Advances in Gaussian Processes

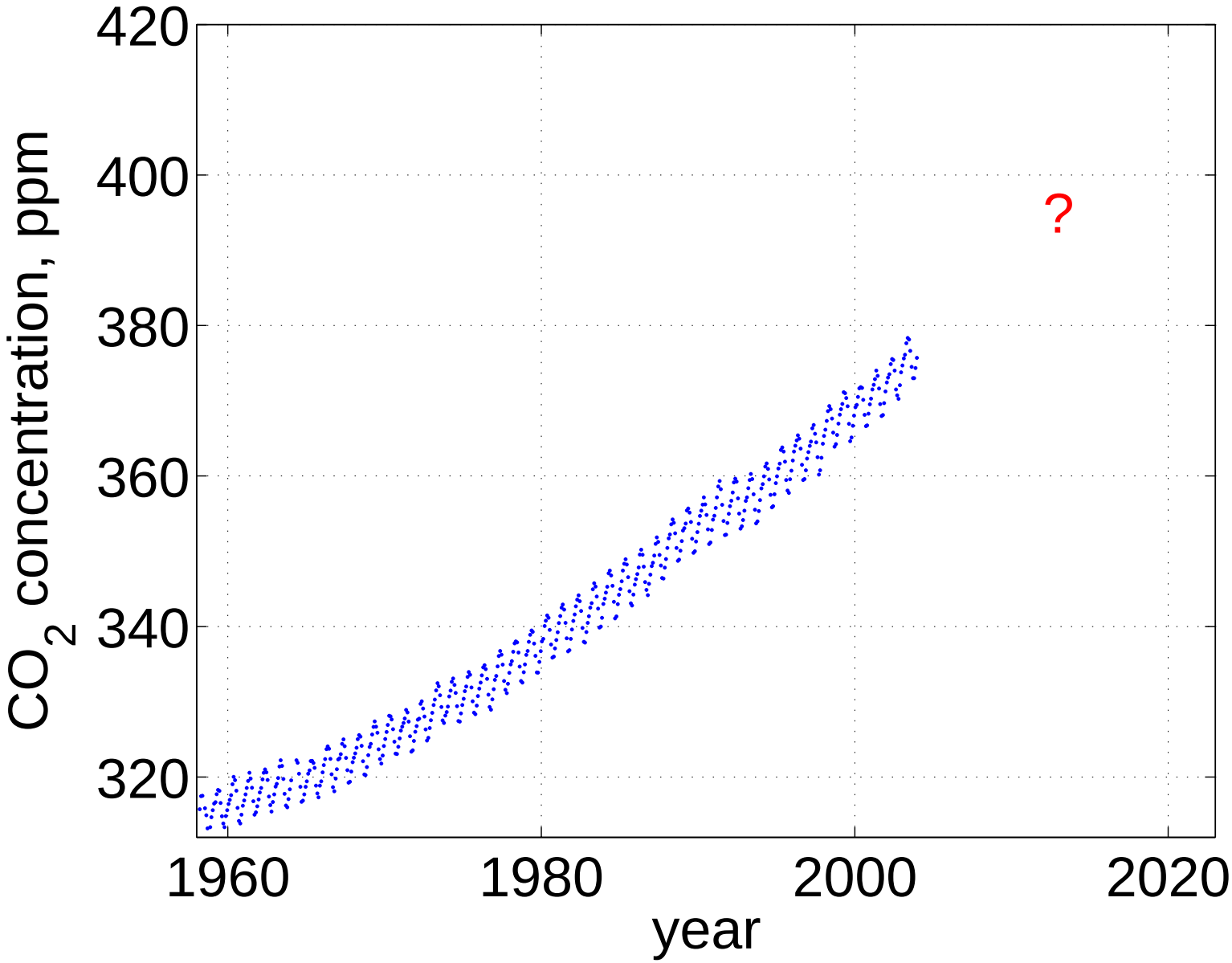
Tutorial at NIPS 2006 in Vancouver

Carl Edward Rasmussen

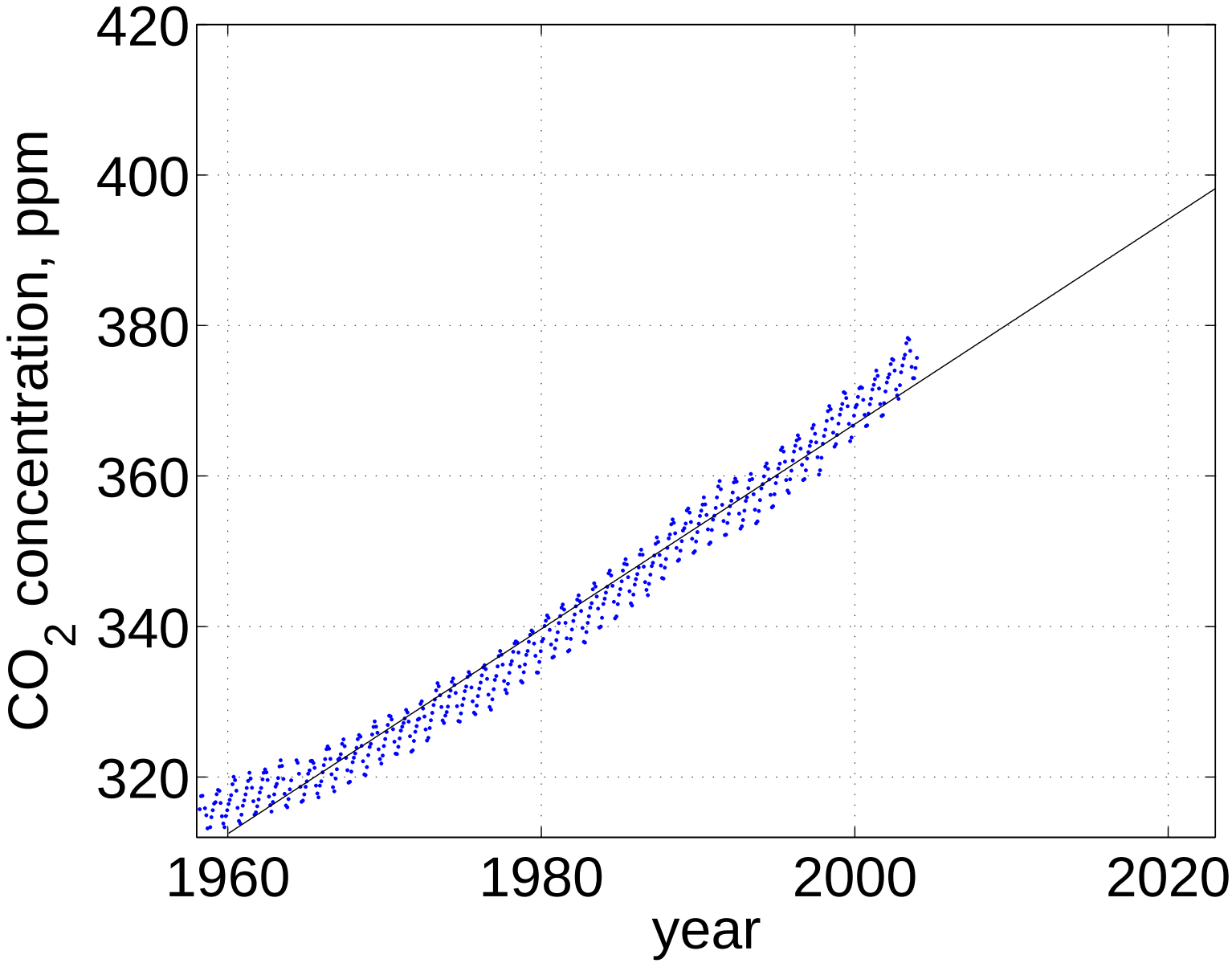
Max Planck Institute for Biological Cybernetics, Tübingen

December 4th, 2006

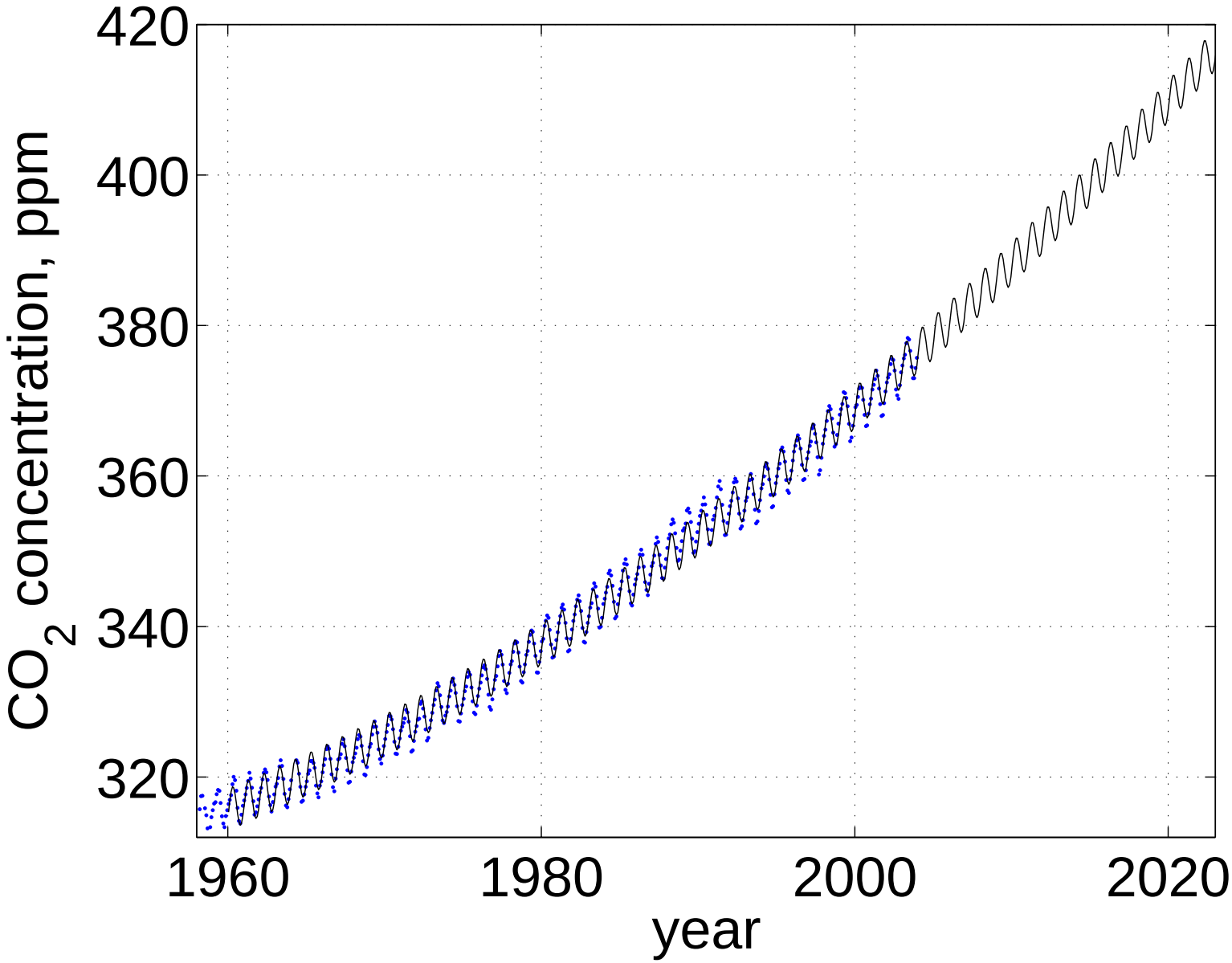
The Prediction Problem



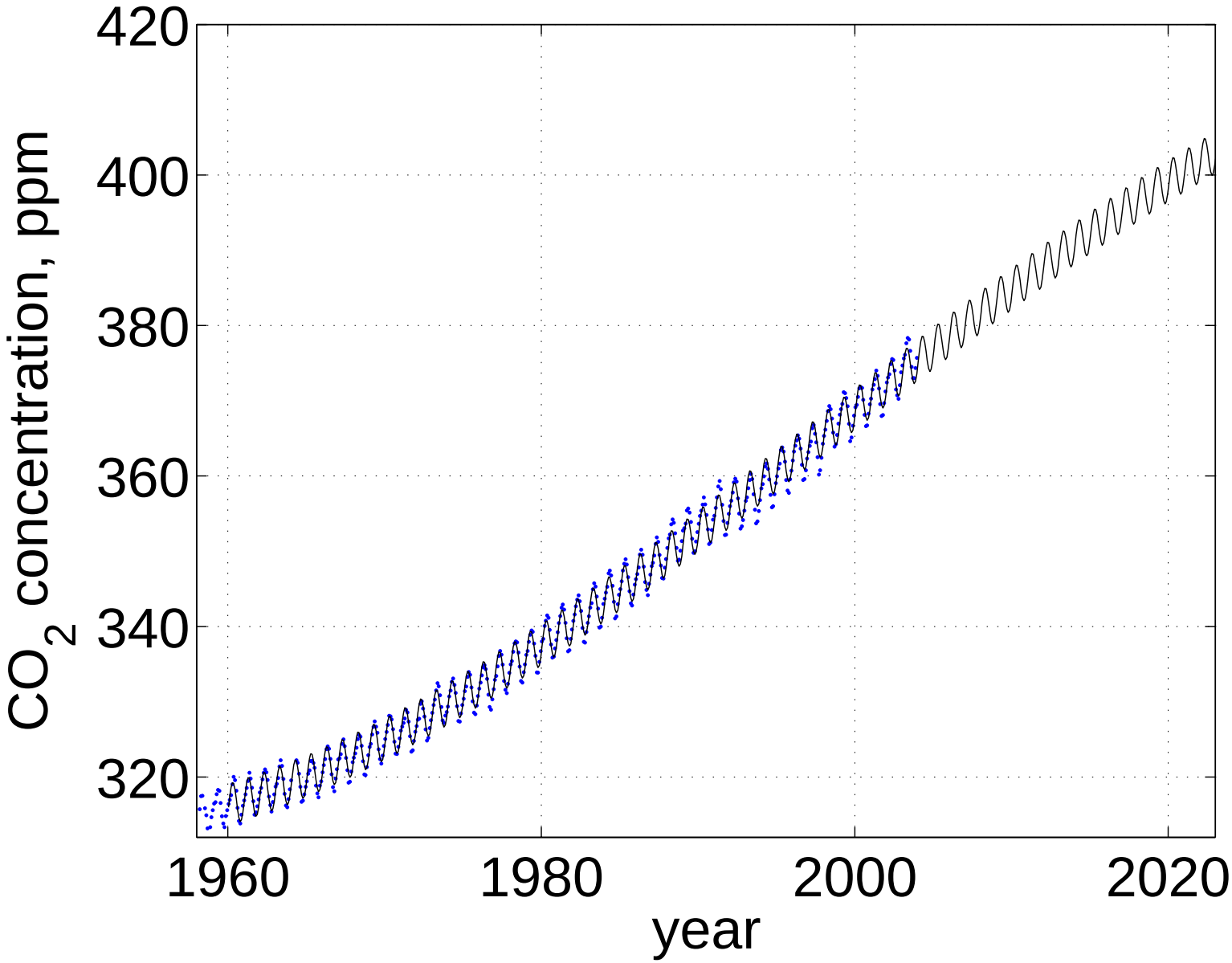
The Prediction Problem



The Prediction Problem



The Prediction Problem



The Prediction Problem

Ubiquitous questions:

- Model fitting
  - how do I fit the parameters?
  - what about overfitting?
- Model Selection
  - how to I find out which model to use?
  - how sure can I be?
- Interpretation
  - what is the accuracy of the predictions?
  - can I trust the predictions, even if
    - . . . I am not sure about the parameters?
    - . . . I am not sure of the model structure?

