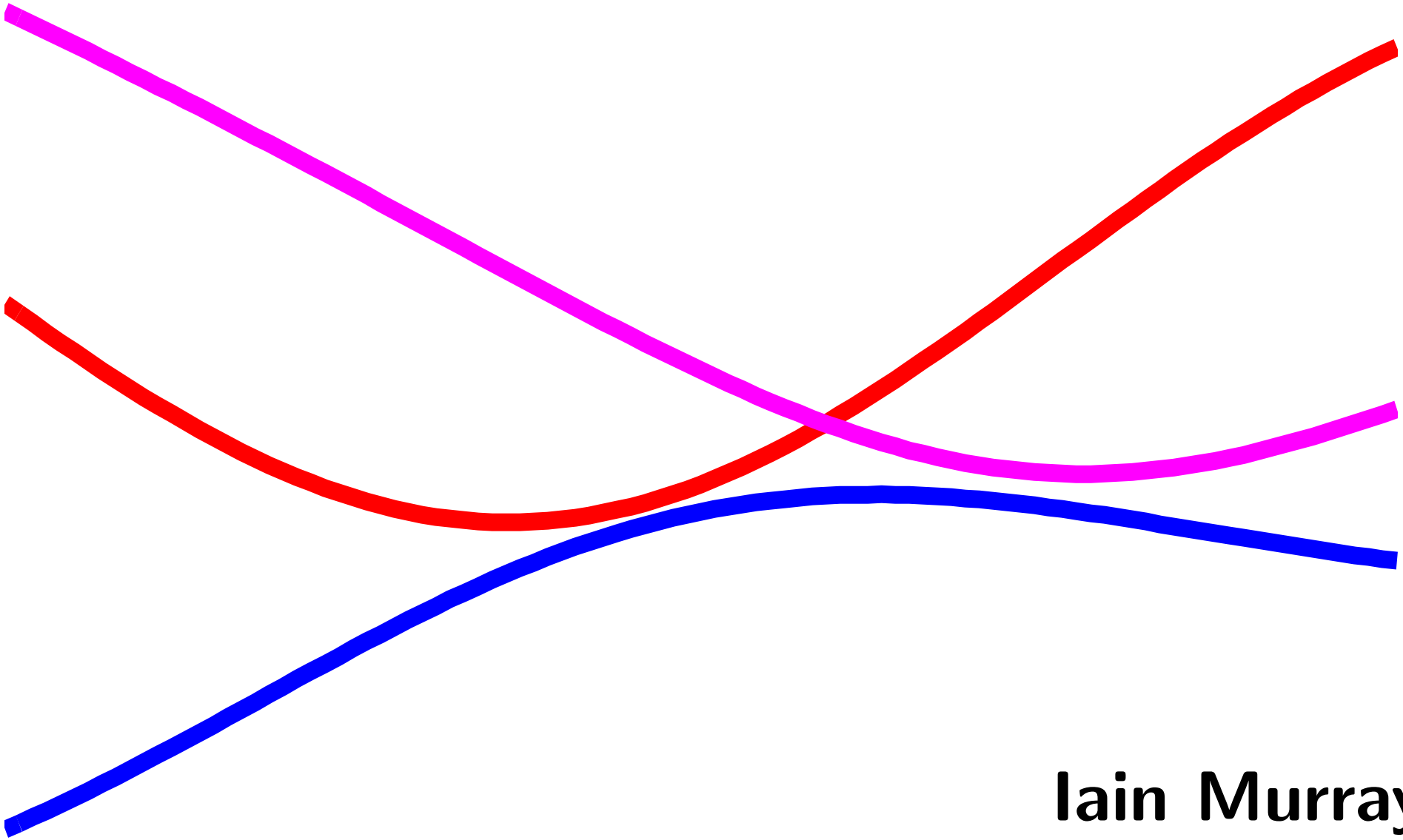
Introduction to Gaussian Processes



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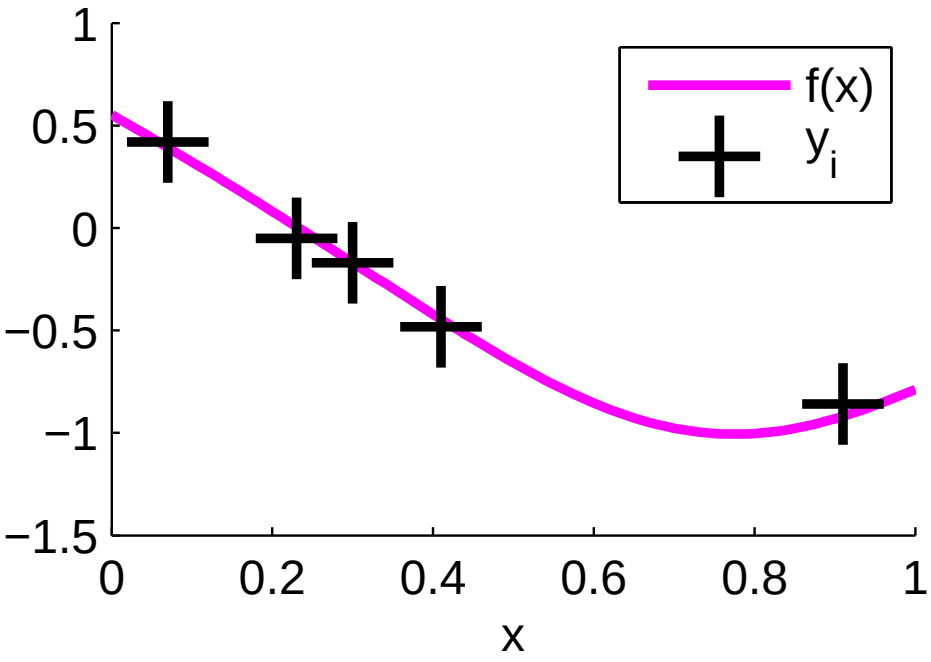
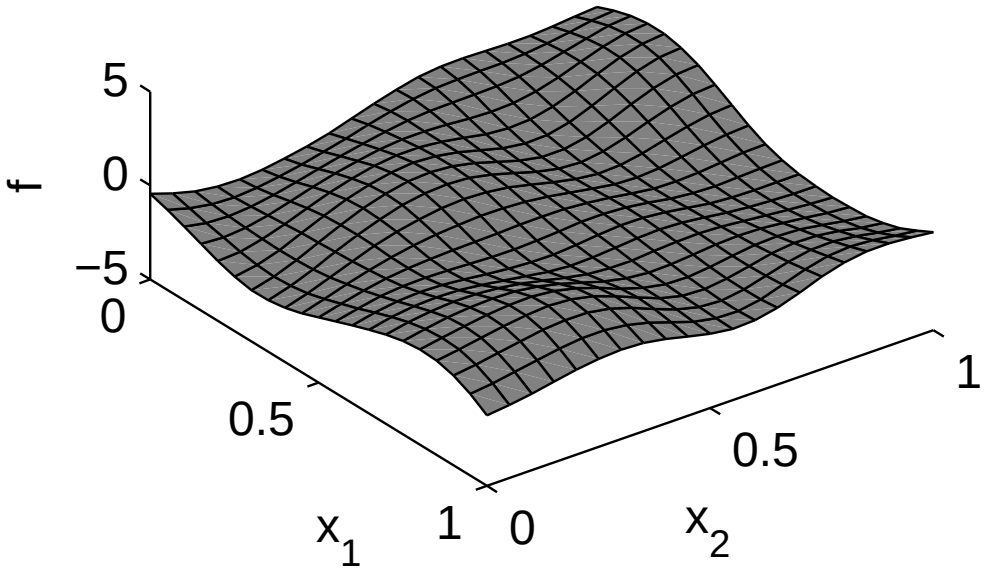
The problem

Learn scalar function of vector values $f(\mathbf{x})$





We have (possibly noisy) observations $\{\mathbf{x}_i, y_i\}_{i=1}^n$

Example Applications

Real-valued regression:

— Robotics: target state $\rightarrow$ required torque

— Process engineering: predicting yield

— Surrogate surfaces for optimization or simulation

Classification:

— Recognition: e.g. handwritten digits on cheques

— Filtering: fraud, interesting science, disease screening

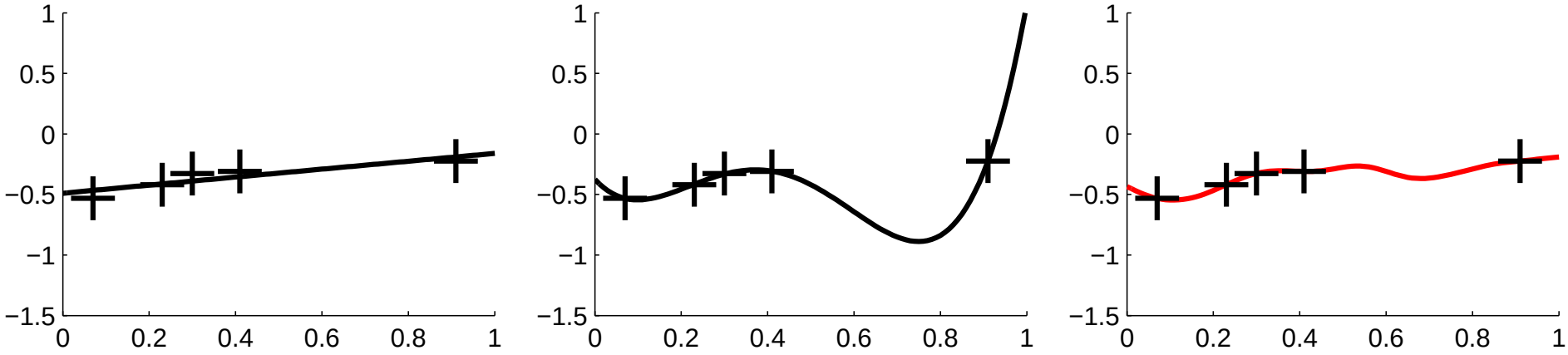
Ordinal regression:

— User ratings (e.g. movies or restaurants)

— Disease screening (e.g. predicting Gleason score)

Model complexity

The world is often complicated:



simple fit

complex fit

truth

Problems:

— Fitting complicated models can be hard

— How do we find an appropriate model?

— How do we avoid over-fitting some aspects of model?

