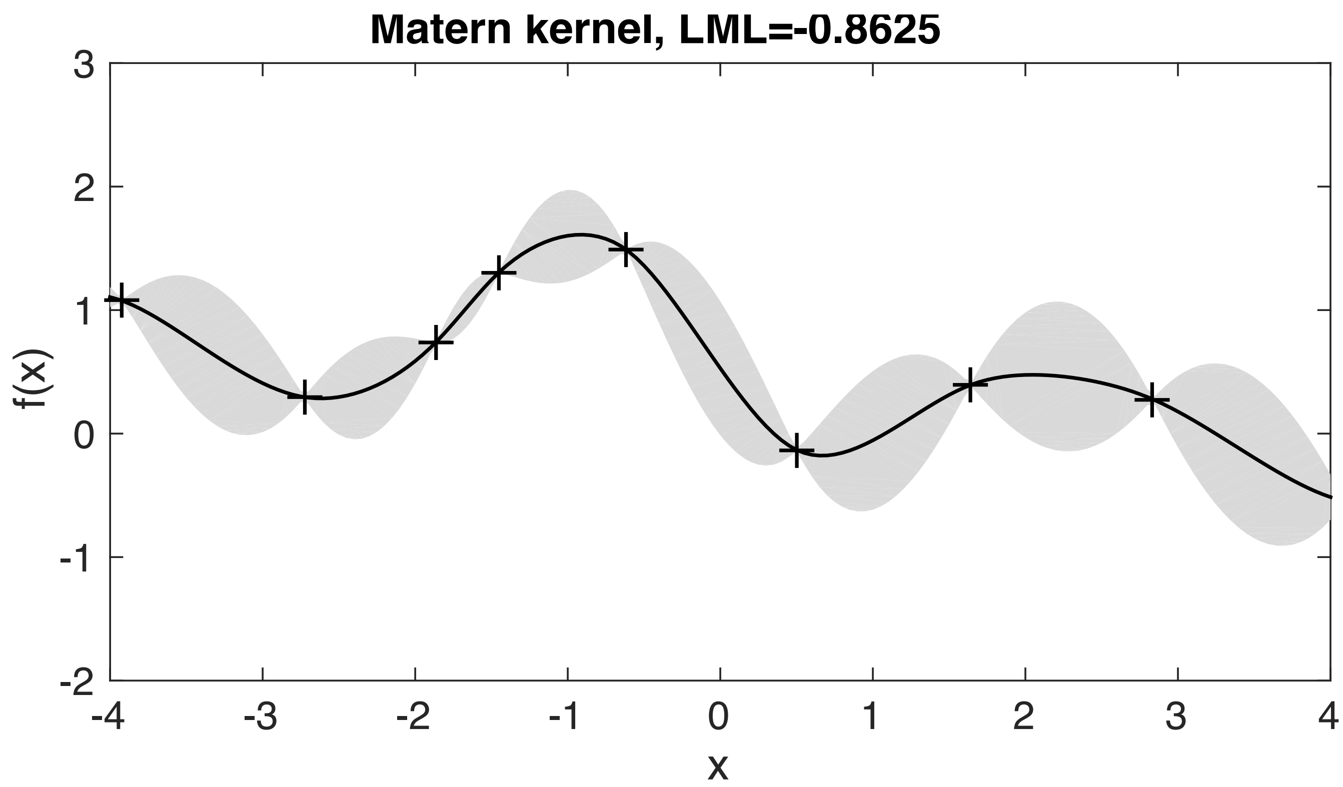

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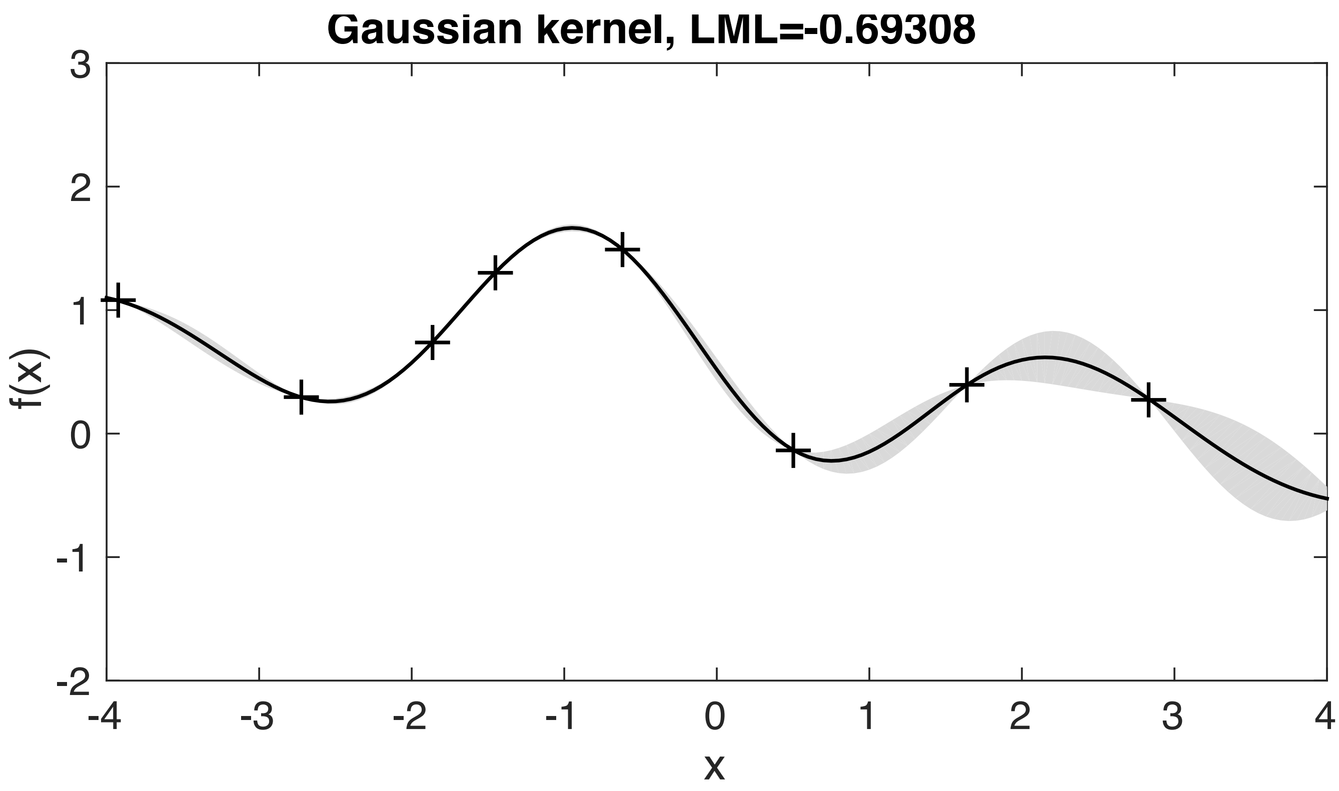