Gaussian processes solve some of the above, and provide a practical framework to address the remaining issues.

Outline

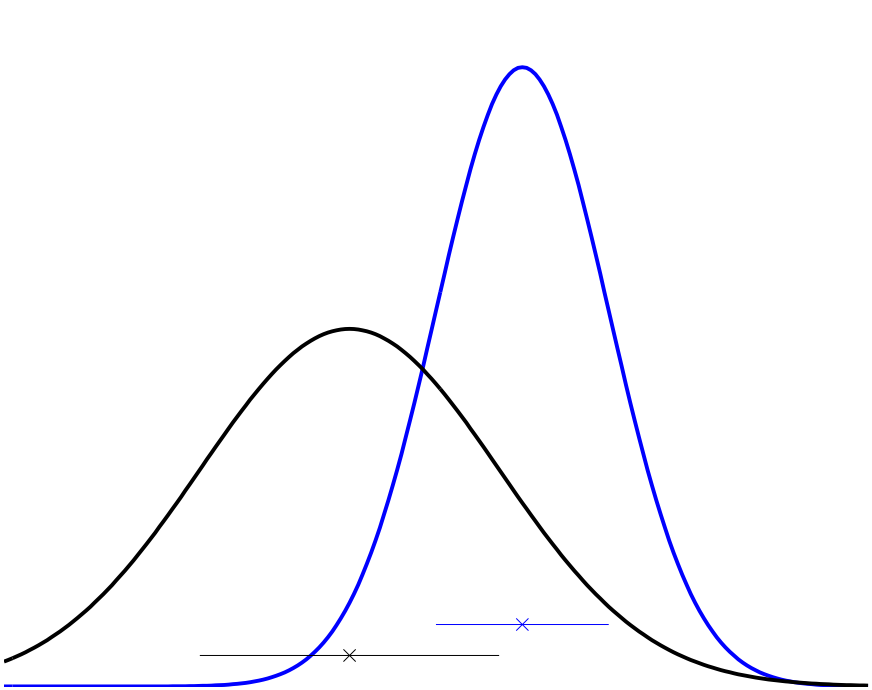
Part I: foundations

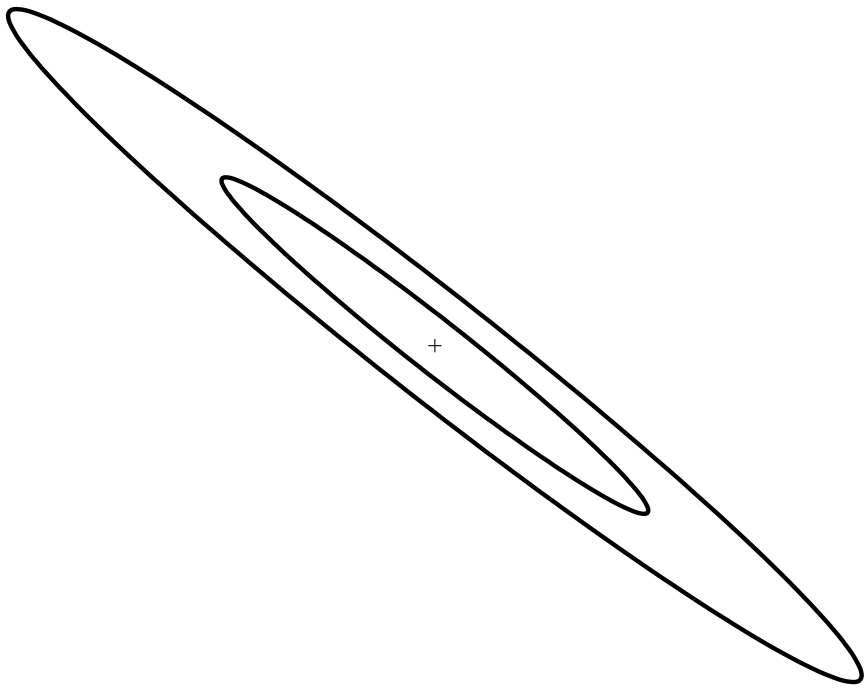
- What is a Gaussian process
  - from distribution to process
  - distribution over *functions*
  - the marginalization property
- Inference
  - Bayesian inference
  - posterior over functions
  - predictive distribution
  - marginal likelihood
  - Occam's Razor
  - automatic complexity penalty

Part II: advanced topics

- Example
  - priors over functions
  - hierarchical priors using hyperparameters
  - learning the covariance function
- Approximate methods for classification
- Gaussian Process latent variable models
- Sparse methods

The Gaussian Distribution



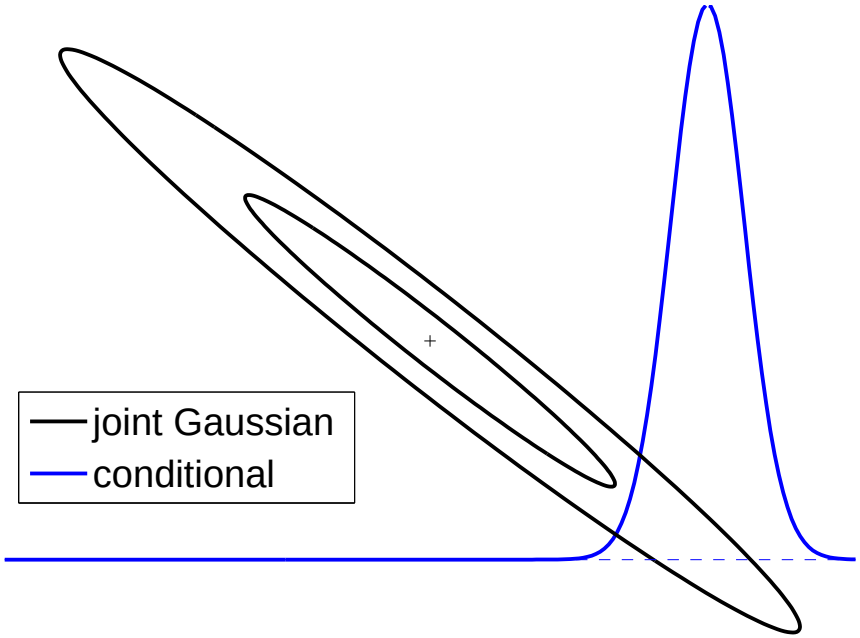


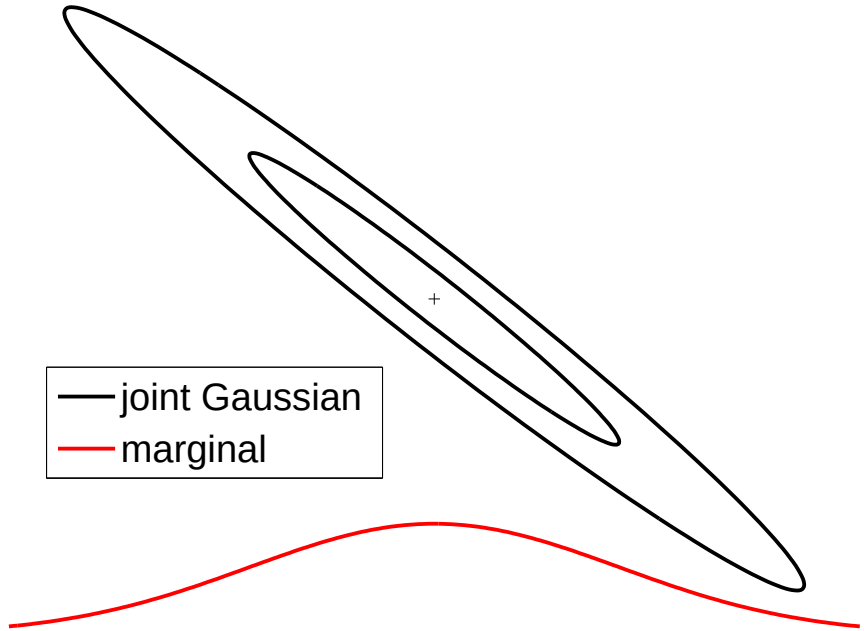
The Gaussian distribution is given by

$$p(\mathbf{x}|\mu,\Sigma) \;=\; \mathcal{N}(\mu,\Sigma) \;=\; (2\pi)^{-D/2}|\Sigma|^{-1/2}\exp\Big(-\tfrac{1}{2}(\mathbf{x}-\mu)^\top\Sigma^{-1}(\mathbf{x}-\mu)\Big)$$

where μ is the mean vector and Σ the covariance matrix.

Conditionals and Marginals of a Gaussian





Both the conditionals and the marginals of a joint Gaussian are again Gaussian.

What is a Gaussian Process?

A *Gaussian process* is a generalization of a multivariate Gaussian distribution to infinitely many variables.

Informally: infinitely long vector $\simeq$ function

> **Definition:** *a Gaussian process is a collection of random variables, any finite number of which have (consistent) Gaussian distributions.* □

A Gaussian distribution is fully specified by a mean vector, μ, and covariance matrix Σ:

$$\mathbf{f} = (f_1, \ldots, f_n)^\top \sim \mathcal{N}(\mu, \Sigma), \quad \text{indexes } i = 1, \ldots, n$$

A Gaussian process is fully specified by a mean function $m(x)$ and covariance function $k(x, x')$:

$$f(x) \sim \mathcal{GP}\big(m(x), k(x, x')\big), \quad \text{indexes: } x$$

The marginalization property

Thinking of a GP as a Gaussian distribution with an infinitely long mean vector and an infinite by infinite covariance matrix may seem impractical...

...luckily we are saved by the *marginalization property*:

Recall:

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}.$$

For Gaussians:

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\right) \implies p(\mathbf{x}) = \mathcal{N}(\mathbf{a}, A)$$

Random functions from a Gaussian Process

Example one dimensional Gaussian process:

$$p(f(x)) \sim \mathcal{GP}\big(m(x) = 0,\ k(x, x') = \exp(-\tfrac{1}{2}(x - x')^2)\big).$$

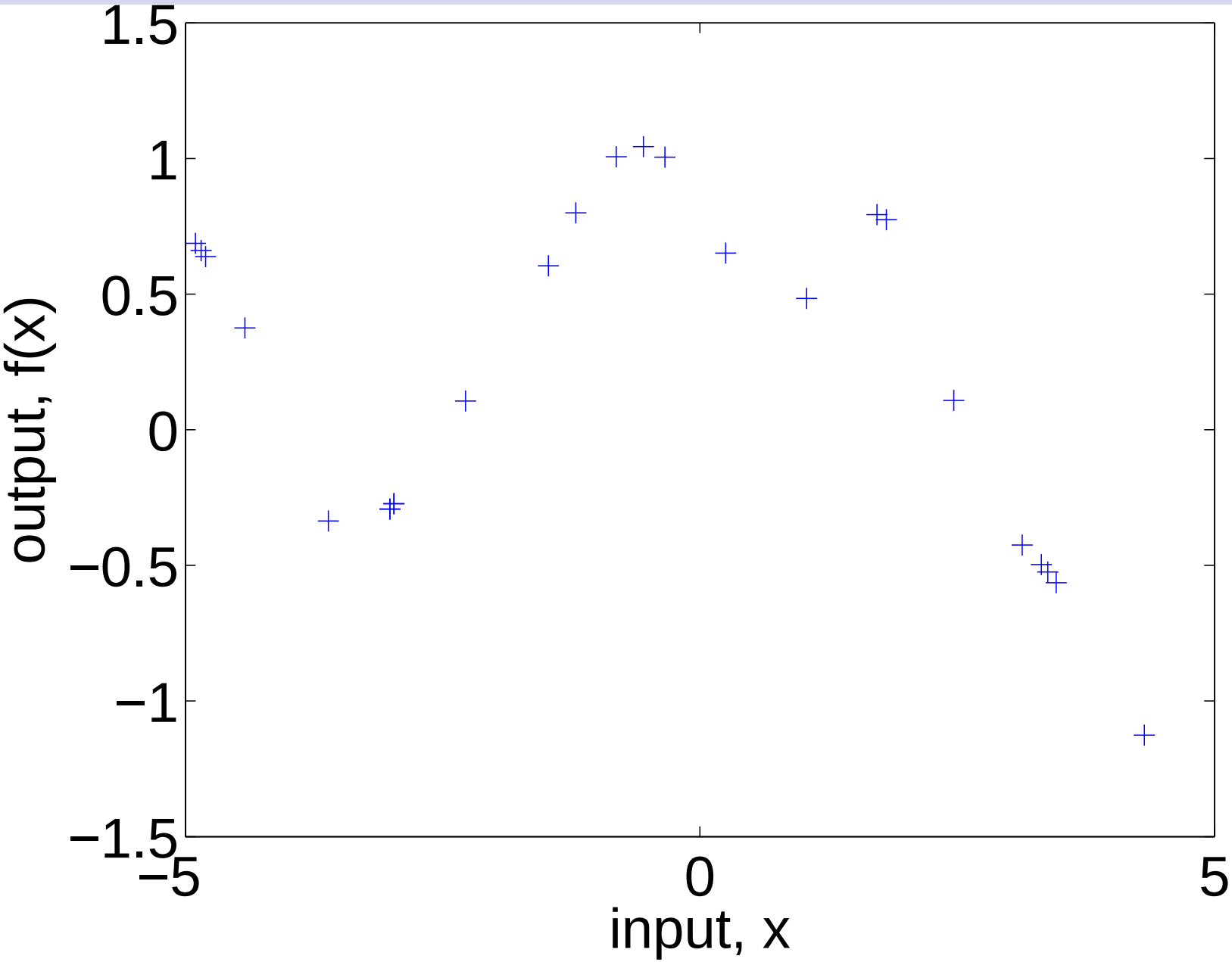
To get an indication of what this distribution over functions looks like, focus on a finite subset of function values $\mathbf{f} = (f(x_1), f(x_2), \ldots, f(x_n))^\top$, for which

$$\mathbf{f} \sim \mathcal{N}(0, \Sigma),$$

where $\Sigma_{ij} = k(x_i, x_j)$.

Then plot the coordinates of f as a function of the corresponding x values.