Predicting yield

Factory settings $\mathbf{x}_1 \rightarrow$ profit of 32 ± 5 monetary units

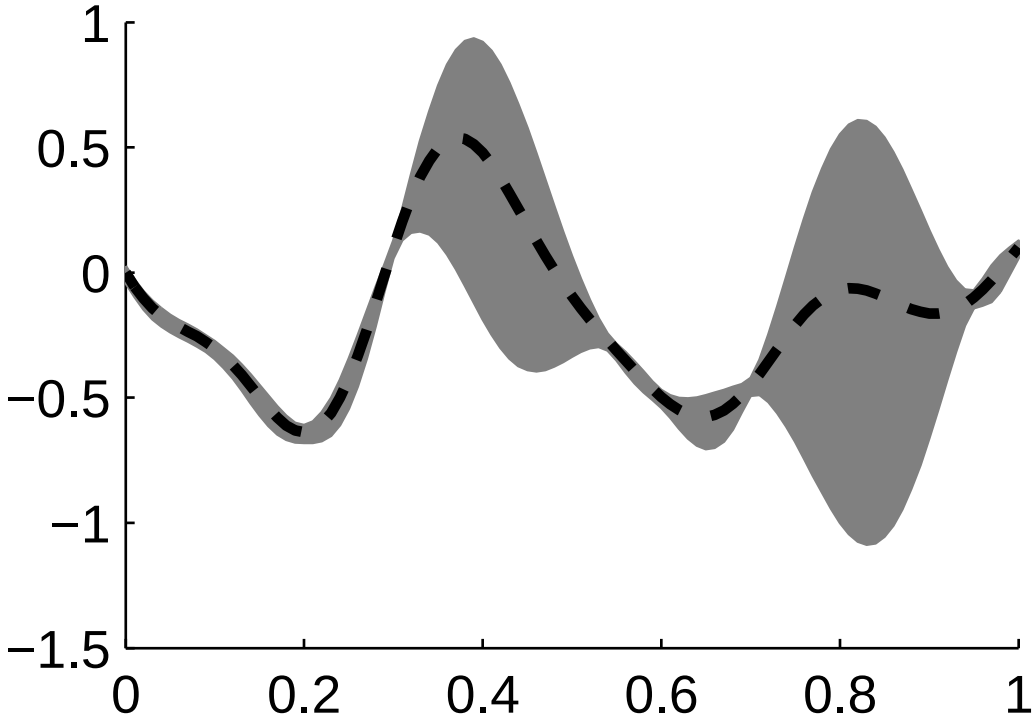
Factory settings $\mathbf{x}_2 \rightarrow$ profit of 100 ± 200 monetary units

Which are the best settings $\mathbf{x}_1$ or $\mathbf{x}_2$?

Knowing the error bars can be important

Optimization

In high dimensions it takes many function evaluations to be certain everywhere. Costly if experiments are involved.

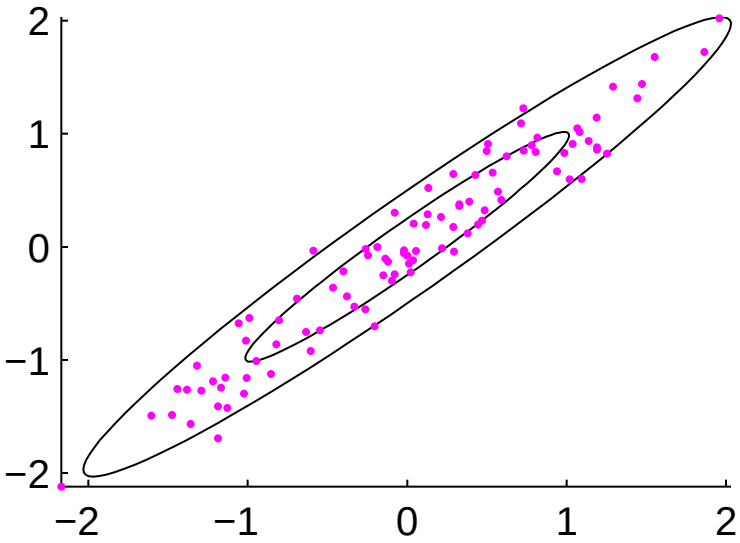


Error bars are needed to see if a region is still promising.

Bayesian modelling

If we come up with a parametric family of functions, $f(\mathbf{x};\theta)$ and define a prior over θ, probability theory tells us how to make predictions given data. For flexible models, this usually involves intractable integrals over θ.

We're really good at integrating Gaussians though



Can we really solve significant machine learning problems with a simple multivariate Gaussian distribution?

Gaussian distributions

Completely described by parameters μ and Σ:

$$p(\mathbf{f} \mid \Sigma, \mu) = |2\pi\Sigma|^{-\frac{1}{2}} \exp\left(-\tfrac{1}{2}(\mathbf{f} - \mu)^T \Sigma^{-1} (\mathbf{f} - \mu) \right)$$

μ and Σ are the mean and covariance of the distribution. For example:

$$\Sigma_{ij} = \mathbb{E}[f_i f_j] - \mu_i \mu_j$$

If we know a distribution is Gaussian and know its mean and covariances, we know its density function.

Marginal of Gaussian

The marginal of a Gaussian distribution is Gaussian.

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

As soon as you convince yourself that the marginal

$$p(\mathbf{f}) = \int p(\mathbf{f}, \mathbf{g}) \, \mathrm{d}\mathbf{g}$$

is Gaussian, you already know the means and covariances:

$$p(\mathbf{f}) = \mathcal{N}(\mathbf{f}; \mathbf{a}, A)$$

Conditional of Gaussian

Any conditional of a Gaussian distribution is also Gaussian:

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

$$p(\mathbf{f} \,|\, \mathbf{g}) = \mathcal{N}(\mathbf{f};\ \mathbf{a}+CB^{-1}(\mathbf{g}-\mathbf{b}),\ A-CB^{-1}C^\top)$$

Showing this result requires some grunt work.
But it is standard, and easily looked up.

Noisy observations

Previously we inferred $\mathbf{f}$ given $\mathbf{g}$.
What if we only saw a noisy observation, $\mathbf{y} \sim \mathcal{N}(\mathbf{g}, S)$?

$p(\mathbf{f}, \mathbf{g}, \mathbf{y}) = p(\mathbf{f}, \mathbf{g})\, p(\mathbf{y} \,|\, \mathbf{g})$ is Gaussian distributed
a quadratic form inside the exponential after multiplying

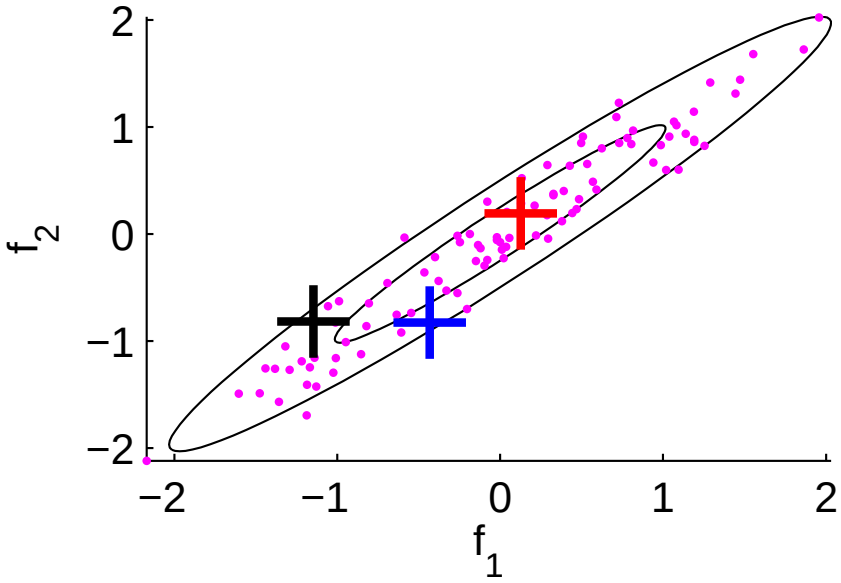
Our posterior over $\mathbf{f}$ is still Gaussian:

$$p(\mathbf{f} \,|\, \mathbf{y}) \propto \int p(\mathbf{f}, \mathbf{g}, \mathbf{y})\, \mathrm{d}\mathbf{g}$$

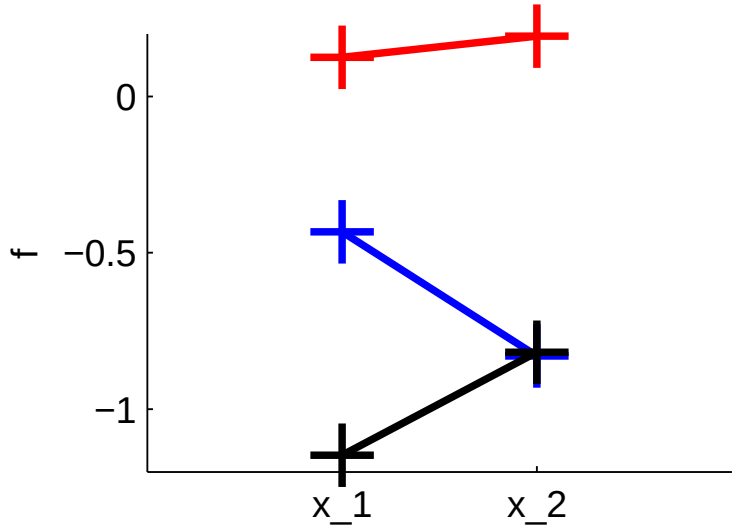
RHS is Gaussian after marginalizing, so still a quadratic form in $\mathbf{f}$ inside an exponential.