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GP Training: Illustration[5]

- 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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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

[5] Thanks to Mark van der Wilk

Limitations and Guidelines

Limitations of Gaussian Processes

Computational and memory complexity

Training set size: N

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

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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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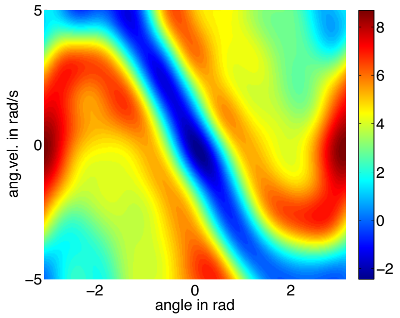
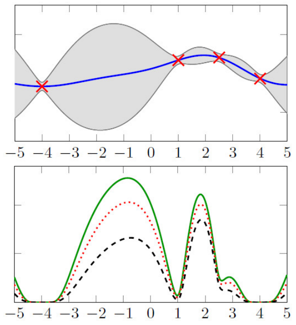
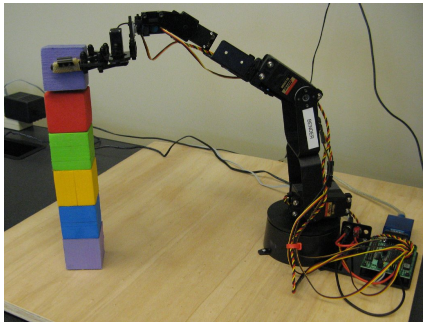
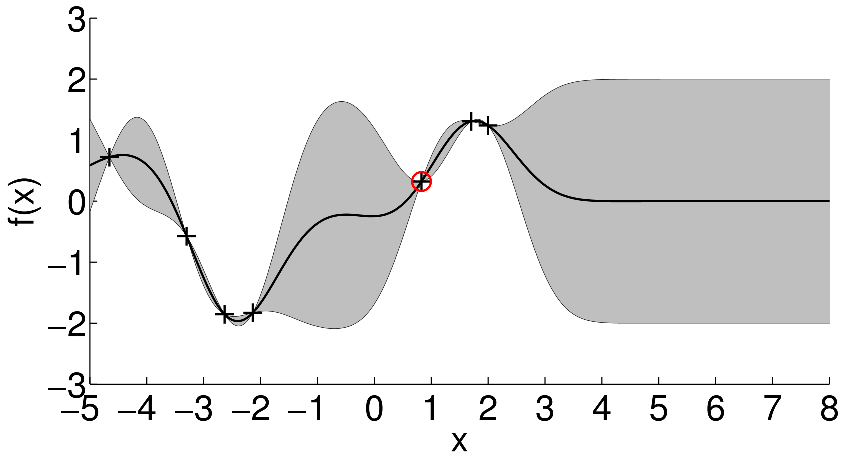


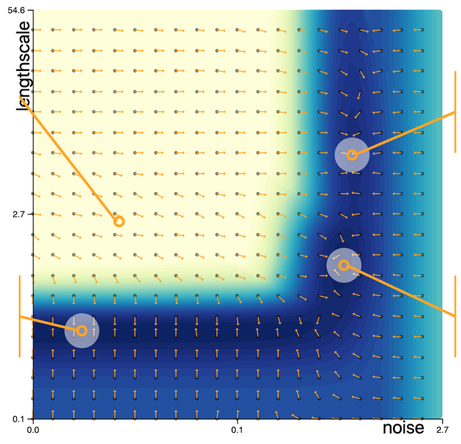




- Reinforcement learning and robotics
  - Model value functions and/or dynamics with GPs
- Bayesian optimization (Experimental Design)
  - Model unknown utility functions with GPs
- Geostatistics
  - Spatial modeling (e.g., landscapes, resources)
- Sensor networks
- Time-series modeling and forecasting

Summary





- 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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