Some values of the random function



Sequential Generation

Factorize the joint distribution

$$p(f_1, \ldots, f_n | \mathbf{x}_1, \ldots \mathbf{x}_n) \;=\; \prod_{i=1}^{n} p(f_i | f_{i-1}, \ldots, f_1, \mathbf{x}_i, \ldots, \mathbf{x}_1),$$

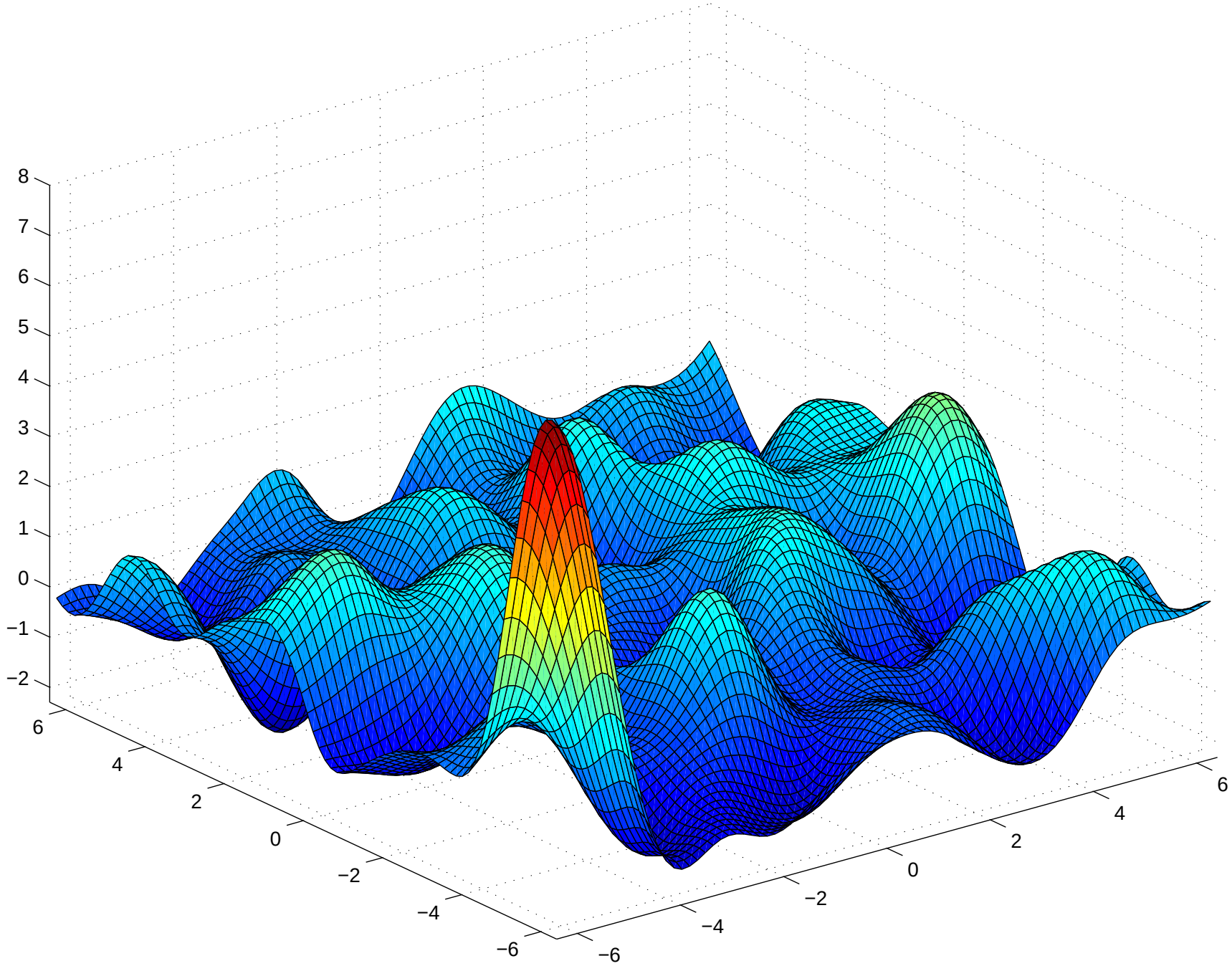
and generate function values sequentially.

What do the individual terms look like? For Gaussians:

$$p(\mathbf{x}, \mathbf{y}) \;=\; \mathcal{N}\Big(\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix}\Big) \;\Longrightarrow\; p(\mathbf{x}|\mathbf{y}) \;=\; \mathcal{N}(\mathbf{a}+BC^{-1}(\mathbf{y}-\mathbf{b}),\; A-BC^{-1}B^\top)$$

Do try this at home!

Function drawn at random from a Gaussian Process with Gaussian covariance



Maximum likelihood, parametric model

Supervised parametric learning:

- data: $\mathbf{x}, \mathbf{y}$
- model: $y = f_{\mathbf{w}}(x) + \varepsilon$

Gaussian likelihood:

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}, M_i) \propto \prod_c \exp(-\tfrac{1}{2}(y_c - f_{\mathbf{w}}(x_c))^2/\sigma^2_{\text{noise}}).$$

Maximize the likelihood:

$$\mathbf{w}_{\text{ML}} = \operatorname*{argmax}_{\mathbf{w}} p(\mathbf{y}|\mathbf{x}, \mathbf{w}, M_i).$$

Make predictions, by plugging in the ML estimate:

$$p(y^*|x^*, \mathbf{w}_{\text{ML}}, M_i)$$

Bayesian Inference, parametric model

Supervised parametric learning:

- data: $\mathbf{x}$, $\mathbf{y}$
- model: $y = f_{\mathbf{w}}(x) + \varepsilon$

Gaussian likelihood:

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}, M_i) \propto \prod_c \exp(-\tfrac{1}{2}(y_c - f_{\mathbf{w}}(x_c))^2/\sigma^2_{\text{noise}}).$$

Parameter prior:

$$p(\mathbf{w}|M_i)$$

Posterior parameter distribution by Bayes rule $p(a|b) = p(b|a)p(a)/p(b)$:

$$p(\mathbf{w}|\mathbf{x}, \mathbf{y}, M_i) = \frac{p(\mathbf{w}|M_i)p(\mathbf{y}|\mathbf{x}, \mathbf{w}, M_i)}{p(\mathbf{y}|\mathbf{x}, M_i)}$$

Bayesian Inference, parametric model, cont.

Making predictions:

$$p(y^*|x^*, \mathbf{x}, \mathbf{y}, M_i) = \int p(y^*|\mathbf{w}, x^*, M_i) p(\mathbf{w}|\mathbf{x}, \mathbf{y}, M_i) d\mathbf{w}$$

Marginal likelihood:

$$p(\mathbf{y}|\mathbf{x}, M_i) = \int p(\mathbf{w}|M_i) p(\mathbf{y}|\mathbf{x}, \mathbf{w}, M_i) d\mathbf{w}.$$

Model probability:

$$p(M_i|\mathbf{x}, \mathbf{y}) = \frac{p(M_i) p(\mathbf{y}|\mathbf{x}, M_i)}{p(\mathbf{y}|\mathbf{x})}$$

Problem: integrals are intractable for most interesting models!

Non-parametric Gaussian process models

In our non-parametric model, the "parameters" is the function itself!

Gaussian likelihood:

$$\mathbf{y}|\mathbf{x}, f(x), M_i \;\sim\; \mathcal{N}(\mathbf{f},\; \sigma^2_{\text{noise}} I)$$

(Zero mean) Gaussian process prior:

$$f(x)|M_i \;\sim\; \mathcal{GP}\big(m(x) \equiv 0,\; k(x, x')\big)$$

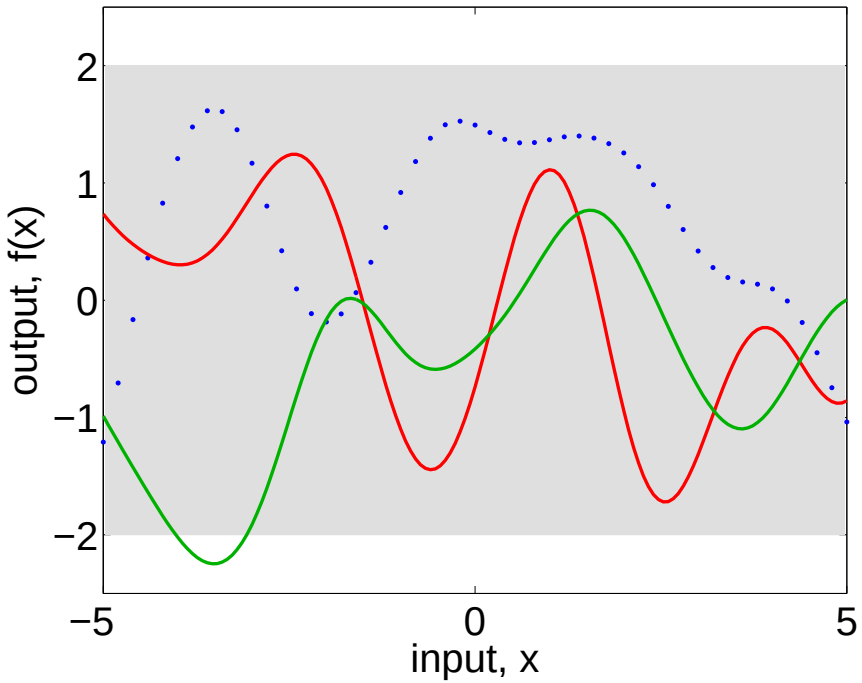
Leads to a Gaussian process posterior

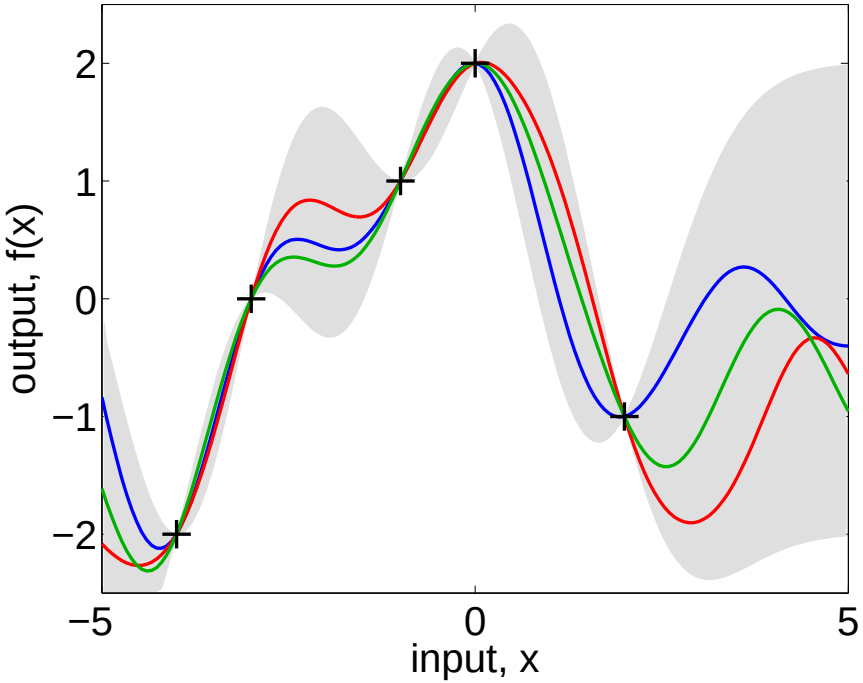
$$f(x)|\mathbf{x}, \mathbf{y}, M_i \;\sim\; \mathcal{GP}\big(m_{\text{post}}(x) = k(x, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1}\mathbf{y},$$
$$k_{\text{post}}(x, x') = k(x, x') - k(x, \mathbf{x})[K(\mathbf{x}, \mathbf{x}) + \sigma^2_{\text{noise}} I]^{-1} k(\mathbf{x}, x')\big).$$

And a Gaussian predictive distribution:

$$y^*|x^*, \mathbf{x}, \mathbf{y}, M_i \;\sim\; \mathcal{N}\big(\mathbf{k}(x^*, \mathbf{x})^\top [K + \sigma^2_{\text{noise}} I]^{-1}\mathbf{y},$$
$$k(x^*, x^*) + \sigma^2_{\text{noise}} - \mathbf{k}(x^*, \mathbf{x})^\top [K + \sigma^2_{\text{noise}} I]^{-1}\mathbf{k}(x^*, \mathbf{x})\big)$$

Prior and Posterior

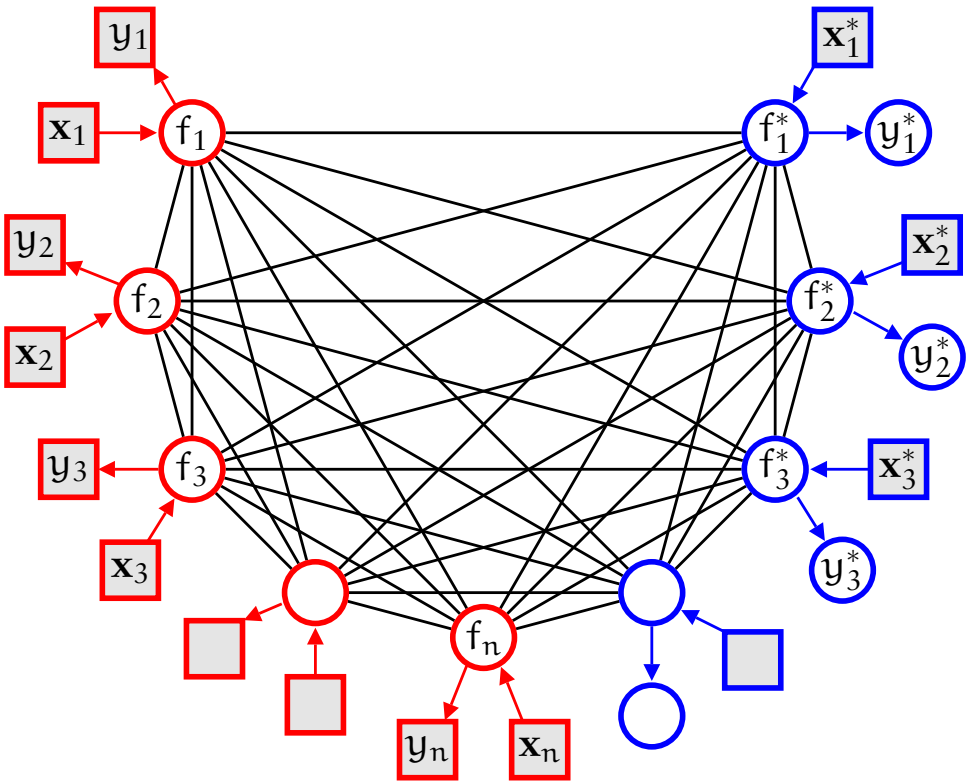




Predictive distribution:

$$p(y^*|x^*, \mathbf{x}, \mathbf{y}) \sim \mathcal{N}\big(\mathbf{k}(x^*, \mathbf{x})^\top [K + \sigma^2_{\text{noise}} I]^{-1} \mathbf{y}, \\ k(x^*, x^*) + \sigma^2_{\text{noise}} - \mathbf{k}(x^*, \mathbf{x})^\top [K + \sigma^2_{\text{noise}} I]^{-1} \mathbf{k}(x^*, \mathbf{x})\big)$$

Graphical model for Gaussian Process



Square nodes are observed (clamped), round nodes stochastic (free).

All pairs of latent variables are connected.

Predictions y^* depend only on the corresponding single latent f^*.

Notice, that adding a triplet x_m^*, f_m^*, y_m^* does not influence the distribution. This is guaranteed by the marginalization property of the GP.

This explains why we can make inference using a finite amount of computation!

Some interpretation

Recall our main result:

$$\mathbf{f}_*|X_*, X, \mathbf{y} \sim \mathcal{N}\big(K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1}\mathbf{y}, \\ K(X_*, X_*) - K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1}K(X, X_*)\big).$$

The mean is linear in two ways:

$$\mu(\mathbf{x}_*) = k(\mathbf{x}_*, X)[K(X, X) + \sigma_n^2]^{-1}\mathbf{y} = \sum_{c=1}^{n} \beta_c y^{(c)} = \sum_{c=1}^{n} \alpha_c k(\mathbf{x}_*, \mathbf{x}^{(c)}).$$

The last form is most commonly encountered in the kernel literature.

The variance is the difference between two terms:

$$V(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}(\mathbf{x}_*, X)[K(X, X) + \sigma_n^2 I]^{-1}\mathbf{k}(X, \mathbf{x}_*),$$

the first term is the *prior variance*, from which we subtract a (positive) term, telling how much the data X has explained. Note, that the variance is independent of the observed outputs $\mathbf{y}$.

The marginal likelihood

Log marginal likelihood:

$$\log p(\mathbf{y}|\mathbf{x}, M_i) = -\frac{1}{2}\mathbf{y}^\top K^{-1}\mathbf{y} - \frac{1}{2}\log|K| - \frac{n}{2}\log(2\pi)$$

is the combination of a data fit term and complexity penalty. Occam's Razor is automatic.