Laying out Gaussians

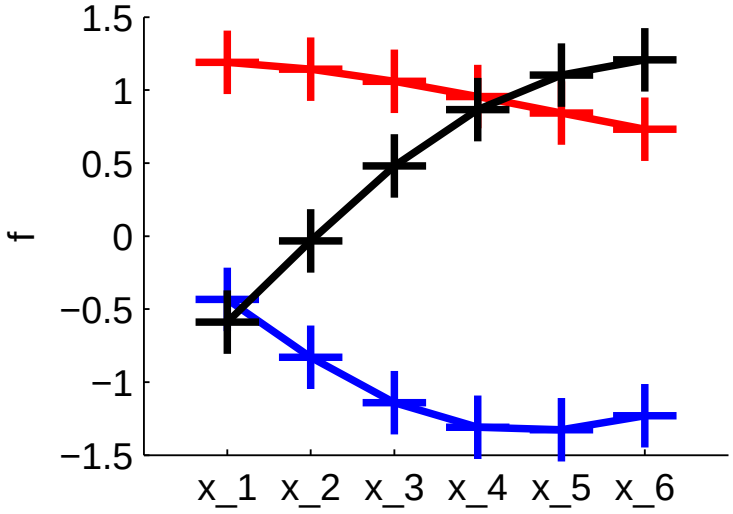
A way of visualizing draws from a 2D Gaussian:



$\Leftrightarrow$

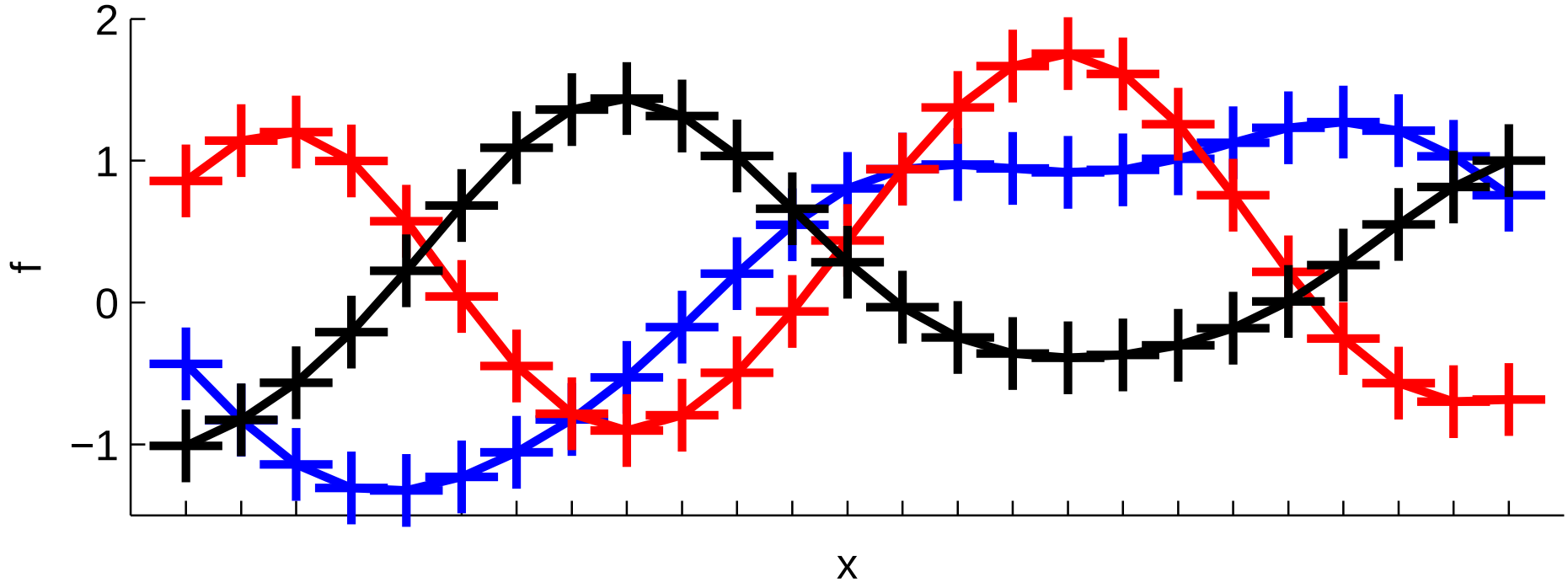


Now it's easy to show three draws from a 6D Gaussian:



Building large Gaussians

Three draws from a 25D Gaussian:



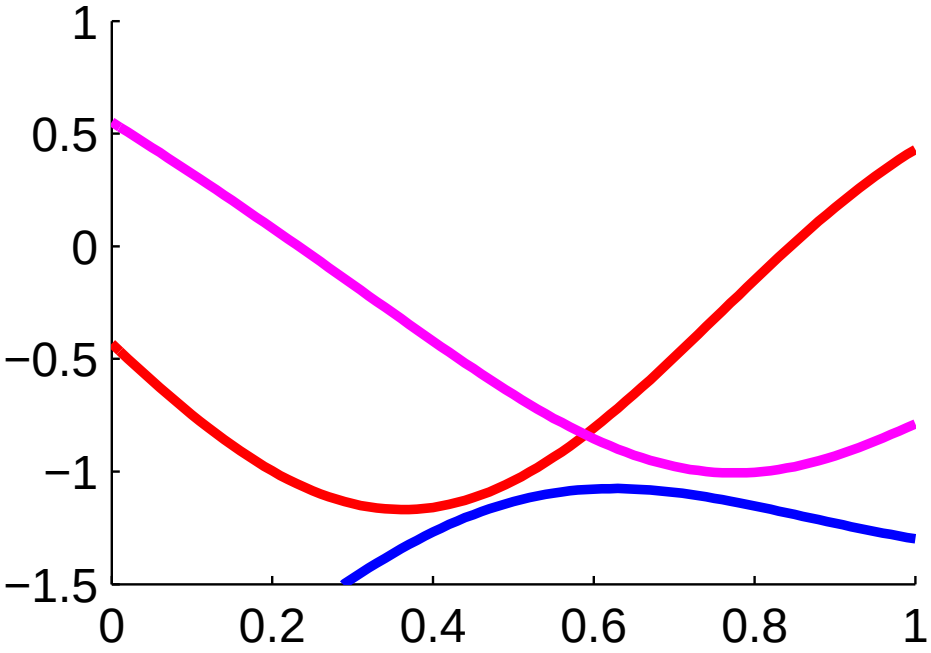
To produce this, we needed a mean: I used `zeros(25,1)`

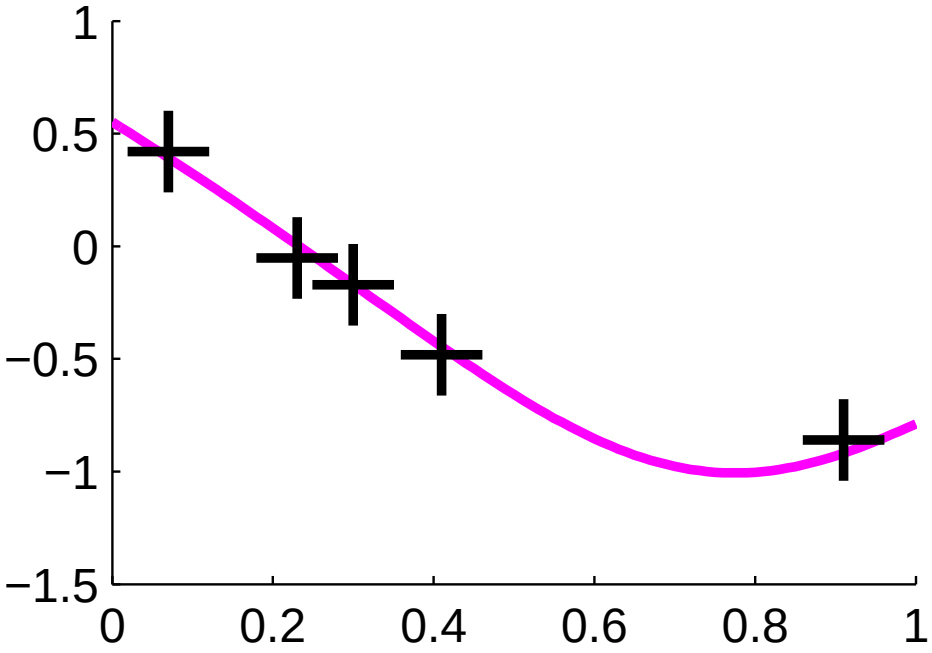
The covariances were set using a *kernel* function: $\Sigma_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$.

The $\mathbf{x}$'s are the positions that I planted the tics on the axis.

Later we'll find k's that ensure Σ is always positive semi-definite.

GP regression model





$$f \sim \mathcal{GP}$$

Noisy observations:

$$y_i \mid f_i \sim \mathcal{N}(f_i, \sigma_n^2)$$

$$\mathbf{f} \sim \mathcal{N}(0, K), \quad K_{ij} = k(x_i, x_j)$$

where $f_i = f(x_i)$

GP Posterior

Our prior over observations and targets is Gaussian:

$$P\left(\begin{bmatrix}\mathbf{y}\\ \mathbf{f}_*\end{bmatrix}\right) = \mathcal{N}\left(\begin{bmatrix}\mathbf{y}\\ \mathbf{f}_*\end{bmatrix}; \mathbf{0}, \begin{bmatrix}K(X,X)+\sigma_n^2\mathbb{I} & K(X,X_*)\\ K(X_*,X) & K(X_*,X_*)\end{bmatrix}\right)$$

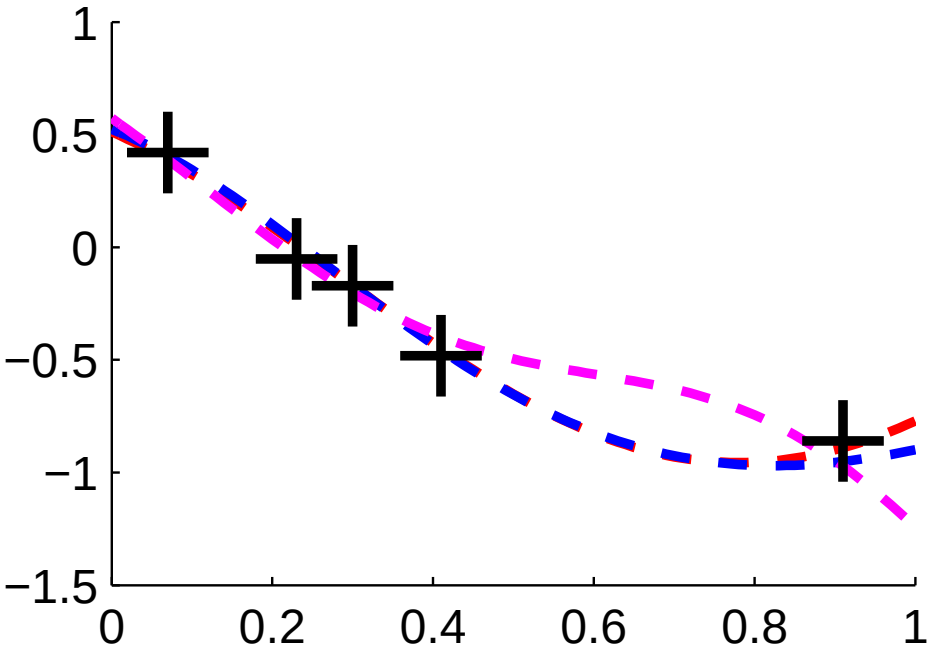
Using the rule for conditionals, $p(\mathbf{f}_* \,|\, \mathbf{y})$ is Gaussian with:

$$\text{mean}, \bar{\mathbf{f}}_* = K(X_*,X)(K(X,X)+\sigma_n^2\mathbb{I})^{-1}\mathbf{y}$$
$$\text{cov}(\mathbf{f}_*) = K(X_*,X_*) - K(X_*,X)(K(X,X)+\sigma_n^2\mathbb{I})^{-1}K(X,X_*)$$