Learning in Gaussian process models involves finding

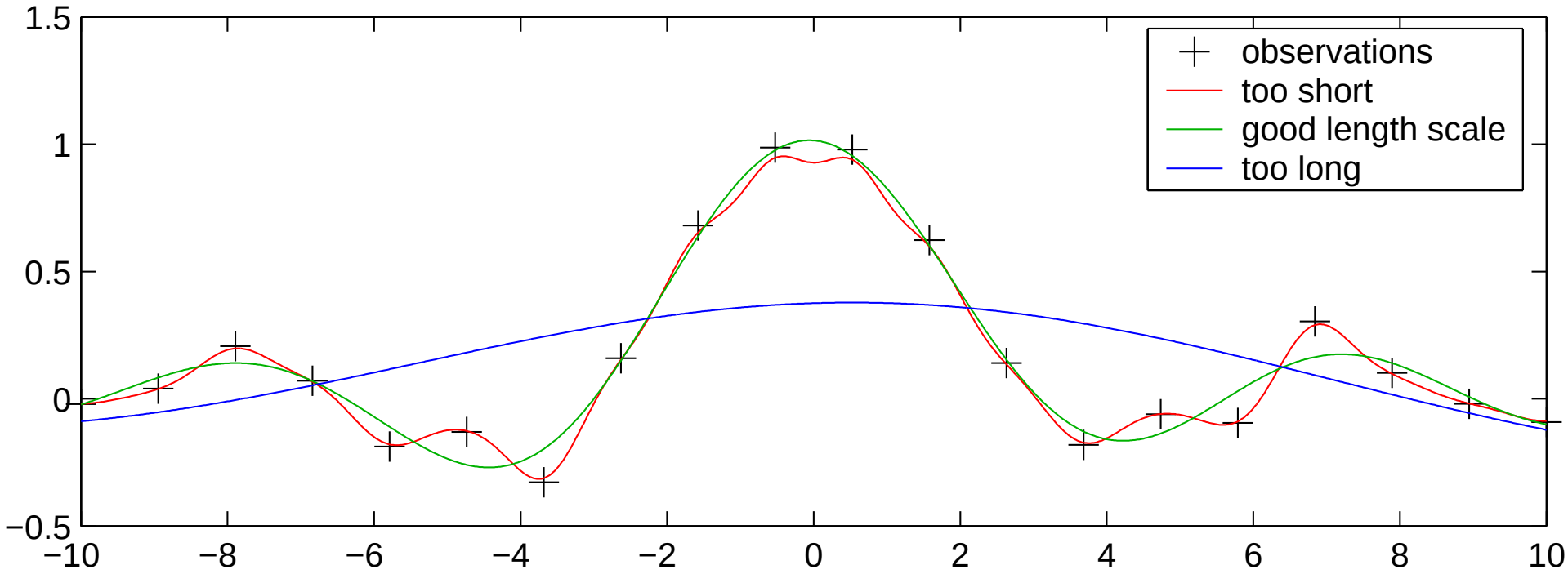
- the form of the covariance function, and
- any unknown (hyper-) parameters θ.

This can be done by optimizing the marginal likelihood:

$$\frac{\partial \log p(\mathbf{y}|\mathbf{x}, \theta, M_i)}{\partial \theta_j} = \frac{1}{2}\mathbf{y}^\top K^{-1}\frac{\partial K}{\partial \theta_j}K^{-1}\mathbf{y} - \frac{1}{2}\mathrm{trace}(K^{-1}\frac{\partial K}{\partial \theta_j})$$

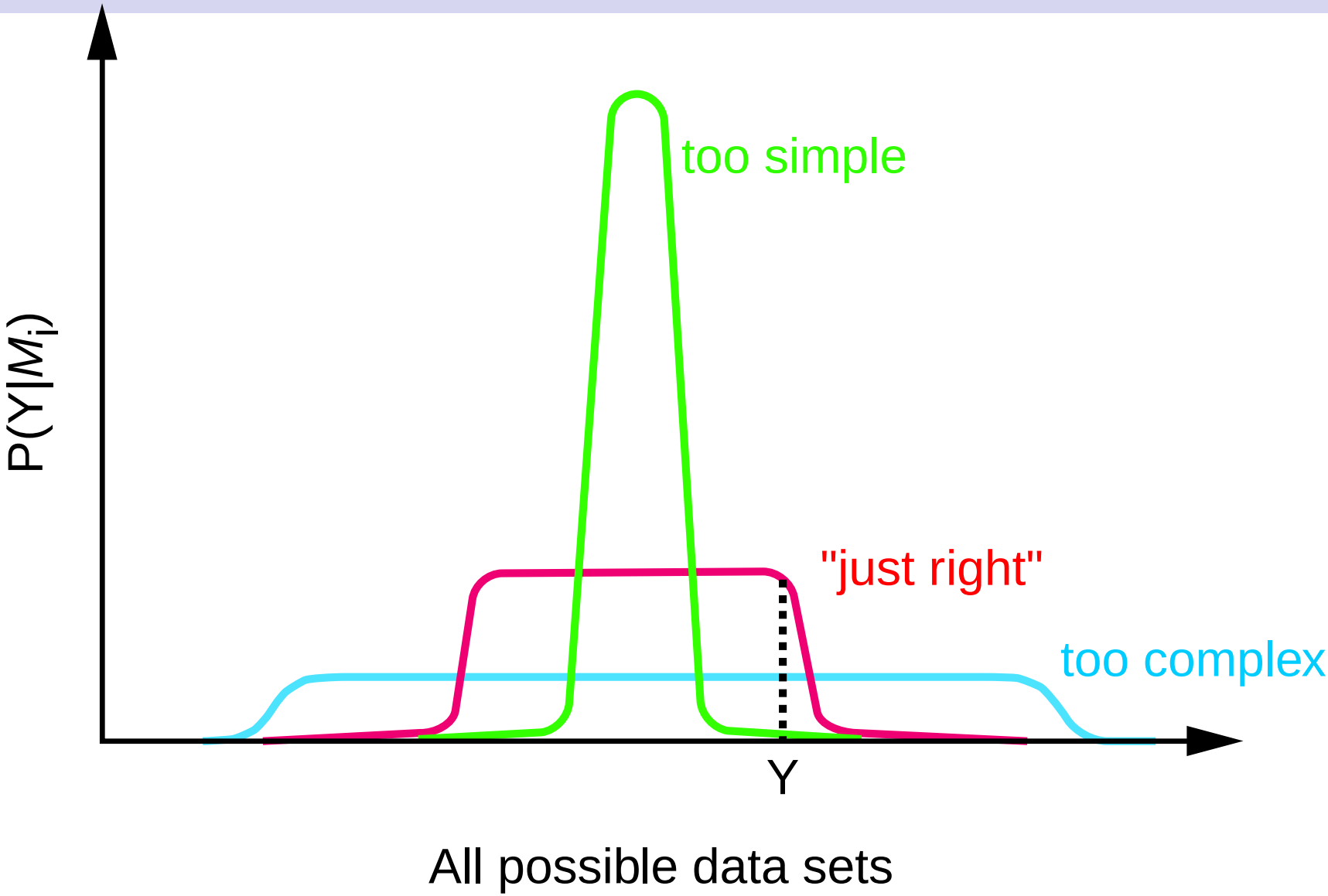
Example: Fitting the length scale parameter

Parameterized covariance function: $k(x, x') = v^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right) + \sigma_n^2 \delta_{xx'}$.



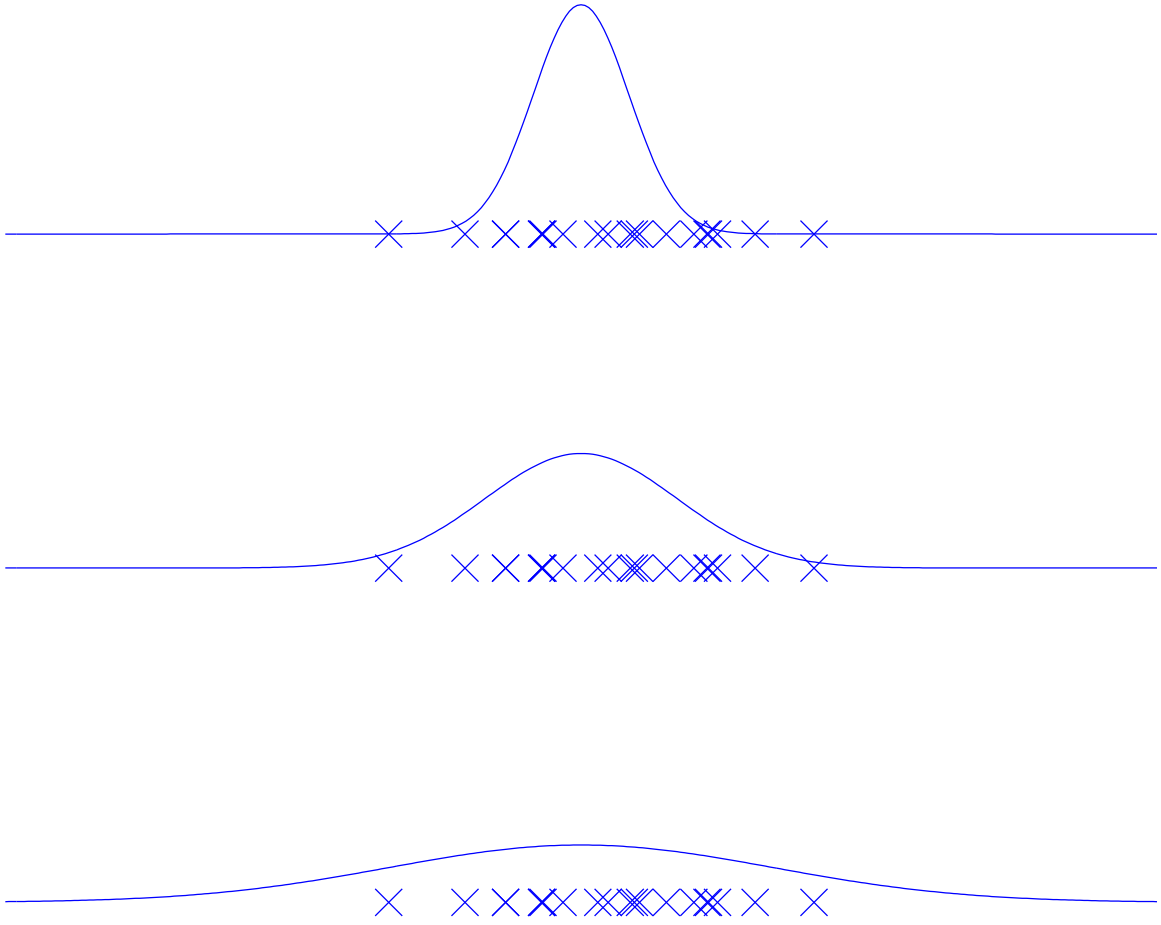
The mean posterior predictive function is plotted for 3 different length scales (the green curve corresponds to optimizing the marginal likelihood). Notice, that an almost exact fit to the data can be achieved by reducing the length scale – but the marginal likelihood does not favour this!

Why, in principle, does Bayesian Inference work? Occam's Razor



An illustrative analogous example

Imagine the simple task of fitting the variance, σ^2, of a zero-mean Gaussian to a set of n scalar observations.



The log likelihood is $\log p(\mathbf{y}|\mu, \sigma^2) = -\frac{1}{2}\sum(y_i - \mu)^2/\sigma^2 - \frac{n}{2}\log(\sigma^2) - \frac{n}{2}\log(2\pi)$

From random functions to covariance functions

Consider the class of linear functions:

$$f(x) = ax + b, \quad \text{where} \quad a \sim \mathcal{N}(0, \alpha), \quad \text{and} \quad b \sim \mathcal{N}(0, \beta).$$

We can compute the mean function:

$$\mu(x) = E[f(x)] = \iint f(x)p(a)p(b)dadb = \int axp(a)da + \int bp(b)db = 0,$$

and covariance function:

$$\begin{aligned} k(x, x') &= E[(f(x) - 0)(f(x') - 0)] = \iint (ax + b)(ax' + b)p(a)p(b)dadb \\ &= \int a^2 xx' p(a)da + \int b^2 p(b)db + (x + x') \int abp(a)p(b)dadb = \alpha xx' + \beta. \end{aligned}$$

From random functions to covariance functions II

Consider the class of functions (sums of squared exponentials):

$$f(x) = \lim_{n\to\infty} \frac{1}{n} \sum_i \gamma_i \exp(-(x - i/n)^2), \quad \text{where } \gamma_i \sim \mathcal{N}(0,1), \ \forall i$$

$$= \int_{-\infty}^{\infty} \gamma(u) \exp(-(x-u)^2) du, \quad \text{where } \gamma(u) \sim \mathcal{N}(0,1), \ \forall u.$$

The mean function is:

$$\mu(x) = E[f(x)] = \int_{-\infty}^{\infty} \exp(-(x-u)^2) \int_{-\infty}^{\infty} \gamma p(\gamma) d\gamma du = 0,$$

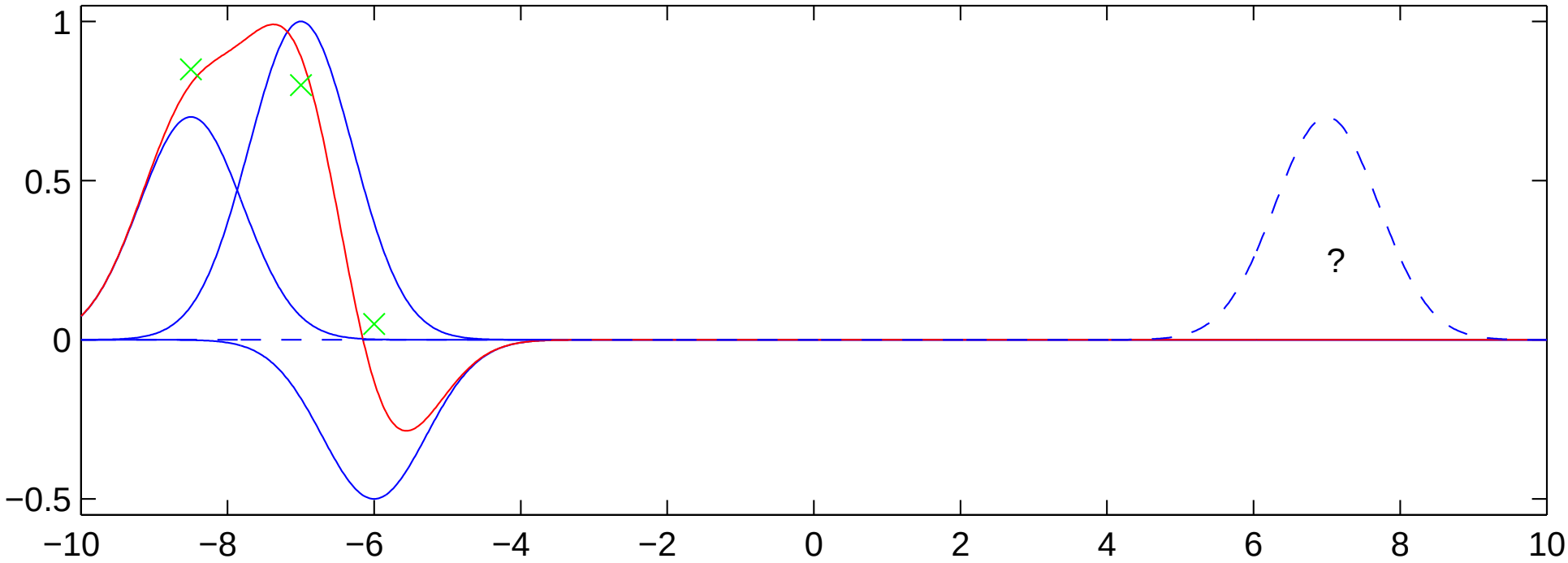
and the covariance function:

$$E[f(x)f(x')] = \int \exp\left(-(x-u)^2 - (x'-u)^2\right) du$$

$$= \int \exp\left(-2(u - \frac{x+x'}{2})^2 + \frac{(x+x')^2}{2} - x^2 - x'^2\right) du \ \propto \ \exp\left(-\frac{(x-x')^2}{2}\right).$$

Thus, the squared exponential covariance function is equivalent to regression using infinitely many Gaussian shaped basis functions placed everywhere, not just at your training points!