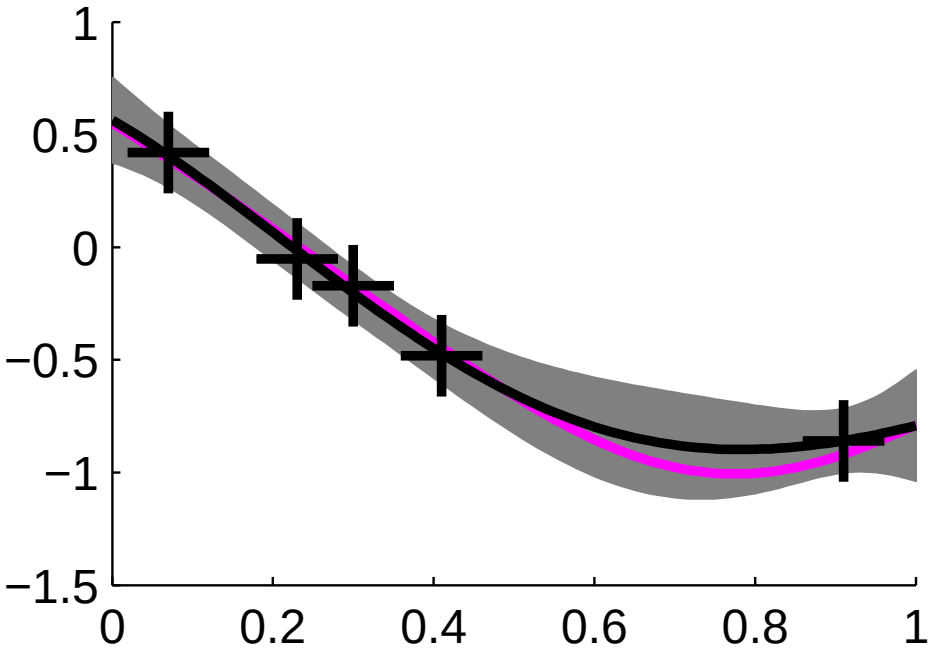
The posterior over functions is a Gaussian Process.

GP Posterior

Two incomplete ways of visualizing what we know:



Draws $\sim p(\mathbf{f} \,|\, \mathrm{data})$



Mean and error bars

Point predictions

Conditional at one point $\mathbf{x}_*$ is a simple Gaussian:

$$p(f(\mathbf{x}_*) \,|\, \text{data}) = \mathcal{N}(f;\, m,\, s^2)$$

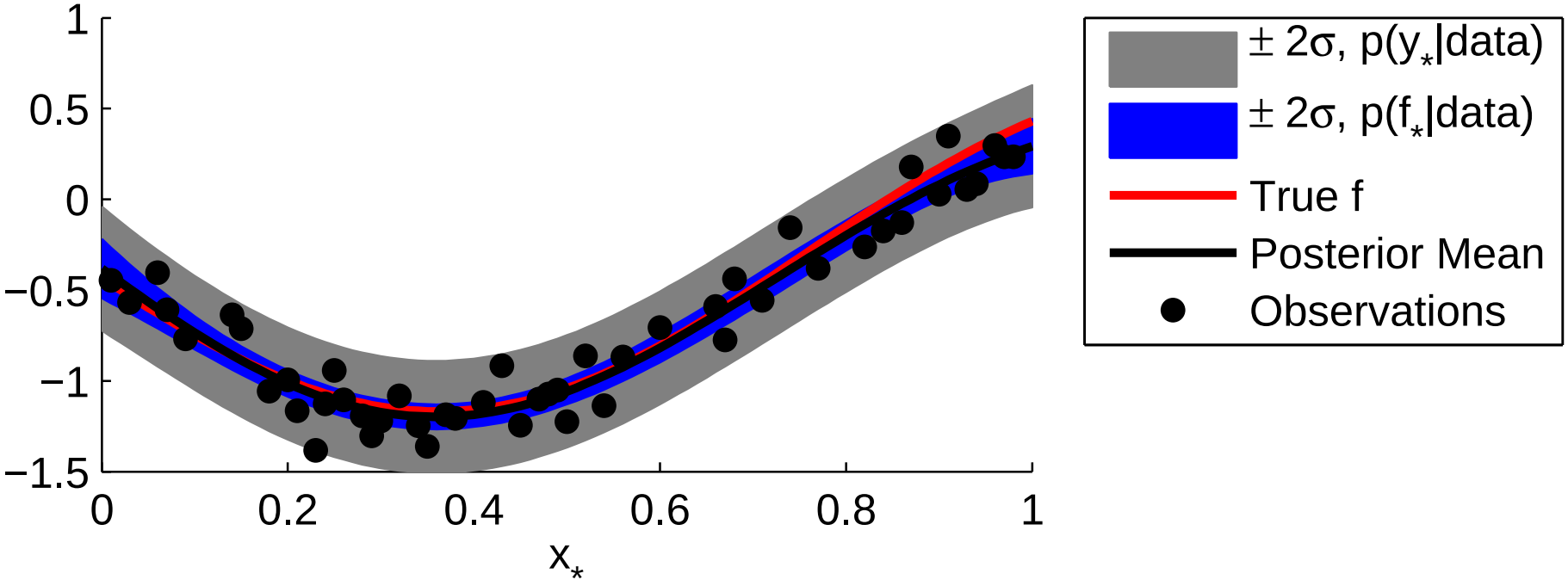
Need covariances:

$$K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j), \quad (\mathbf{k}_*)_i = k(\mathbf{x}_*, \mathbf{x}_i)$$

Special case of joint posterior:

$$M = K + \sigma_n^2 \mathbb{I}$$
$$m = \mathbf{k}_*^\top M^{-1} \mathbf{y}$$
$$s^2 = k(\mathbf{x}_*, \mathbf{x}_*) - \underbrace{\mathbf{k}_*^\top M^{-1} \mathbf{k}_*}_{\text{positive}}$$

Discovery or prediction?



$p(f_* \,|\, \text{data}) = \mathcal{N}(f_*;\ m,\ s^2)$

says what we know about the noiseless function.

$p(y_* \,|\, \text{data}) = \mathcal{N}(y_*;\ m,\ s^2 + \sigma_n^2)$

predicts what we'll see next.

Review so far

We can represent a function as a *big* vector $\mathbf{f}$

We assume that this unknown vector was drawn from a *big* correlated Gaussian distribution, a *Gaussian process*.

(This might upset some mathematicians, but for all practical machine learning and statistical problems, this is fine.)

Observing elements of the vector (optionally corrupted by Gaussian noise) creates a Gaussian posterior distribution. The posterior over functions is still a Gaussian process.

Marginalization in Gaussians is trivial: just ignore all of the positions $\mathbf{x}_i$ that are neither observed nor queried.

Covariance functions

The main part that has been missing so far is where the covariance function $k(\mathbf{x}_i, \mathbf{x}_j)$ comes from.

Also, other than making nearby points covary, what can we express with covariance functions, and what do do they mean?

Covariance functions

We can construct covariance functions from parametric models

Simplest example: **Bayesian linear regression:**

$$f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i + b, \qquad \mathbf{w} \sim \mathcal{N}(0, \sigma_w^2 \mathbb{I}), \;\; b \sim \mathcal{N}(0, \sigma_b^2)$$

$$\begin{aligned}
\mathrm{cov}(f_i, f_j) &= \langle f_i f_j \rangle - \cancelto{0}{\langle f_i \rangle} \cancelto{0}{\langle f_j \rangle} \\
&= \left\langle (\mathbf{w}^\top \mathbf{x}_i + b)^\top (\mathbf{w}^\top \mathbf{x}_j + b) \right\rangle \\
&= \sigma_w^2 \mathbf{x}_i^\top \mathbf{x}_j + \sigma_b^2 = k(\mathbf{x}_i, \mathbf{x}_j)
\end{aligned}$$

Kernel parameters σ_w^2 and σ_b^2 are *hyper-parameters* in the Bayesian hierarchical model.

More interesting kernels come from models with a large or infinite feature space: $k(\mathbf{x}_i, \mathbf{x}_j) = \sigma_w^2 \Phi(\mathbf{x}_i)^\top \Phi(\mathbf{x}_j) + \sigma_b^2$, the 'kernel trick'.

Squared-exponential kernel

An ∞ number of radial-basis functions can give

$$k(\mathbf{x}_i, \mathbf{x}_j) \;=\; \sigma_f^2 \exp\!\left(-\tfrac{1}{2} \sum_{d=1}^{D} (x_{d,i} - x_{d,j})^2 / \ell_d^2 \right),$$

the most commonly-used kernel in machine learning.

It looks like an (unnormalized) Gaussian, so is commonly called the Gaussian kernel. *Please* remember that this has nothing to do with it being a *Gaussian* process.