Using finitely many basis functions may be dangerous!



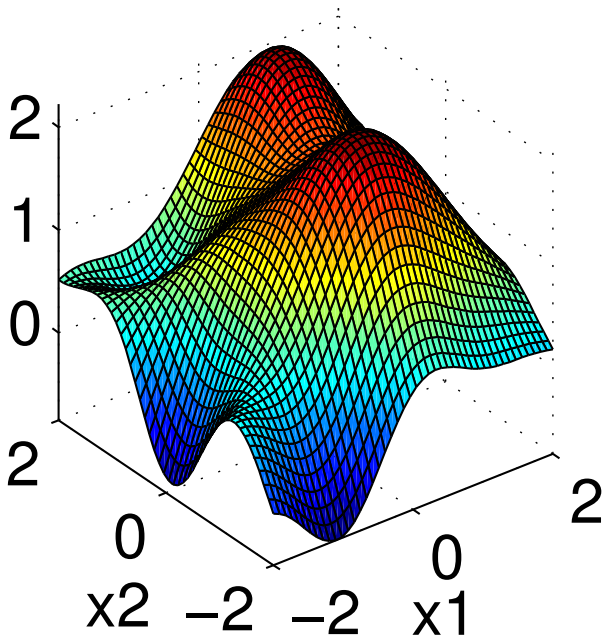
Model Selection in Practise; Hyperparameters

There are two types of task: *form* and *parameters* of the covariance function.

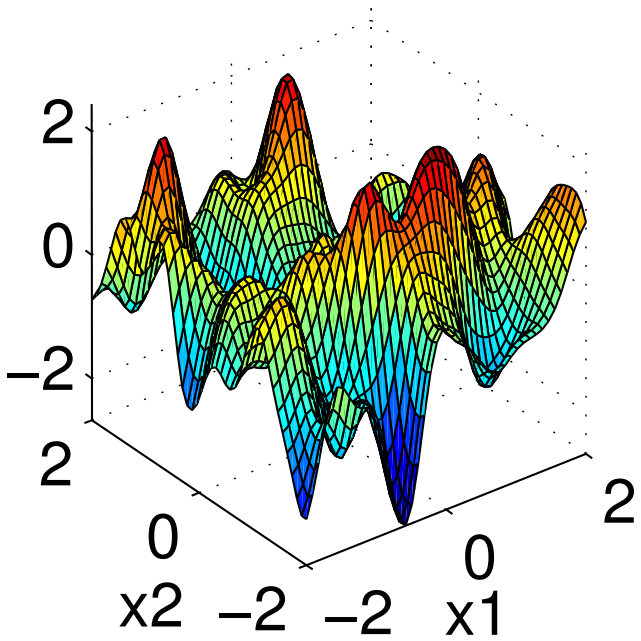
Typically, our prior is too weak to quantify aspects of the covariance function.
We use a hierarchical model using hyperparameters. Eg, in ARD:

$$k(\mathbf{x}, \mathbf{x}') = v_0^2 \exp\left(-\sum_{d=1}^{D} \frac{(x_d - x'_d)^2}{2v_d^2}\right), \qquad \text{hyperparameters } \theta = (v_0, v_1, \ldots, v_d, \sigma_n^2).$$

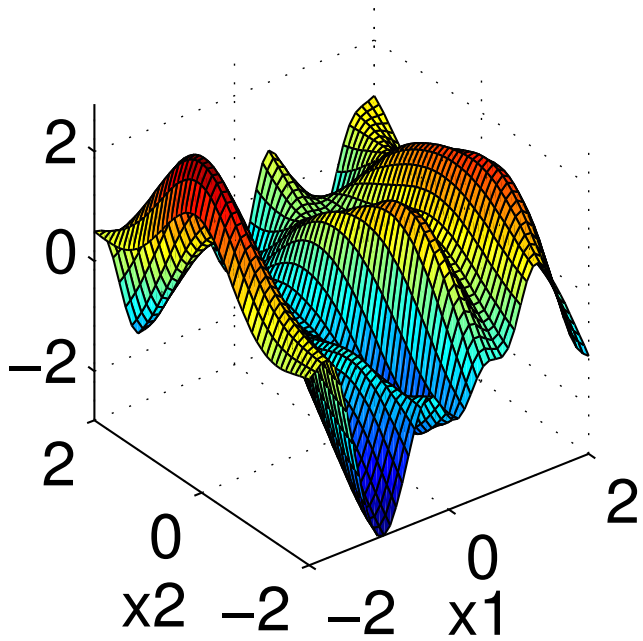
v1=v2=1



v1=v2=0.32



v1=0.32 and v2=1



Rational quadratic covariance function

The *rational quadratic* (RQ) covariance function:

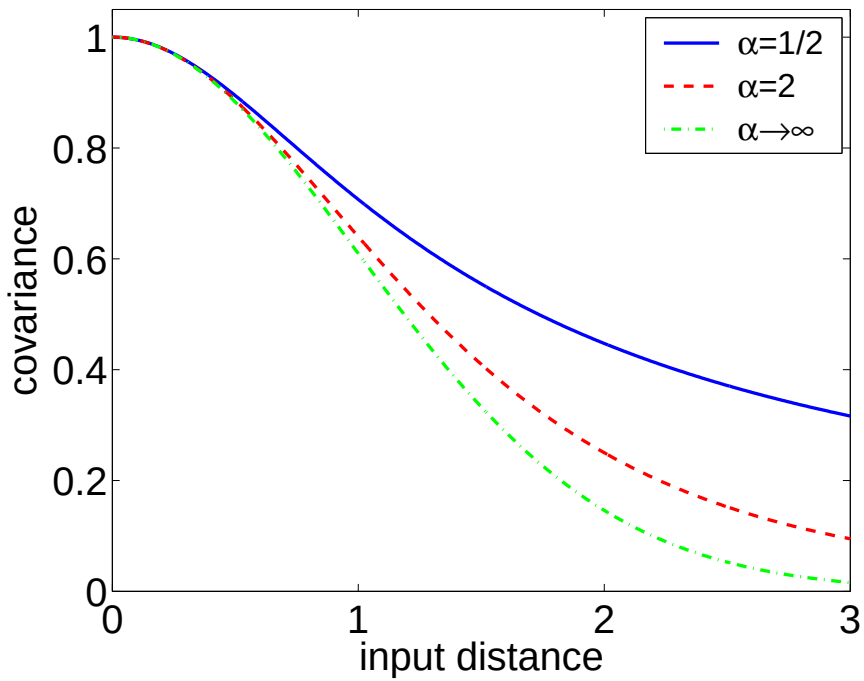
$$k_{\mathrm{RQ}}(r) \;=\; \left(1 + \frac{r^2}{2\alpha\ell^2}\right)^{-\alpha}$$

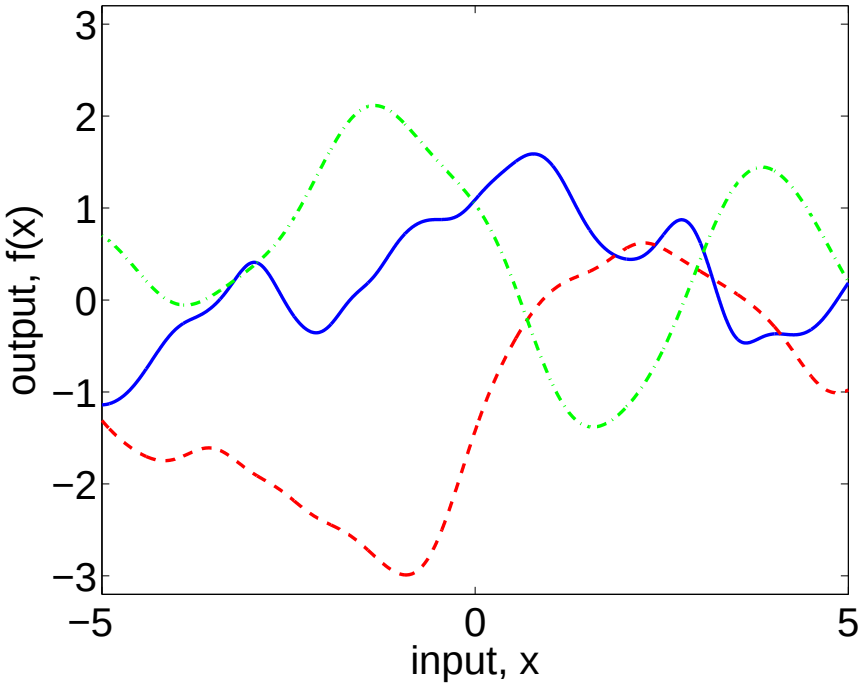
with $\alpha,\ \ell > 0$ can be seen as a *scale mixture* (an infinite sum) of squared exponential (SE) covariance functions with different characteristic length-scales.

Using $\tau = \ell^{-2}$ and $p(\tau|\alpha, \beta) \propto \tau^{\alpha-1}\exp(-\alpha\tau/\beta)$:

$$\begin{aligned} k_{\mathrm{RQ}}(r) \;&=\; \int p(\tau|\alpha, \beta) k_{\mathrm{SE}}(r|\tau) d\tau \\ &\propto \int \tau^{\alpha-1} \exp\left(-\frac{\alpha\tau}{\beta}\right) \exp\left(-\frac{\tau r^2}{2}\right) d\tau \;\propto\; \left(1 + \frac{r^2}{2\alpha\ell^2}\right)^{-\alpha}, \end{aligned}$$

Rational quadratic covariance function II





The limit $\alpha \to \infty$ of the RQ covariance function is the SE.

Matérn covariance functions

Stationary covariance functions can be based on the Matérn form:

$$k(\mathbf{x}, \mathbf{x}') = \frac{1}{\Gamma(\nu)2^{\nu-1}}\left[\frac{\sqrt{2\nu}}{\ell}|\mathbf{x}-\mathbf{x}'|\right]^{\nu} K_{\nu}\left(\frac{\sqrt{2\nu}}{\ell}|\mathbf{x}-\mathbf{x}'|\right),$$

where K_ν is the modified Bessel function of second kind of order ν, and ℓ is the characteristic length scale.

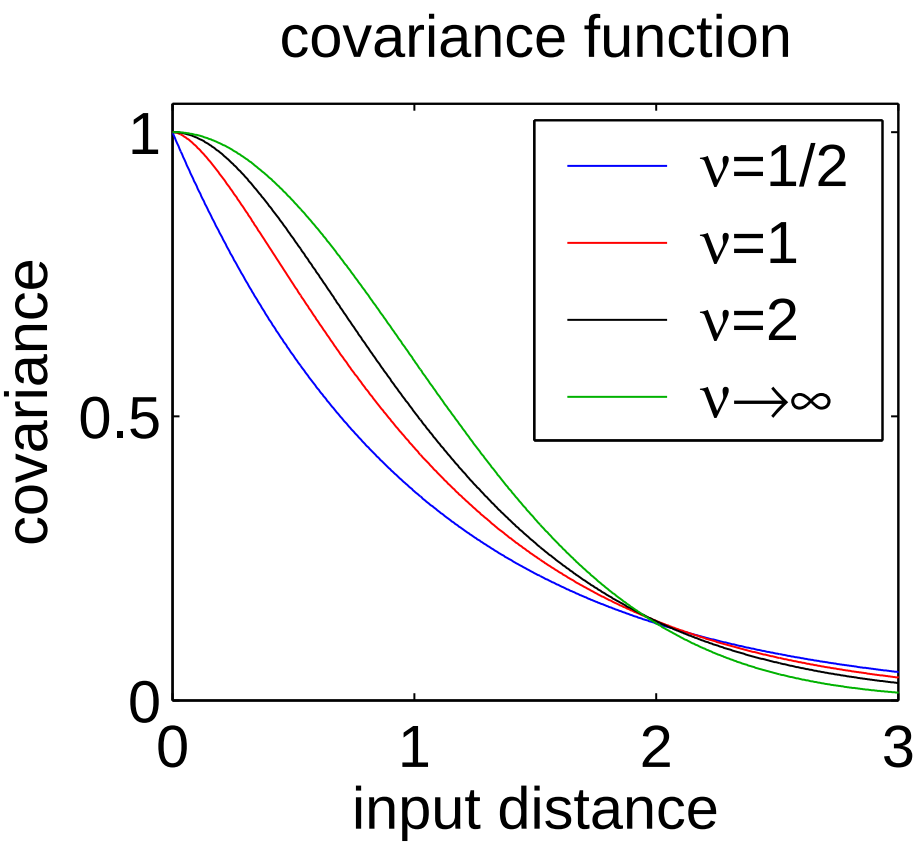
Sample functions from Matérn forms are $\lfloor \nu - 1 \rfloor$ times differentiable. Thus, the hyperparameter ν can control the degree of smoothness

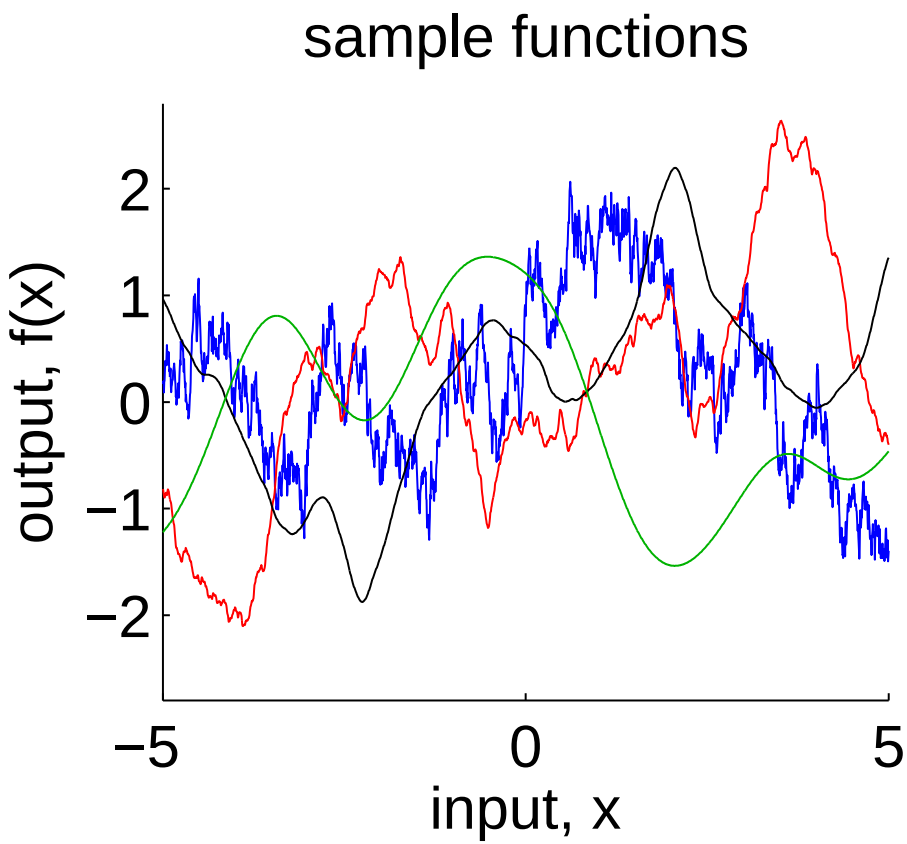
Special cases:

- $k_{\nu=1/2}(r) = \exp(-\frac{r}{\ell})$: Laplacian covariance function, Browninan motion (Ornstein-Uhlenbeck)
- $k_{\nu=3/2}(r) = \left(1 + \frac{\sqrt{3}r}{\ell}\right)\exp\left(-\frac{\sqrt{3}r}{\ell}\right)$ (once differentiable)
- $k_{\nu=5/2}(r) = \left(1 + \frac{\sqrt{5}r}{\ell} + \frac{5r^2}{3\ell^2}\right)\exp\left(-\frac{\sqrt{5}r}{\ell}\right)$ (twice differentiable)
- $k_{\nu\to\infty} = \exp(-\frac{r^2}{2\ell^2})$: smooth (infinitely differentiable)

Matérn covariance functions II

Univariate Matérn covariance function with unit characteristic length scale and unit variance:

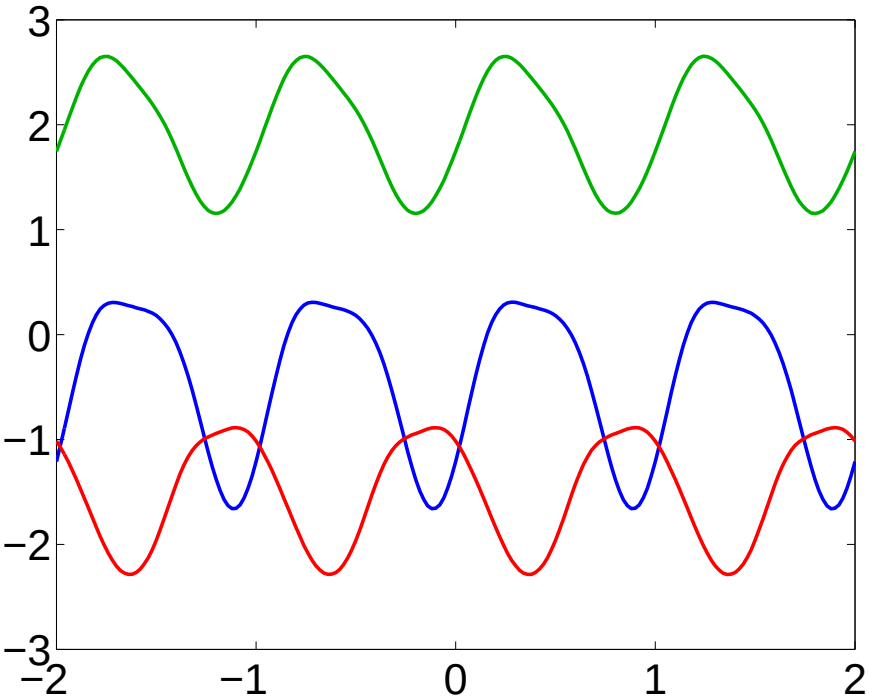


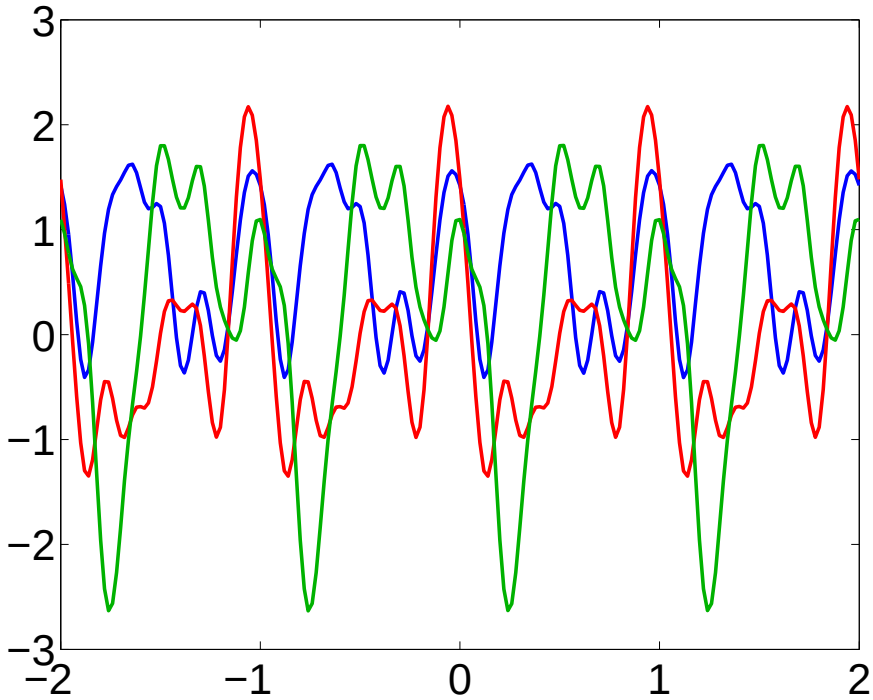


Periodic, smooth functions

To create a distribution over periodic functions of x, we can first map the inputs to $u = (\sin(x), \cos(x))^\top$, and then measure distances in the u space. Combined with the SE covariance function, which characteristic length scale ℓ, we get:

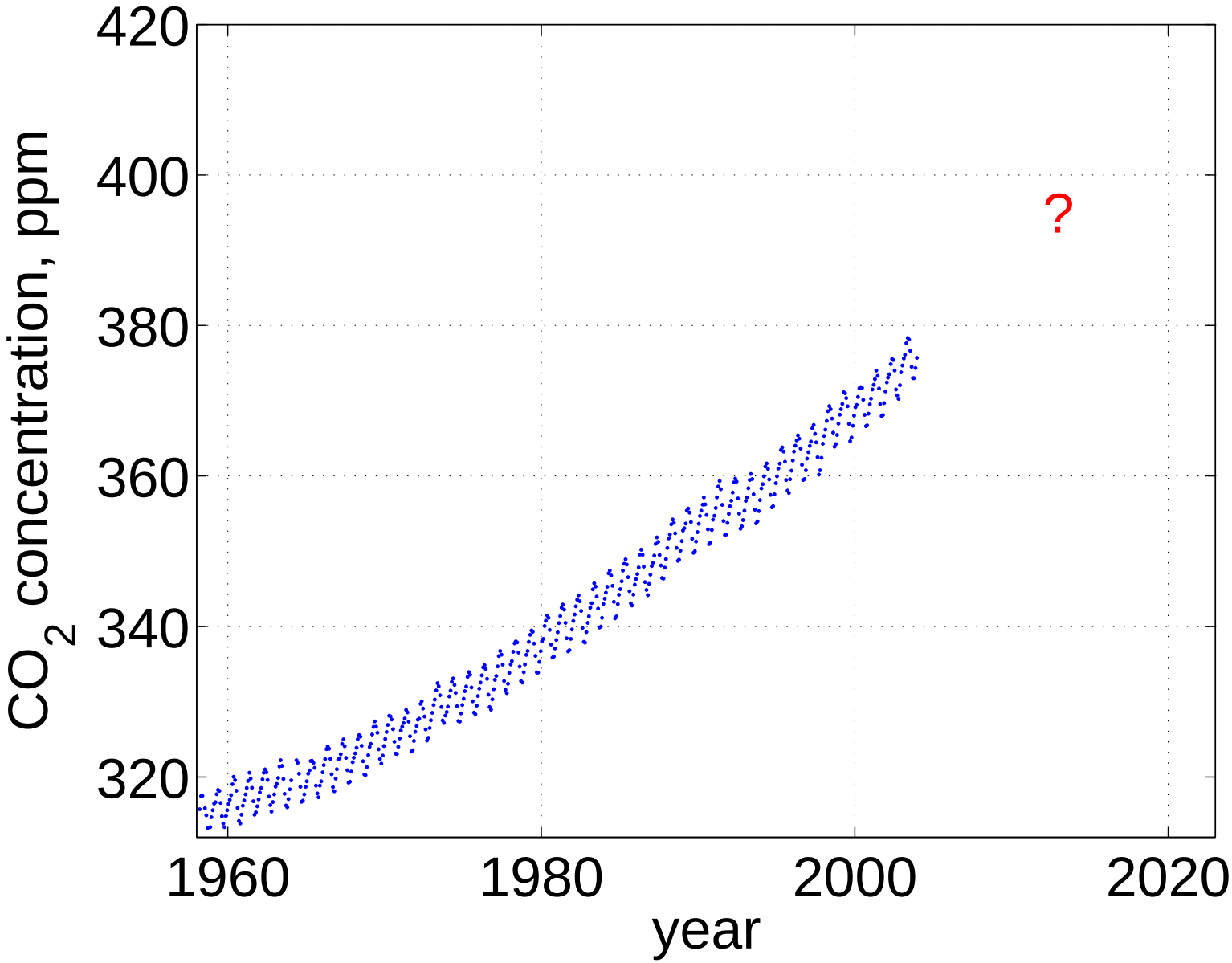
$$k_{\text{periodic}}(x, x') = \exp(-2\sin^2(\pi(x - x'))/\ell^2)$$





Three functions drawn at random; left $\ell > 1$, and right $\ell < 1$.

The Prediction Problem



Covariance Function

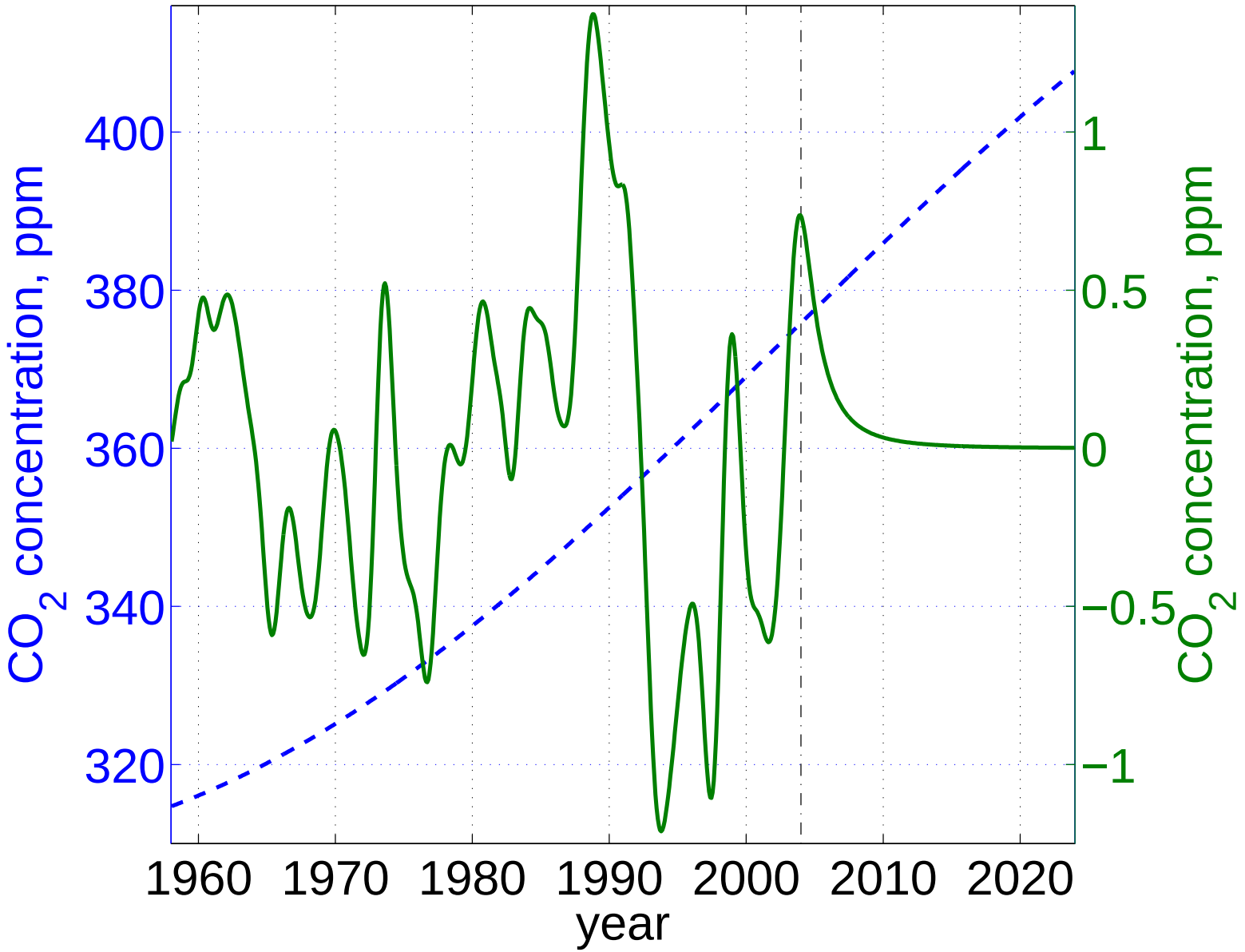
The covariance function consists of several terms, parameterized by a total of 11 *hyperparameters*:

- long-term smooth trend (squared exponential)
  $k_1(x,x') = \theta_1^2 \exp(-(x-x')^2/\theta_2^2)$,
- seasonal trend (quasi-periodic smooth)
  $k_2(x,x') = \theta_3^2 \exp\left(-2\sin^2(\pi(x-x'))/\theta_5^2\right) \times \exp\left(-\frac{1}{2}(x-x')^2/\theta_4^2\right)$,
- short- and medium-term anomaly (rational quadratic)
  $k_3(x,x') = \theta_6^2\left(1+\frac{(x-x')^2}{2\theta_8\theta_7^2}\right)^{-\theta_8}$
- noise (independent Gaussian, and dependent)
  $k_4(x,x') = \theta_9^2 \exp\left(-\frac{(x-x')^2}{2\theta_{10}^2}\right) + \theta_{11}^2\delta_{xx'}$.

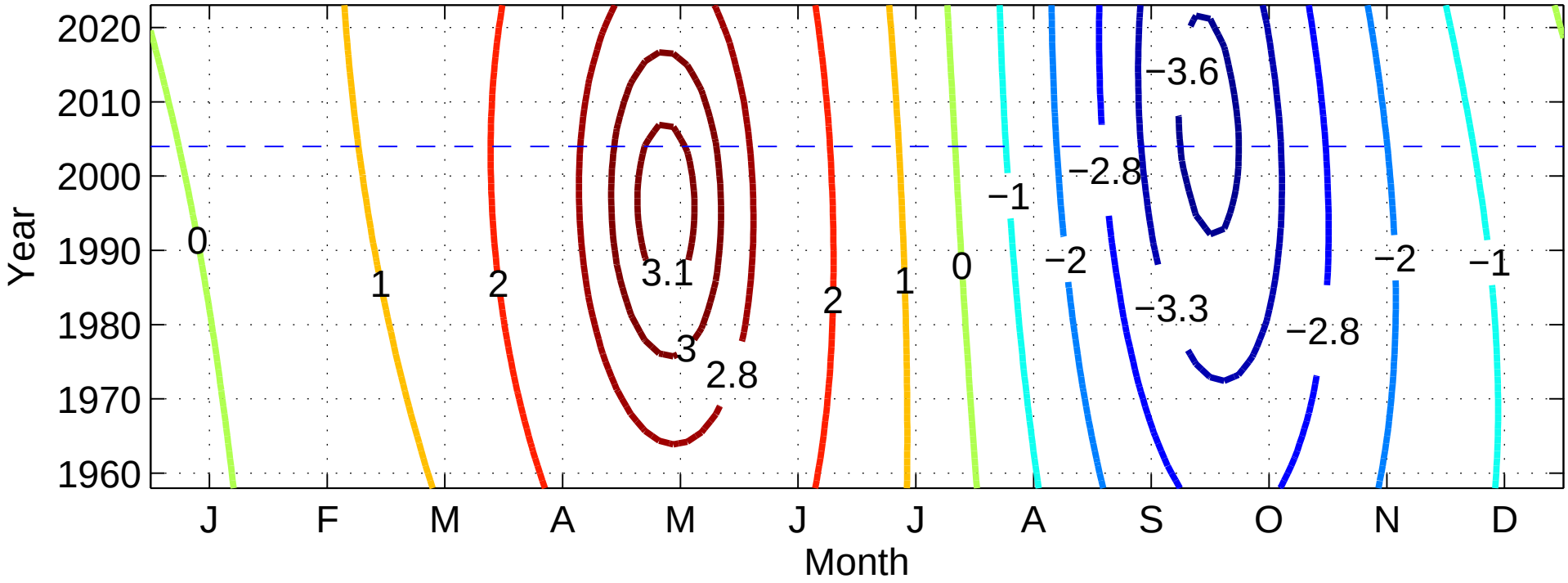
$$k(x,x') = k_1(x,x') + k_2(x,x') + k_3(x,x') + k_4(x,x')$$

Let's try this with the `gpml` software (`http://www.gaussianprocess.org/gpml`).