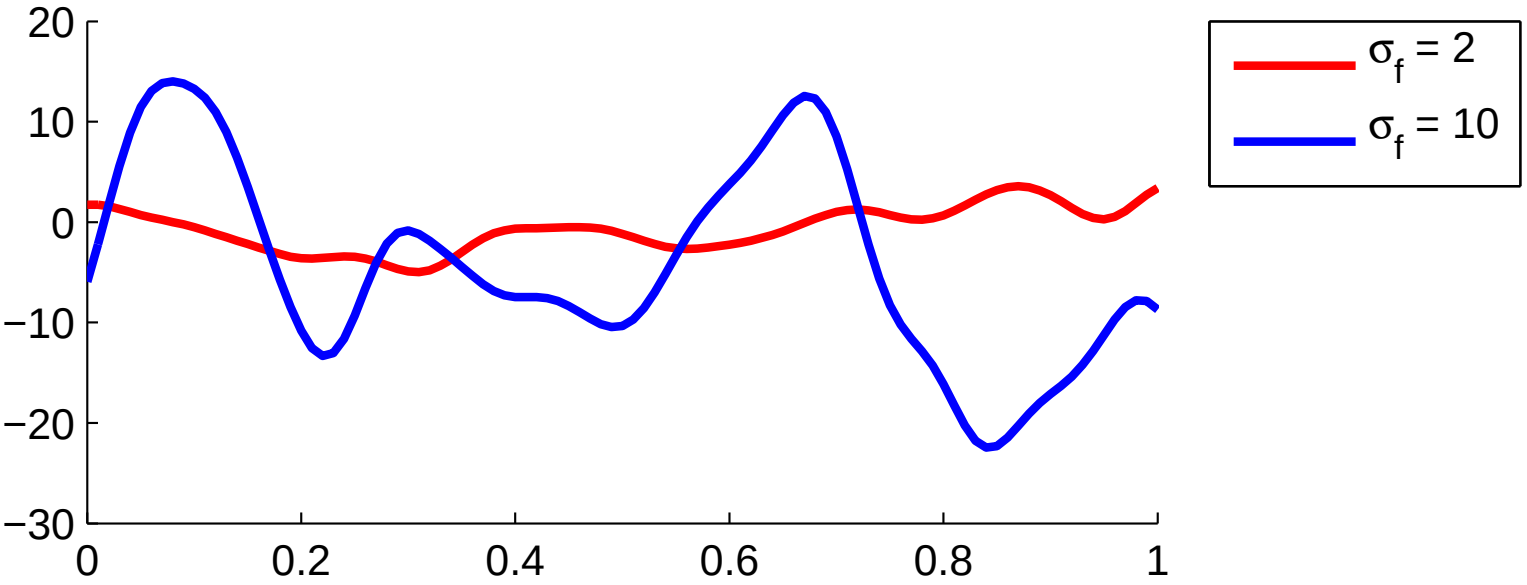
A Gaussian process need not use the "Gaussian" kernel. In fact, other choices will often be better.

Meaning of hyper-parameters

Many kernels have similar types of parameters:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(-\frac{1}{2} \sum_{d=1}^{D} (x_{d,i} - x_{d,j})^2 / \ell_d^2 \right),$$

Consider $\mathbf{x}_i = \mathbf{x}_j$, $\Rightarrow$ marginal function variance is σ_f^2

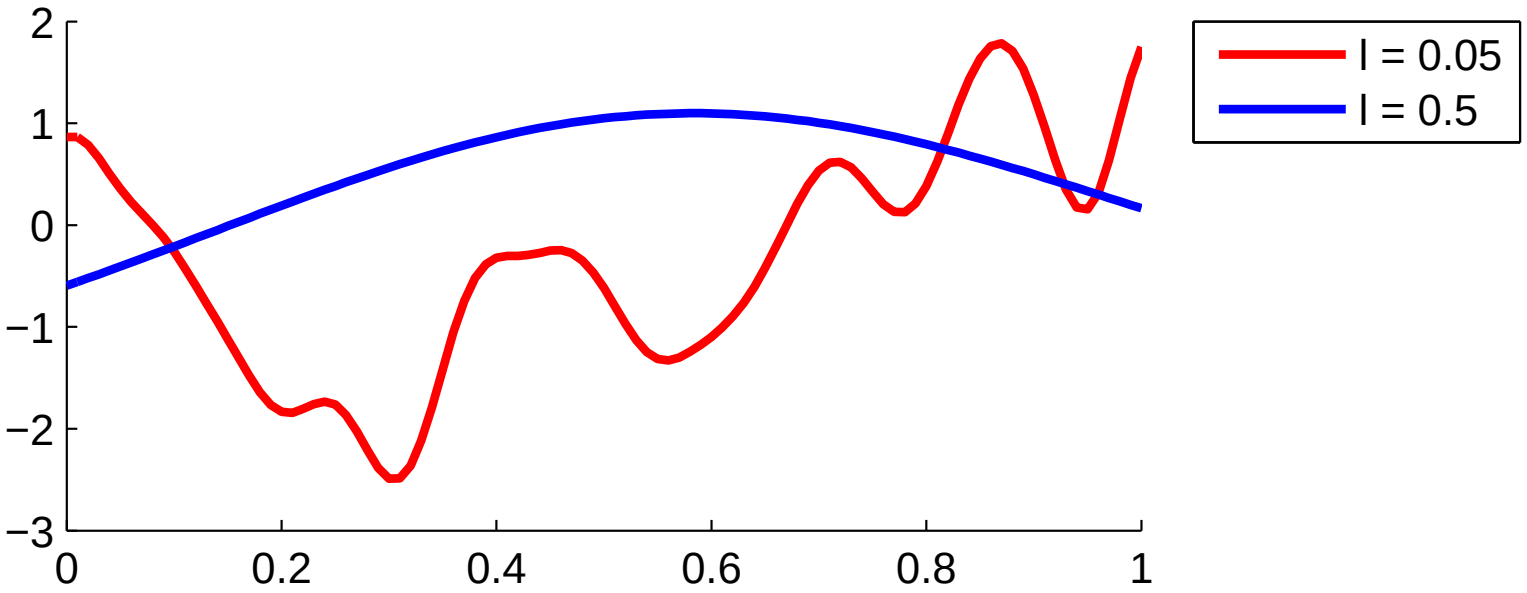


Meaning of hyper-parameters

ℓ_d parameters give the length-scale in dimension-d

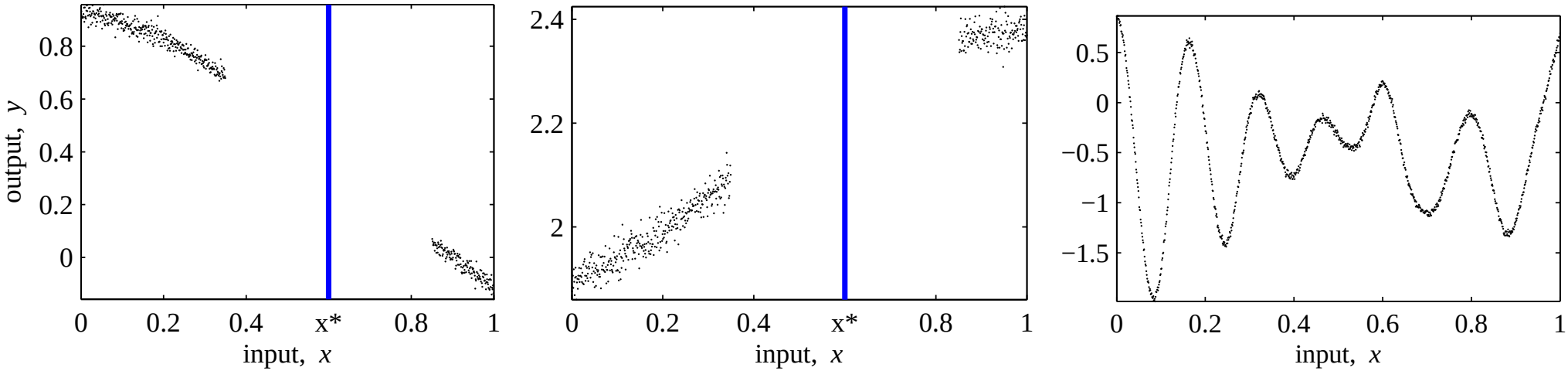
$$k(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(-\frac{1}{2} \sum_{d=1}^{D} (x_{d,i} - x_{d,j})^2 / \ell_d^2 \right),$$

Typical distance between peaks $\approx \ell$



Typical GP lengthscales

What is the covariance matrix like?



— Zeros in the covariance $\Rightarrow$ marginal independence

— Short length scales usually don't match my beliefs

— Empirically, I often learn $\ell \approx 1$ giving a dense K

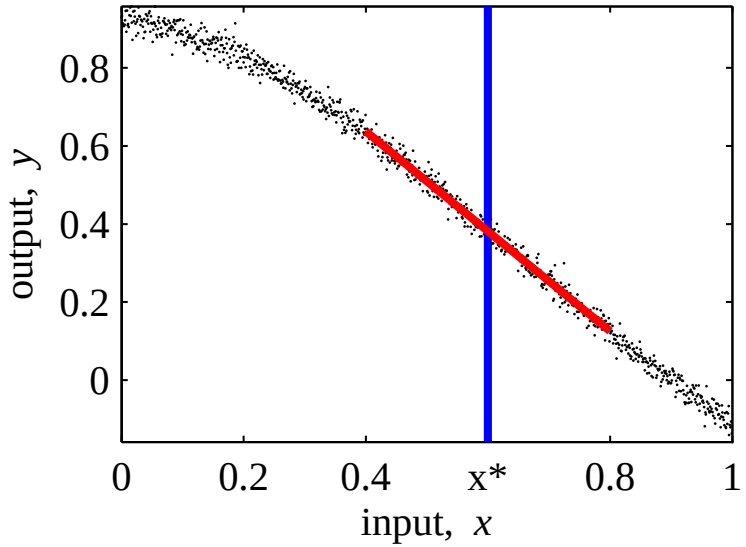
Common exceptions:

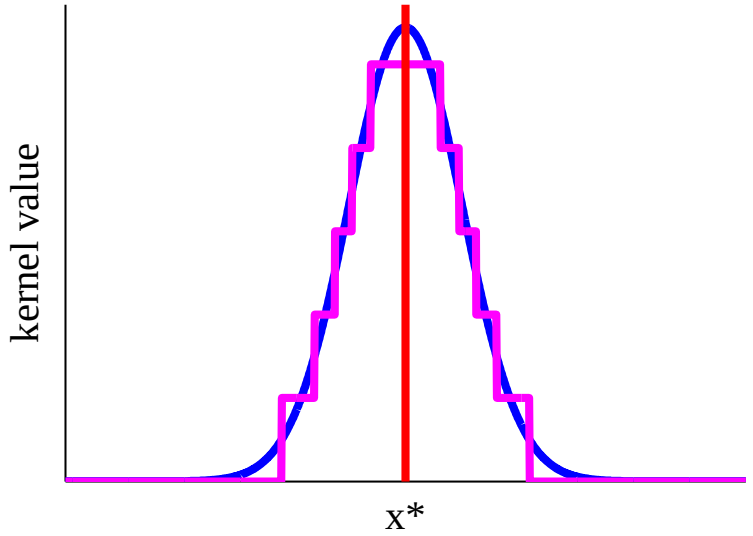
Time series data, ℓ small. Irrelevant dimensions, ℓ large.

In high dimensions, can have $K_{ij} \approx 0$ with $\ell \approx 1$.

What GPs are not

Locally-Weighted Regression weights points with a kernel before fitting a simple model



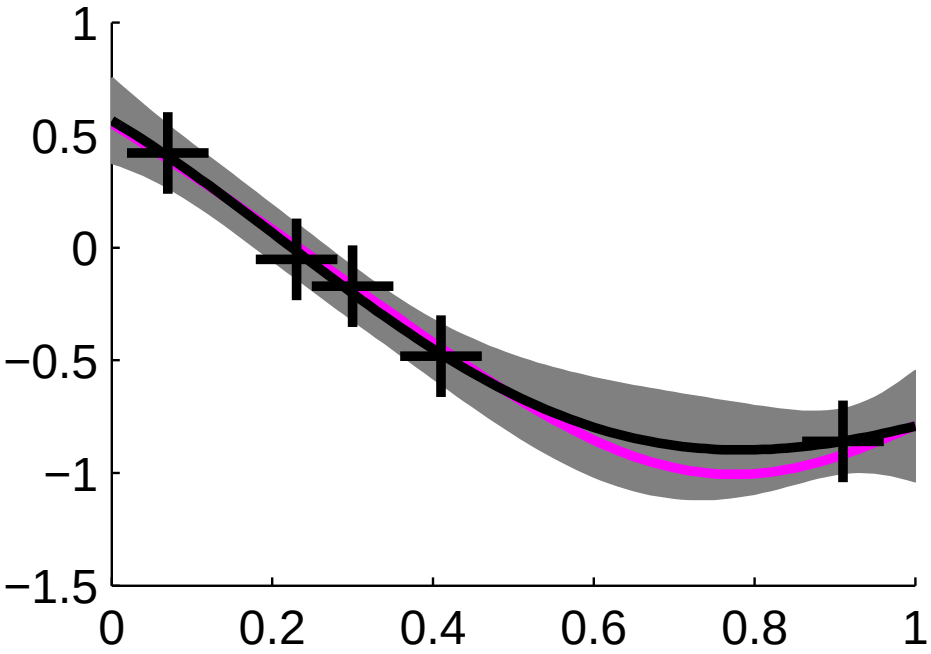


Meaning of kernel zero here: $\approx$ *conditional* independence.

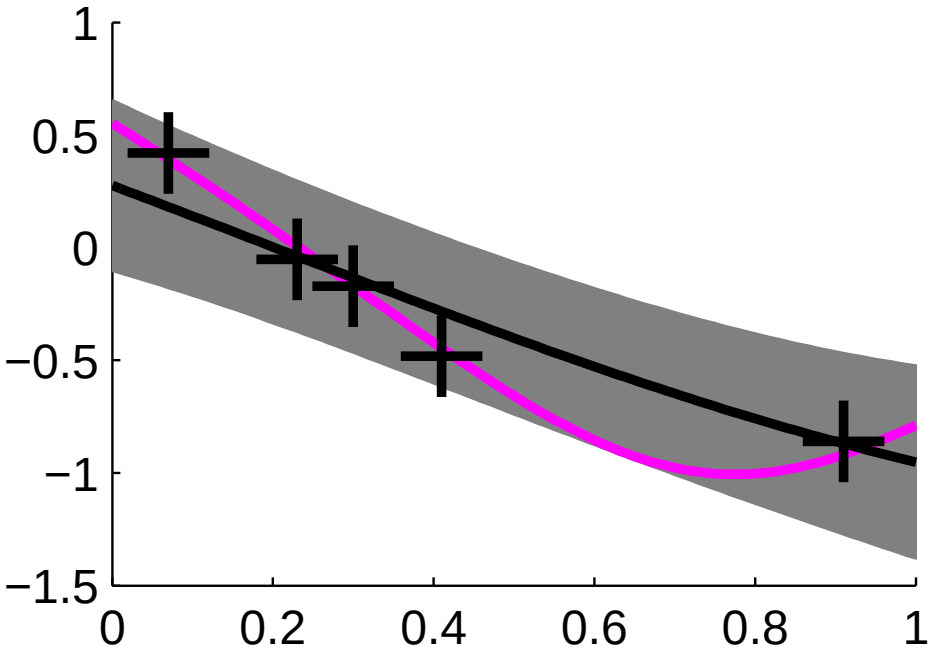
Unlike GP kernel: a) shrinks to small ℓ with many data points; b) does not need to be positive definite.

Effect of hyper-parameters

Different (SE) kernel parameters give different explanations of the data:



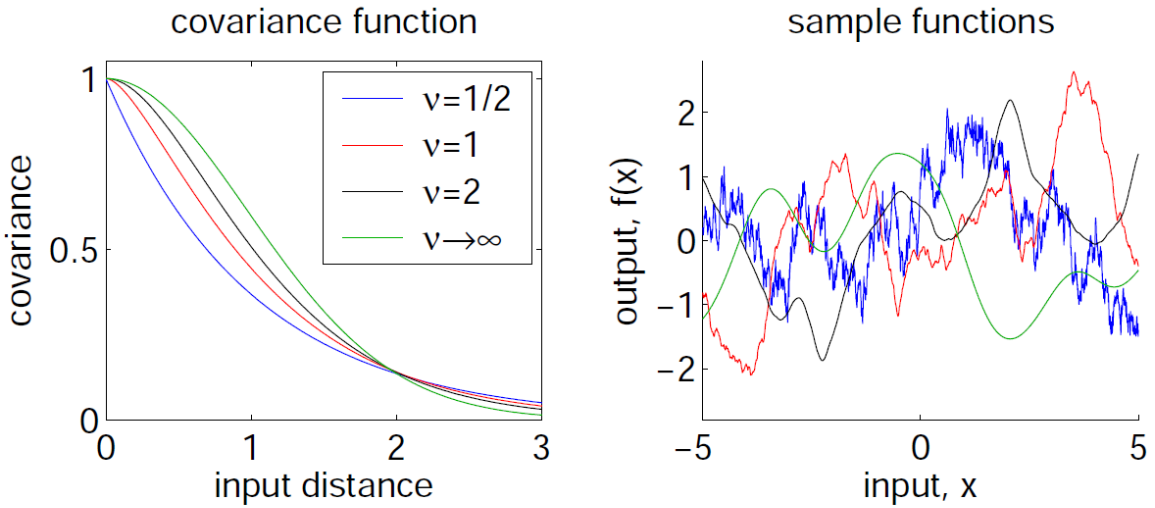
$\ell = 0.5, \quad \sigma_n = 0.05$



$\ell = 1.5, \quad \sigma_n = 0.15$

Other kernels

The squared-exponential kernel produces *very* smooth functions. For some problems the Matérn covariances functions may be more appropriate:



Periodic kernels are available, and some that vary their noise and lengthscales across space.

Kernels can be combined in many ways (Bishop p296). For example, add kernels with long and short lengthscales

The (marginal) likelihood

The probability of the data is just a Gaussian:

$$\log p(\mathbf{y} \mid X, \theta) = -\tfrac{1}{2}\mathbf{y}^\top M^{-1}\mathbf{y} - \tfrac{1}{2}\log|M| - \tfrac{n}{2}\log 2\pi$$

— likelihood of the kernel parameters, $\theta = \{\ell, \sigma_n, \dots\}$
— used to choose amongst kernels

Gradients of the likelihood wrt the hyper-parameters can be computed to find (local) maximum likelihood fits.

Because the GP can be viewed as having an infinite number of weight parameters that have been integrated out, $\log p(\mathbf{y} \mid X, \theta)$ is often called the *marginal* likelihood.

Learning hyper-parameters

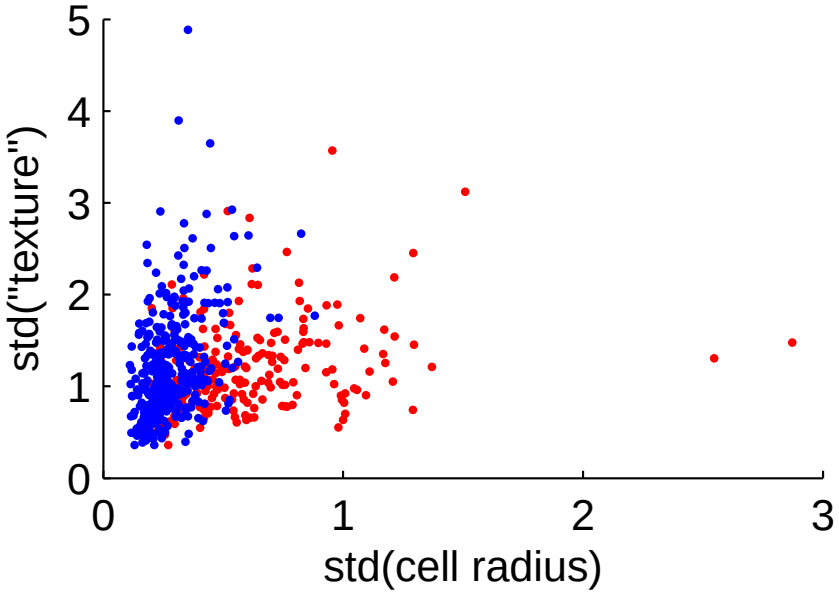
The **fully Bayesian solution** computes the function posterior:

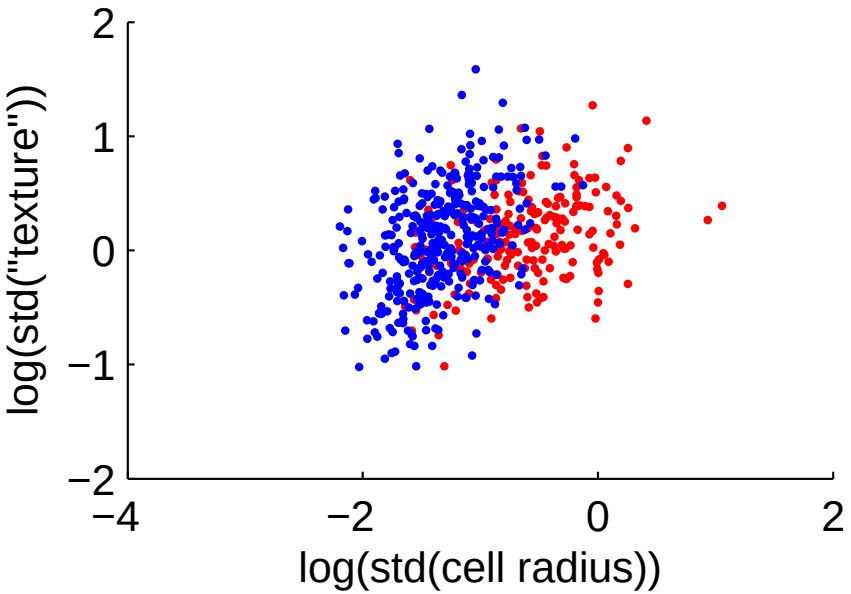
$$p(f_* \,|\, \mathbf{y}, X) = \int p(f_* \,|\, \mathbf{y}, X, \theta)\, p(\theta \,|\, \mathbf{y}, X)\, \mathrm{d}\theta$$

The first term in the integrand is tractable.