Long- and medium-term mean predictions



Mean Seasonal Component

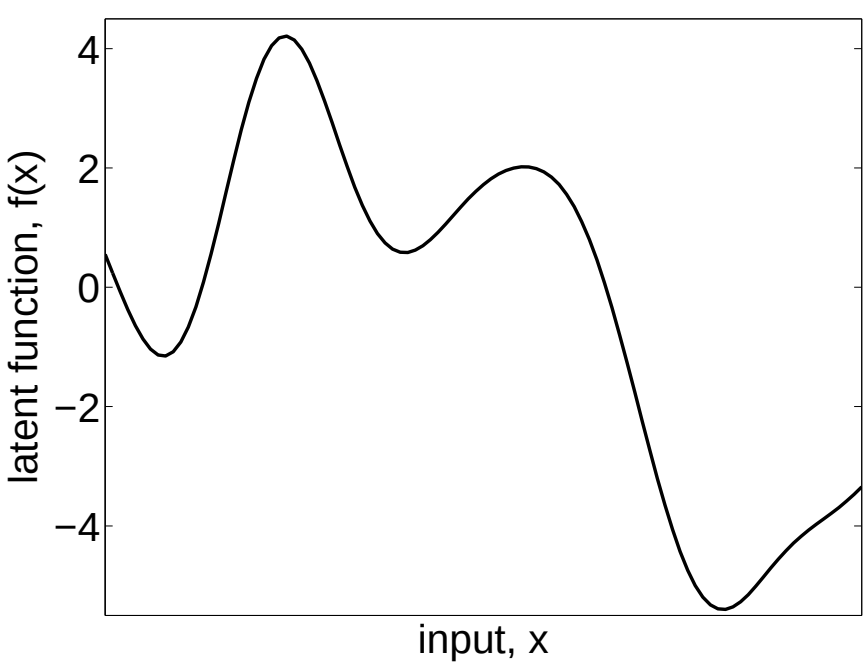


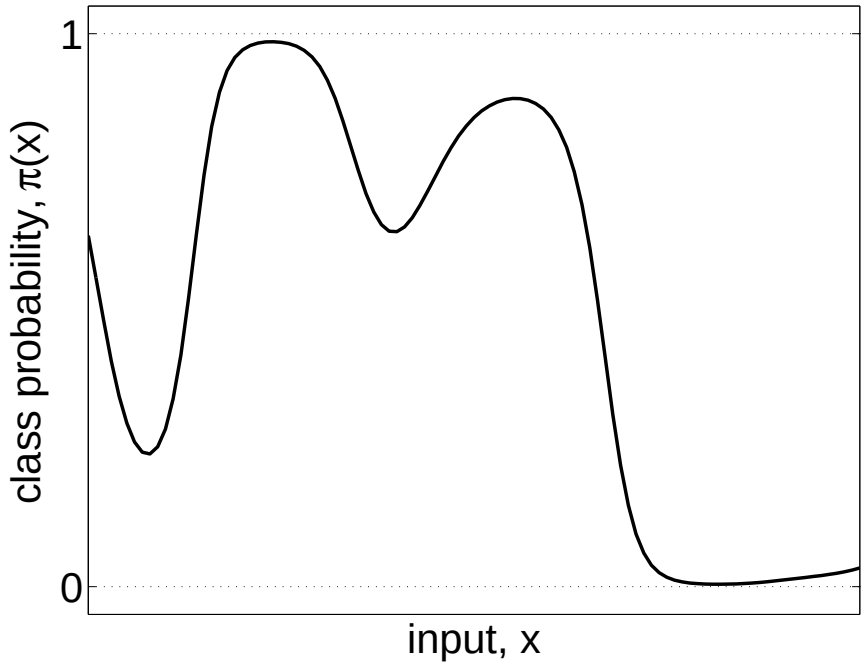
Seasonal component: magnitude $\theta_3 = 2.4$ ppm, decay-time $\theta_4 = 90$ years.

Dependent noise, magnitude $\theta_9 = 0.18$ ppm, decay $\theta_{10} = 1.6$ months.
Independent noise, magnitude $\theta_{11} = 0.19$ ppm.

Optimize or integrate out? See MacKay [5].

Binary Gaussian Process Classification





The class probability is related to the *latent* function, f, through:

$$p(y = 1|f(\mathbf{x})) \;=\; \pi(\mathbf{x}) \;=\; \Phi\big(f(\mathbf{x})\big),$$

where Φ is a sigmoid function, such as the logistic or cumulative Gaussian.
Observations are independent given f, so the likelihood is

$$p(\mathbf{y}|\mathbf{f}) \;=\; \prod_{i=1}^{n} p(y_i|f_i) \;=\; \prod_{i=1}^{n} \Phi(y_i f_i).$$

Prior and Posterior for Classification

We use a Gaussian process prior for the latent function:

$$\mathbf{f}|X,\theta \;\sim\; \mathcal{N}(\mathbf{0},\; K)$$

The posterior becomes:

$$p(\mathbf{f}|\mathcal{D},\theta) \;=\; \frac{p(\mathbf{y}|\mathbf{f})\,p(\mathbf{f}|X,\theta)}{p(\mathcal{D}|\theta)} \;=\; \frac{\mathcal{N}(\mathbf{f}|\mathbf{0},\; K)}{p(\mathcal{D}|\theta)}\prod_{i=1}^{m}\Phi(y_i f_i),$$

which is non-Gaussian.

The latent value at the test point, $f(\mathbf{x}^*)$ is

$$p(f_*|\mathcal{D},\theta,\mathbf{x}_*) \;=\; \int p(f_*|\mathbf{f},X,\theta,\mathbf{x}_*)p(\mathbf{f}|\mathcal{D},\theta)d\mathbf{f},$$

and the predictive class probability becomes

$$p(y_*|\mathcal{D},\theta,\mathbf{x}_*) \;=\; \int p(y_*|f_*)p(f_*|\mathcal{D},\theta,\mathbf{x}_*)df_*,$$

both of which are intractable to compute.

Gaussian Approximation to the Posterior

We approximate the non-Gaussian posterior by a Gaussian:

$$p(\mathbf{f}|\mathcal{D},\theta) \;\simeq\; q(\mathbf{f}|\mathcal{D},\theta) \;=\; \mathcal{N}(\mathbf{m},\; A)$$

then $q(f_*|\mathcal{D},\theta,\mathbf{x}_*) = \mathcal{N}(f_*|\mu_*,\sigma_*^2)$, where

$$\begin{aligned}\mu_* &= \mathbf{k}_*^\top K^{-1}\mathbf{m}\\ \sigma_*^2 &= k(\mathbf{x}_*,\mathbf{x}_*) - \mathbf{k}_*^\top(K^{-1} - K^{-1}AK^{-1})\mathbf{k}_*.\end{aligned}$$

Using this approximation with the cumulative Gaussian likelihood

$$q(y_*=1|\mathcal{D},\theta,\mathbf{x}_*) \;=\; \int \Phi(f_*)\,\mathcal{N}(f_*|\mu_*,\sigma_*^2)df_* \;=\; \Phi\left(\frac{\mu_*}{\sqrt{1+\sigma_*^2}}\right)$$

Laplace's method and Expectation Propagation

How do we find a good Gaussian approximation $\mathcal{N}(\mathbf{m}, A)$ to the posterior?

Laplace's method: Find the Maximum A Posteriori (MAP) lantent values $\mathbf{f}_{\text{MAP}}$, and use a local expansion (Gaussian) around this point as suggested by Williams and Barber [10].

Variational bounds: bound the likelihood by some tractable expression
A **local variational bound for each likelihood term** was given by Gibbs and MacKay [1]. A **lower bound based on Jensen's inequality** by Opper and Seeger [7].

Expectation Propagation: use an approximation of the likelihood, such that the moments of the marginals of the approximate posterior match the (approximate) moment of the posterior, Minka [6].

Laplace's method and EP were compared by Kuss and Rasmussen [3].

Gaussian process latent variable models

GP's can be used for non-linear dimensionality reduction (unsupervised learning).

Observed (high-dimensional) data Y_{dc}, where $1 \leqslant d \leqslant D$ indexes dimensions and $1 \leqslant c \leqslant n$ indexes dimensions.

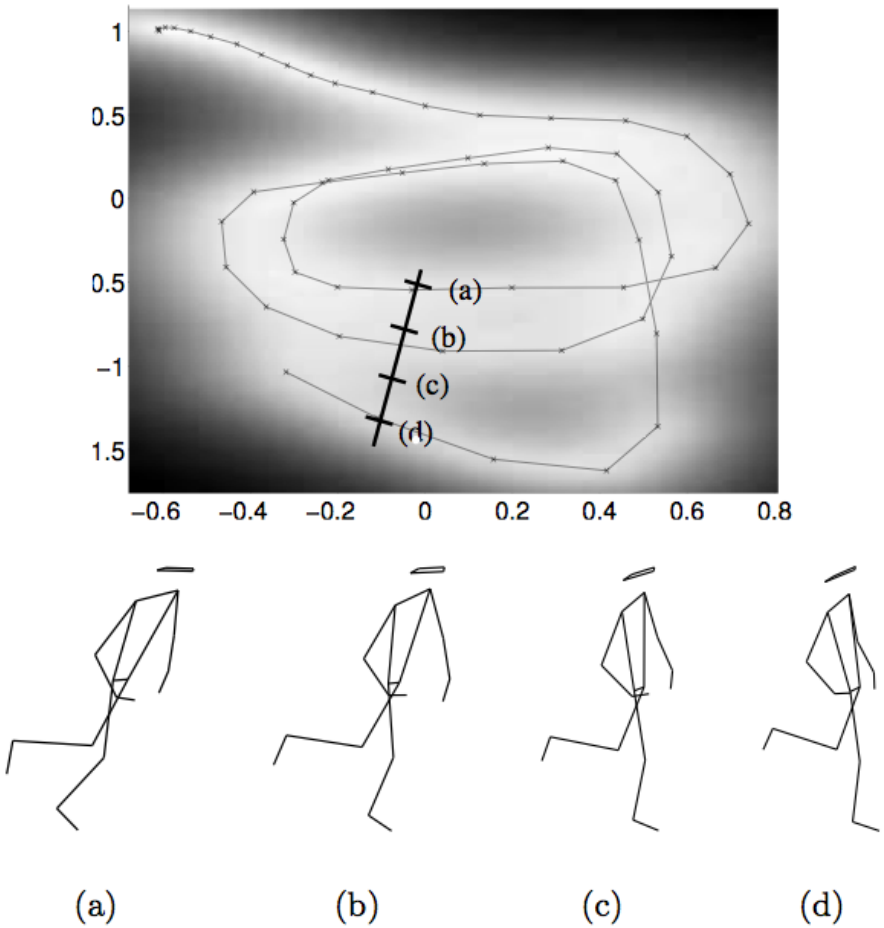
Assume that each visible coordinate, $\mathbf{y}_d$, is modeled by a separate GP using some latent (low dimensional) inputs $\mathbf{x}$.

Find the best latent inputs by maximizing the marginal likelihood under the constraint that all visible variables must share the same latent values.

Computationally, this isn't too expensive, as all dimensions are modeled using the same covariance matrix K.

This is the GPLVM model proposed by Lawrence [4].

Gaussian process latent variable models



Motion capture example, representing 102-D data in 2-D, borrowed from Neil Lawrence.

Finding the latent variables is a high-dimensional, non-linear, optimization problem with local optima.

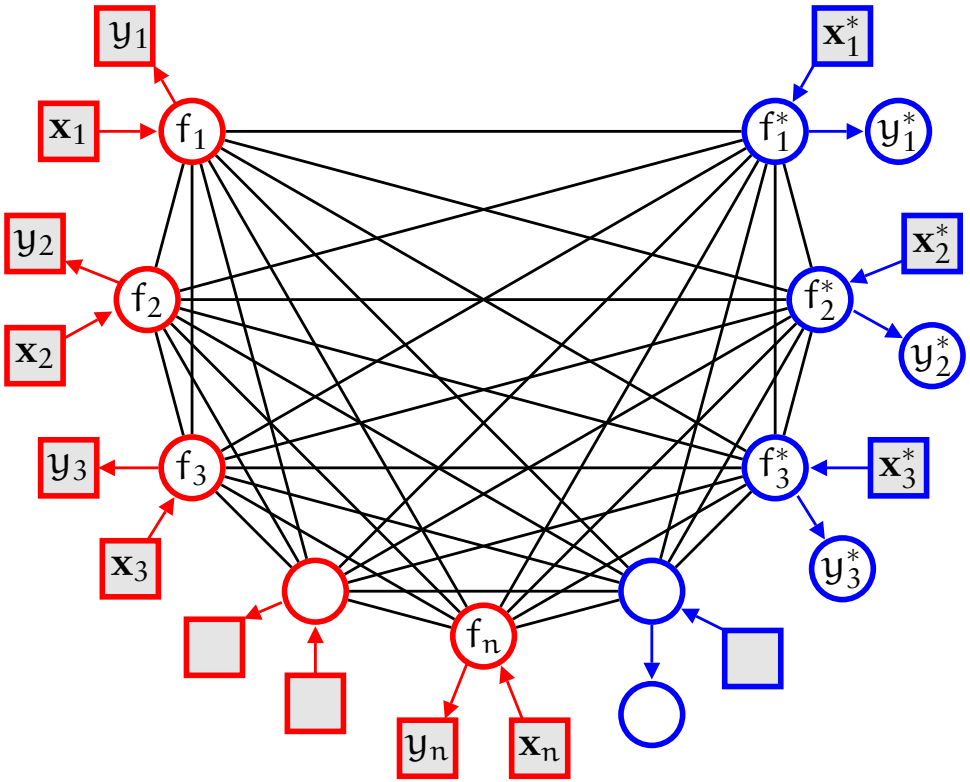
GPLVM defines a map from latent to observed space, not a generative model.

Mapping new latent coordinates to (distributions over) observations is easy.

Finding the latent coordinates (pre-image) for new cases is difficult.

Sparse Approximations

Recall the graphical model for a Gaussian process. Inference is expensive because the latent variables are fully connected.



Exact inference: $\mathcal{O}(n^3)$.