The second term is the posterior over hyper-parameters. This can be sampled using Markov chain Monte Carlo to **average predictions over plausible hyper-parameters**.

Log-transform +ve inputs





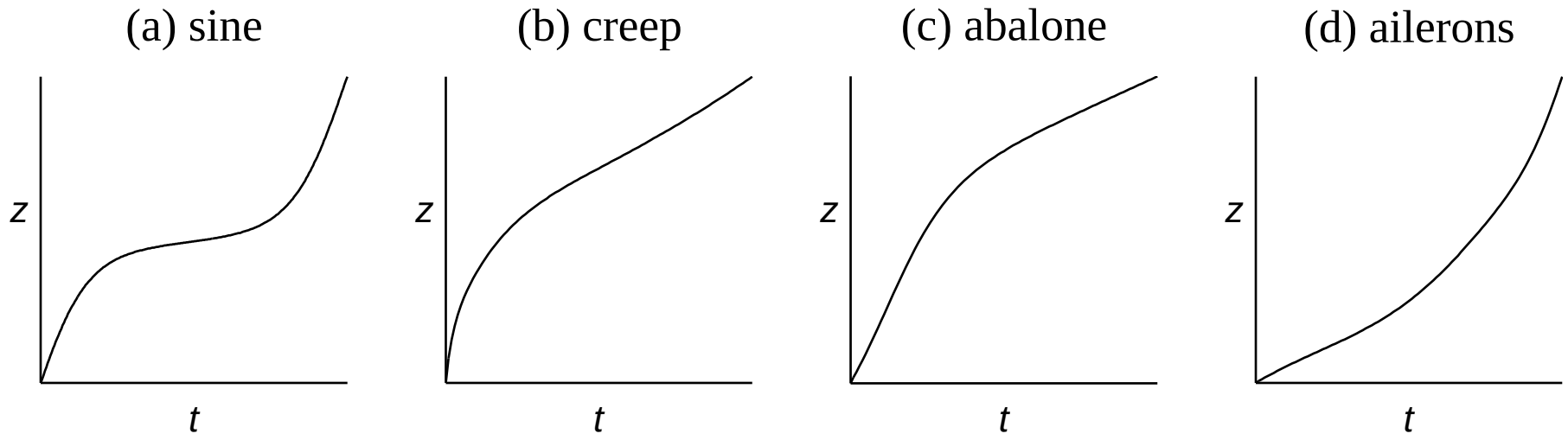
(Wisconsin breast cancer data from the UCI repository)

Positive quantities are often highly skewed
The log-domain is often a much more natural space

A better transformation could be learned:
Schmidt and O'Hagan, JRSSB, 65(3):743–758, (2003).

Log-transform +ve outputs

Warped Gaussian processes, Snelson et al. (2003)

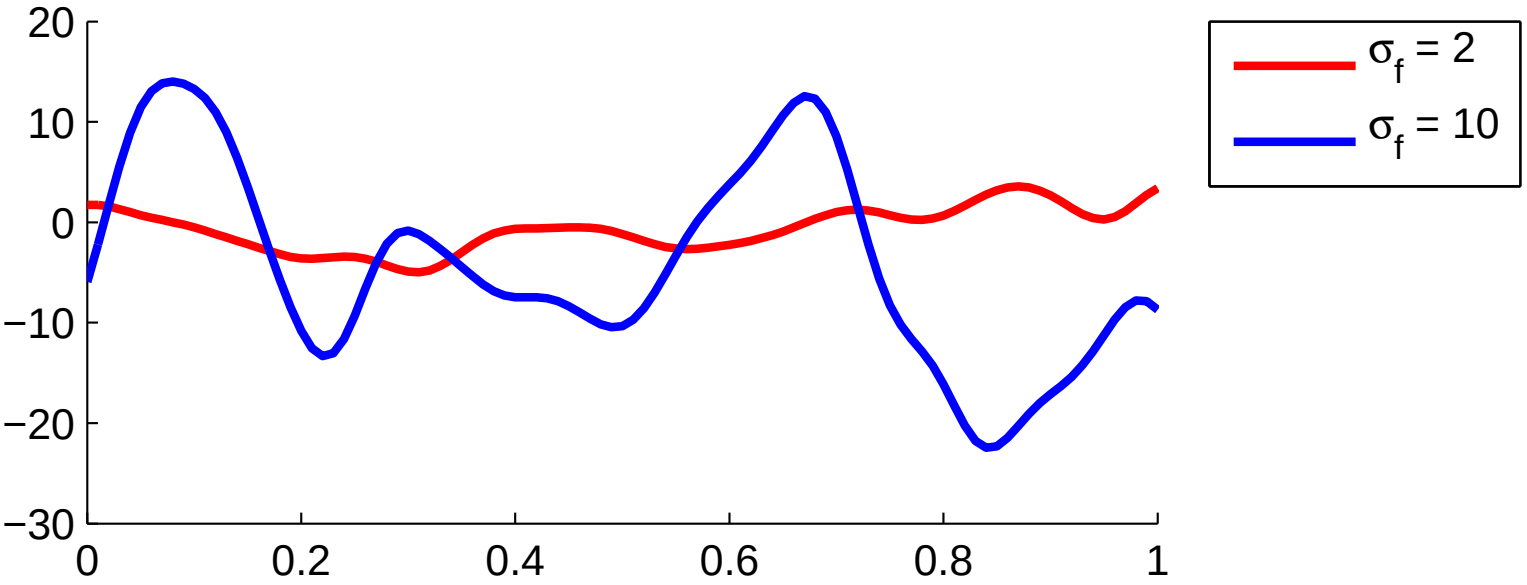


Learned transformations for positive data were log-like.
Always consider log transforming postive data.

However, other transformations (or none at all)
are sometimes the best option.

Mean function

Using $\mathbf{f} \sim \mathcal{N}(\mathbf{0}, K)$ is common



If your data is not zero-mean this is a poor model.

Center your data, or use a parametric mean function $m(\mathbf{x})$.

Other tricks

To set initial hyper-parameters, **use domain knowledge wherever possible**. Otherwise. . .

Standardize input data and set lengthscales to ~ 1.

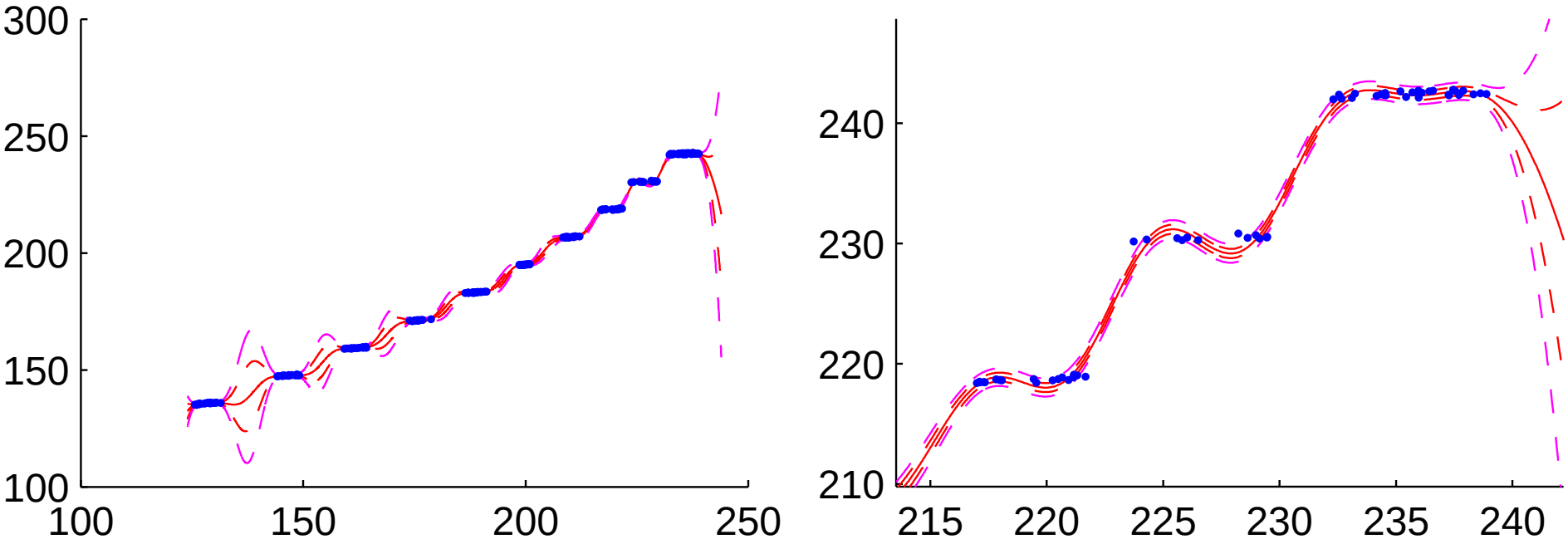
Standardize targets and set function variance to ~ 1.

Often useful: **set initial noise level high**, even if you think your data have low noise. The optimization surface for your other parameters will be easier to move in.

If optimizing hyper-parameters, (as always) random restarts or other tricks to **avoid local optima** are advised.

Real data can be nasty

A projection of a robot arm problem:



Common artifacts: thresholding, ju^{mps}, clumps, $_{k}$i^{n}k$_{s}$

How might we fix these problems? [discussion]

Non-Gaussian likelihoods

GP regression is tractable because both the prior and likelihood are Gaussian.

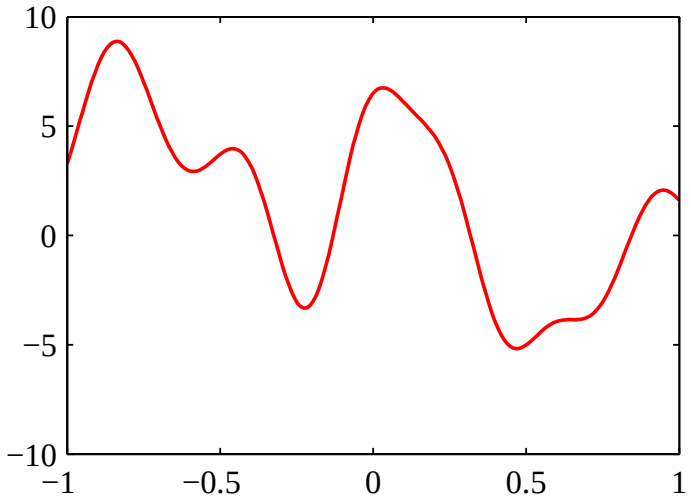
There are many reasons to want to use non-Gaussian likelihoods, although we can no longer marginalize out the unknown function values at the observations. We can use approximate inference methods such as MCMC, EP, Laplace or Variational Bayes.