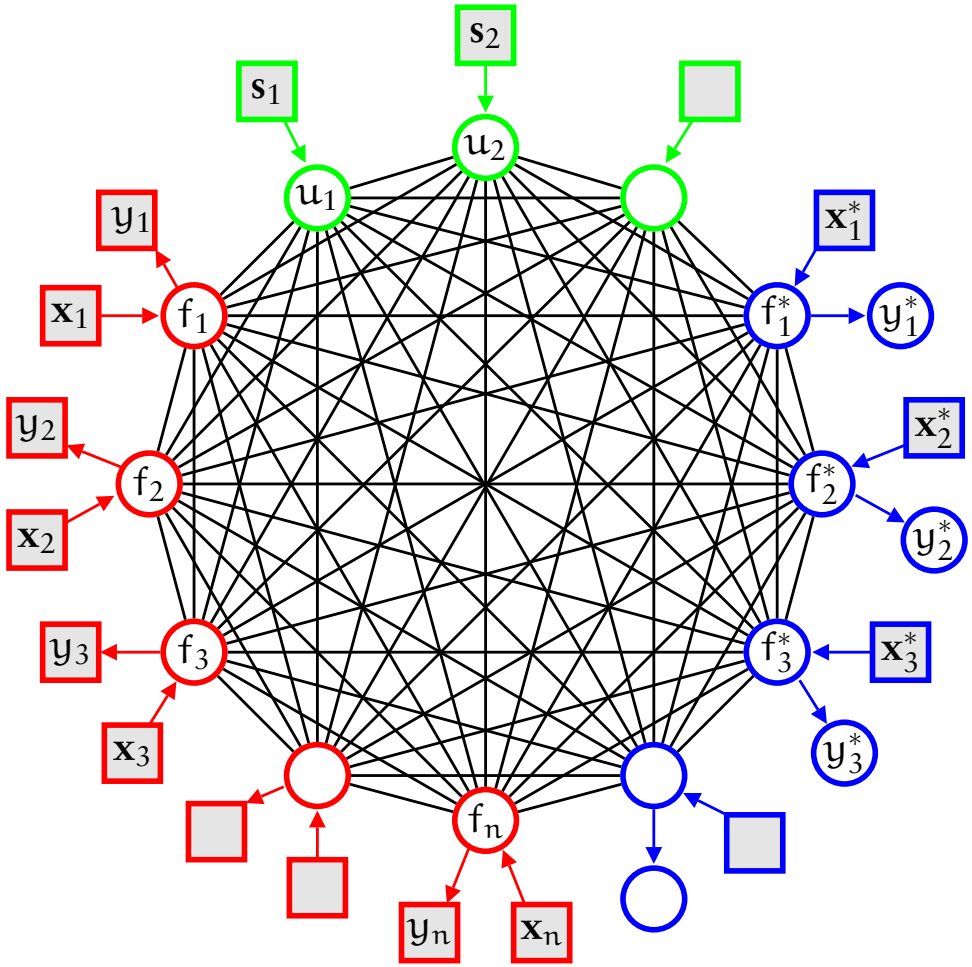
Sparse approximations: solve a smaller, sparse, approximation of the original problem.

Algorithm: Subset of data.

Are there better ways to sparsify?

Inducing Variables

Because of the marginalization property, we can introduce more latent variables without changing the distribution of the original variables.



The $\mathbf{u} = (u_1, u_2, \ldots)^\top$ are called *inducing variables*.

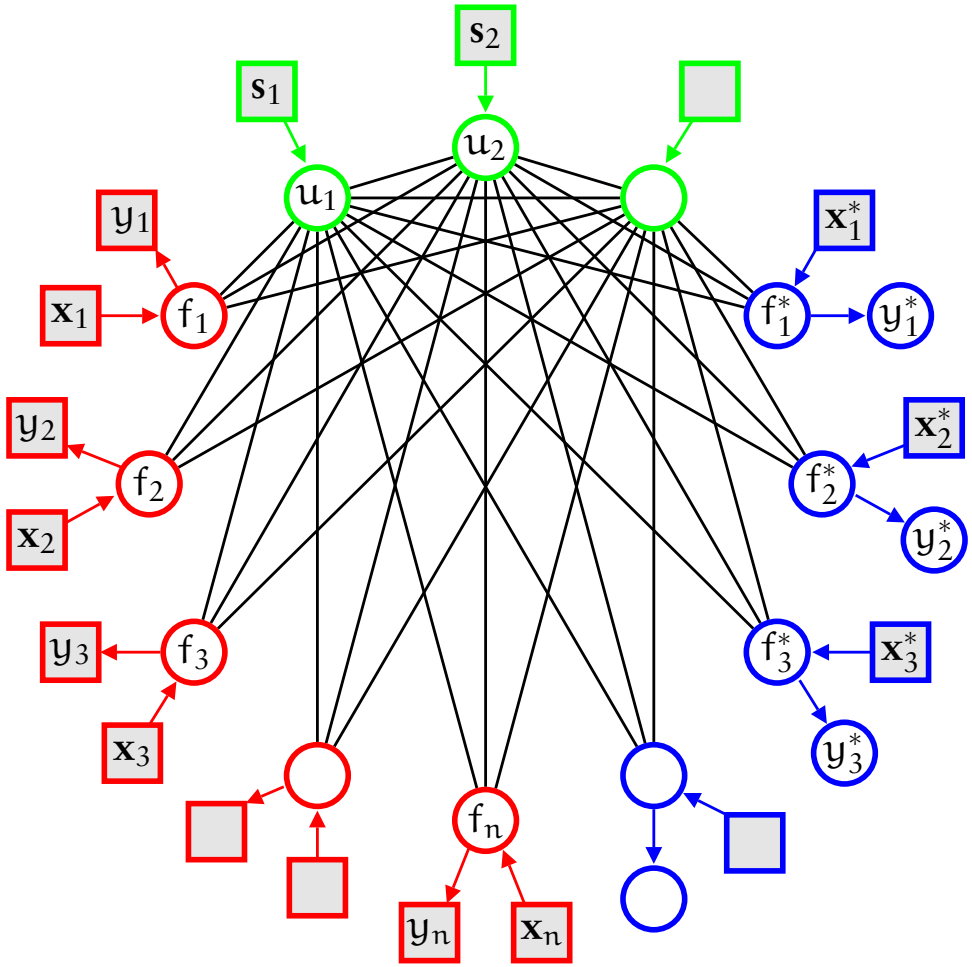
The inducing variables have associated *inducing inputs*, $\mathbf{s}$, but no associated output values.

The marginalization property ensures that

$$p(\mathbf{f}, \mathbf{f}^*) = \int p(\mathbf{f}, \mathbf{f}^*, \mathbf{u}) d\mathbf{u}$$

The Central Approximations

In a unifying treatment, Candela and Rasmussen [2] assume that training and test sets are *conditionally independent* given $\mathbf{u}$.



Assume: $p(\mathbf{f}, \mathbf{f}_*) \simeq q(\mathbf{f}, \mathbf{f}_*)$, where

$$q(\mathbf{f}, \mathbf{f}_*) = \int q(\mathbf{f}_*|\mathbf{u}) q(\mathbf{f}|\mathbf{u}) p(\mathbf{u}) d\mathbf{u}.$$

The inducing variables *induce* the dependencies between training and test cases.

Different sparse algorithms in the literature correspond to different

- choices of the inducing inputs
- further approximations

Training and test conditionals

The exact training and test conditionals are:

$$\begin{aligned} p(\mathbf{f}|\mathbf{u}) &= \mathcal{N}(K_{\mathbf{f},\mathbf{u}}K_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{u}, K_{\mathbf{f},\mathbf{f}} - Q_{\mathbf{f},\mathbf{f}}) \\ p(\mathbf{f}_*|\mathbf{u}) &= \mathcal{N}(K_{\mathbf{f}_*,\mathbf{u}}K_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{u}, K_{\mathbf{f}_*,\mathbf{f}_*} - Q_{\mathbf{f}_*,\mathbf{f}_*}), \end{aligned}$$

where $Q_{\mathbf{a},\mathbf{b}} = K_{\mathbf{a},\mathbf{u}}K_{\mathbf{u},\mathbf{u}}^{-1}K_{\mathbf{u},\mathbf{b}}$.

These equations are easily recognized as the usual predictive equations for GPs.

The *effective prior* is:

$$q(\mathbf{f}, \mathbf{f}_*) = \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K_{\mathbf{f},\mathbf{f}} & Q_{*,\mathbf{f}} \\ Q_{\mathbf{f},*} & K_{*,*} \end{bmatrix}\right)$$

Example: Subset of Regressors

Replace both training and test conditionals by *deterministic* relations:

$$\begin{aligned} q(\mathbf{f}|\mathbf{u}) &= \mathcal{N}(K_{\mathbf{f},\mathbf{u}}K_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{u}, 0) \\ q(\mathbf{f}_*|\mathbf{u}) &= \mathcal{N}(K_{\mathbf{f}_*,\mathbf{u}}K_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{u}, 0). \end{aligned}$$

The effective prior becomes

$$q_{\mathrm{SOR}}(\mathbf{f}, \mathbf{f}_*) = \mathcal{N}\Big(\mathbf{0}, \begin{bmatrix} Q_{\mathbf{f},\mathbf{f}} & Q_{*,\mathbf{f}} \\ Q_{\mathbf{f},*} & Q_{*,*} \end{bmatrix}\Big),$$

showing that SOR is just a GP with (degenerate) covariance function Q.

Example: Sparse parametric Gaussian processes

Snelson and Ghahramani [8] introduced the idea of sparse GP inference based on a pseudo data set, integrating out the targets, and optimizing the inputs.

Equivalently, in the unifying scheme:

$$\begin{aligned} q(\mathbf{f}|\mathbf{u}) &= \mathcal{N}(K_{\mathbf{f},\mathbf{u}}K_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{u}, \operatorname{diag}[K_{\mathbf{f},\mathbf{f}} - Q_{\mathbf{f},\mathbf{f}}]) \\ q(\mathbf{f}_*|\mathbf{u}) &= p(\mathbf{f}_*|\mathbf{u}). \end{aligned}$$

The effective prior becomes

$$q_{\text{FITC}}(\mathbf{f}, \mathbf{f}_*) = \mathcal{N}\Big(\mathbf{0}, \begin{bmatrix} Q_{\mathbf{f},\mathbf{f}} - \operatorname{diag}[Q_{\mathbf{f},\mathbf{f}} - K_{\mathbf{f},\mathbf{f}}] & Q_{*,\mathbf{f}} \\ Q_{\mathbf{f},*} & K_{*,*} \end{bmatrix}\Big),$$

which can be computed efficiently.

The Bayesian Committee Machine [9] uses block diag instead of diag, and the inducing variables to be the test cases.

Sparse approximations

Most published sparse approximations can be understood in a single graphical model framework.

The *inducing inputs* (or expansion points, or support vectors) may be a subset of the training data, or completely free.

The approximations are understood as exact inference in a modified model (rather than approximate inference for the exact model).

Conclusions

Complex non-linear inference problems can be solved by manipulating plain old Gaussian distributions

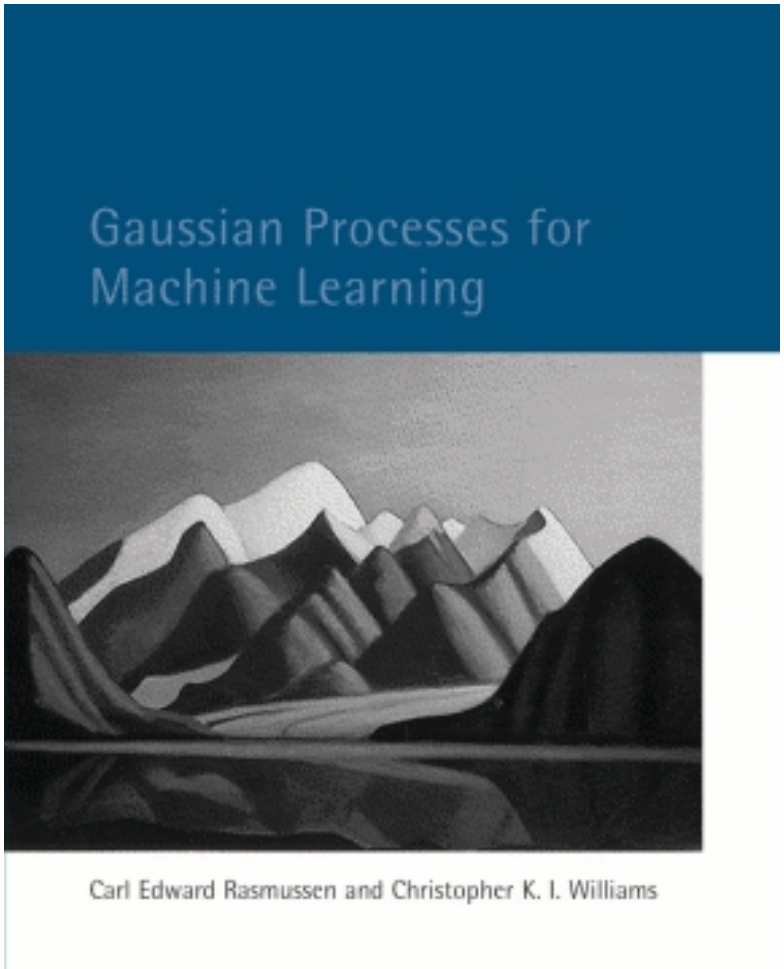
- Bayesian inference is tractable for GP regression and
- Approximations exist for classification
- predictions are probabilistic
- compare different models (via the marginal likelihood)

GPs are a simple and intuitive means of specifying prior information, and explaining data, and equivalent to other models: RVM's, splines, closely related to SVMs.

Outlook:

- new interesting covariance functions
- application to structured data
- better understanding of sparse methods

More on Gaussian Processes



Rasmussen and Williams
Gaussian Processes for Machine Learning,
MIT Press, 2006.
`http://www.GaussianProcess.org/gpml`

Gaussian process web (code, papers, etc): `http://www.GaussianProcess.org`

A few references

[1] Gibbs, M. N. and MacKay, D. J. C. (2000). Variational Gaussian Process Classifiers. *IEEE Transactions on Neural Networks*, 11(6):1458–1464.

[2] Joaquin Quiñonero-Candela and Carl Edward Rasmussen (2005). A unifying view of sparse approximate gaussian process regression. *Journal of Machine Learning Research*, 6:1939–1959.

[3] Kuss, M. and Rasmussen, C. E. (2005). Assessing approximate inference for binary gaussian process classification. *Journal of Machine Learning Research*, 6:1679–1704.

[4] Lawrence, N. (2005). Probabilistic non-linear principal component analysis with Gaussian process latent variable models. *Journal of Machine Learning Research*, 6:1783–1816.

[5] MacKay, D. J. C. (1999). Comparison of Approximate Methods for Handling Hyperparameters. *Neural Computation*, 11(5):1035–1068.

[6] Minka, T. P. (2001). *A Family of Algorithms for Approximate Bayesian Inference*. PhD thesis, Massachusetts Institute of Technology.

[7] Seeger, M. (2003). *Bayesian Gaussian Process Models: PAC-Bayesian Generalisation Error Bounds and Sparse Approximations*. PhD thesis, School of Informatics, University of Edinburgh. `http://www.cs.berkeley.edu/~mseeger`.

[8] Snelson, E. and Ghahramani, Z. (2006). Sparse gaussian processes using pseudo-inputs. In *Advances in Neural Information Processing Systems 18*. MIT Press.

[9] Tresp, V. (2000). A Bayesian Committee Machine. *Neural Computation*, 12(11):2719–2741.

[10] Williams, C. K. I. and Barber, D. (1998). Bayesian Classification with Gaussian Processes. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 20(12):1342–1351.