A common application of a non-Gaussian likelihood is a model of heavy-tailed noise to account for large outliers. This is intractable, but there are computational tricks to help deal with t-distributions.

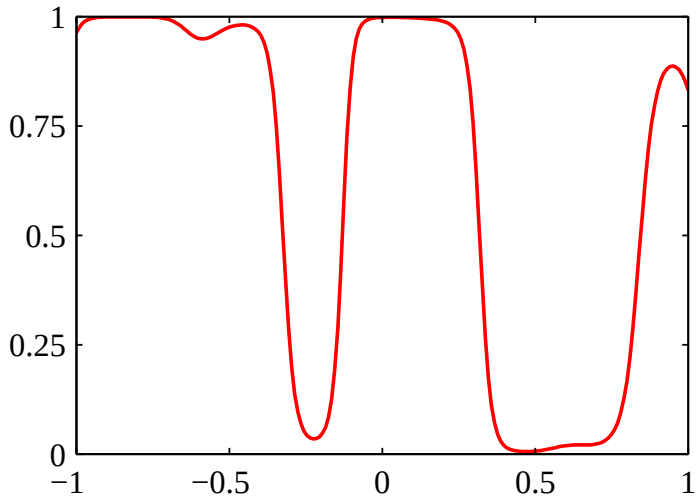
Classification

Special case of a non-Gaussian noise model

Assume $y_i \sim \text{Bernoulli}(\text{sigmoid}(f_i))$



f(x)



logistic(f(x))

MCMC can be used to sum over the latent function values.
EP (Expectation Propagation) also works very well.

Figures from Bishop textbook

Regressing on the labels

If we give up on a Bayesian modelling interpretation, **we could just apply standard GP regression code** on binary classification data with $y \in \{-1, +1\}$.

The sign of the mean function is a reasonable hard classifier. Asymptotically the posterior function will be peaked around $f(\mathbf{x}) = 2p(\mathbf{x}) - 1$.

Multiway classification: regressing $y \in \{1, 2, \ldots, C\}$ would be a bad idea. Instead, train C "one-against all" classifiers and pick class with largest mean function.

Not really Gaussian process modelling any more: this is just regularized least squares fitting

Exploding costs

GPs scale poorly with large datasets

$\mathcal{O}(n^3)$ computation usually takes the blame:

$$M^{-1} \quad \text{or} \quad M^{-1}\mathbf{y},\ M^{-1}\mathbf{k}_* \quad \text{and} \quad \det(M)$$

Not the only story:

$$K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

$\mathcal{O}(dn^2)$ computation

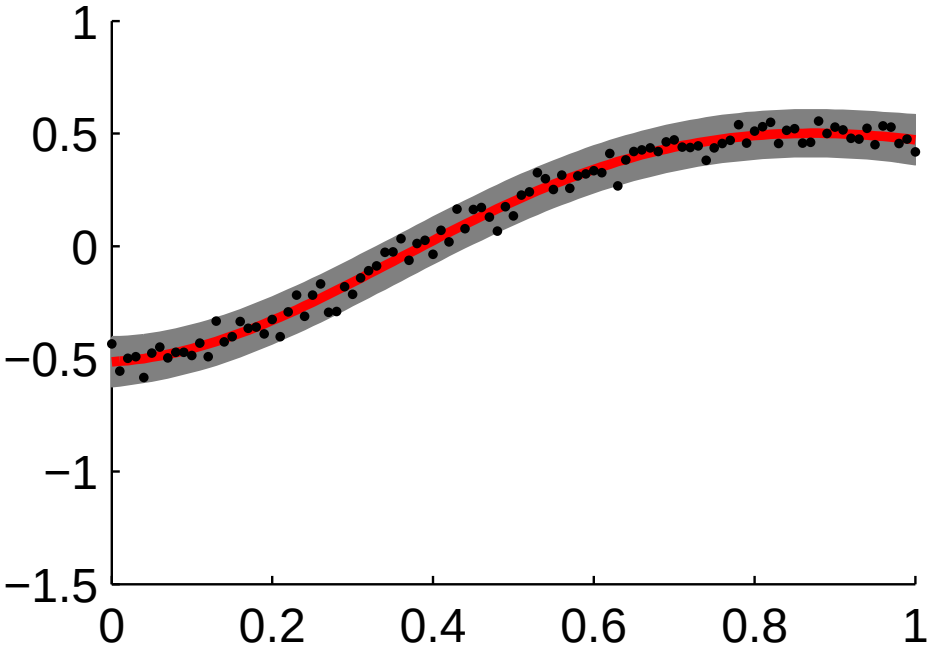
$\mathcal{O}(n^2)$ memory

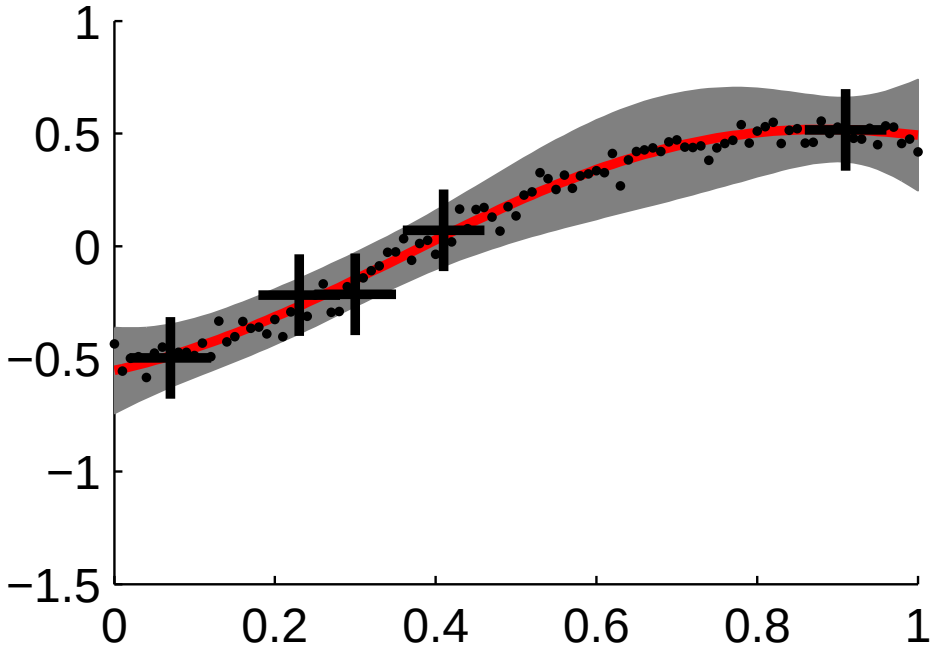
Large literature on GP approximations

Subset of Data

Trivial, obvious solution:

randomly throw away most of the data





e.g. keeping 1/20 points

There are also methods to choose greedily, cheaply choose which points to keep.

Mixtures and committees

Because the costs scale super-linearly, splitting up the dataset helps:

A mixture of K experts potentially involves much cheaper matrix operations:

$$n^3 > K(n/K)^3 = n^3/K^2$$

Alternatively K trained GPs can be simply averaged. The Bayesian Committee Machine (BCM) provides a sensible weighted averaging and error bars.

Inducing point methods

Approximate the GP prior:

$$
\begin{aligned}
p(\mathbf{f}, \mathbf{f}_*) &= \int p(\mathbf{f}, \mathbf{f}_* \,|\, \mathbf{u})\, p(\mathbf{u})\, \mathrm{d}\mathbf{u} \\
&\simeq q(\mathbf{f}, \mathbf{f}_*) = \int q(\mathbf{f} \,|\, \mathbf{u})\, q(\mathbf{f}_* \,|\, \mathbf{u})\, p(\mathbf{u})\, \mathrm{d}\mathbf{u}
\end{aligned}
$$

Several methods result from choosing different q's:

SoR/DIC, PLV/PP/DTC, FI(T)C/SPGP and BCM

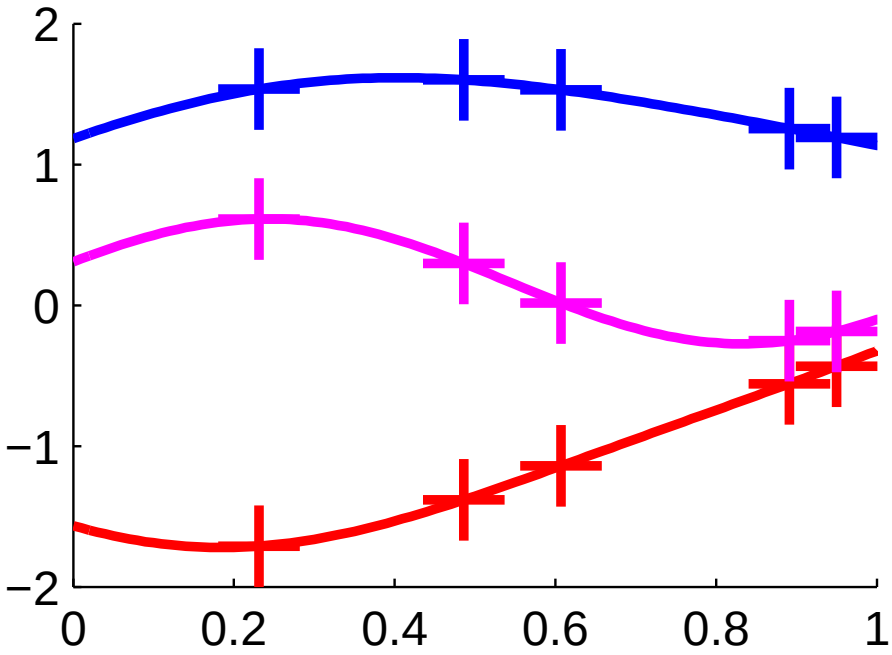
Quiñonero-Candela and Carl Edward Rasmussen (2005)

SoR/DIC, a finite linear model

$q(\mathbf{f} \mid \mathbf{u})$ deterministic:

$$\mathbf{u} \sim \mathcal{N}(0, K_{uu}), \quad \text{set } f_* = \mathbf{k}_*^\top K_{uu}^{-1} \mathbf{u}$$

Draws from the prior:



Costs (m inducing u's):

$\mathcal{O}(m^2 n)$ training

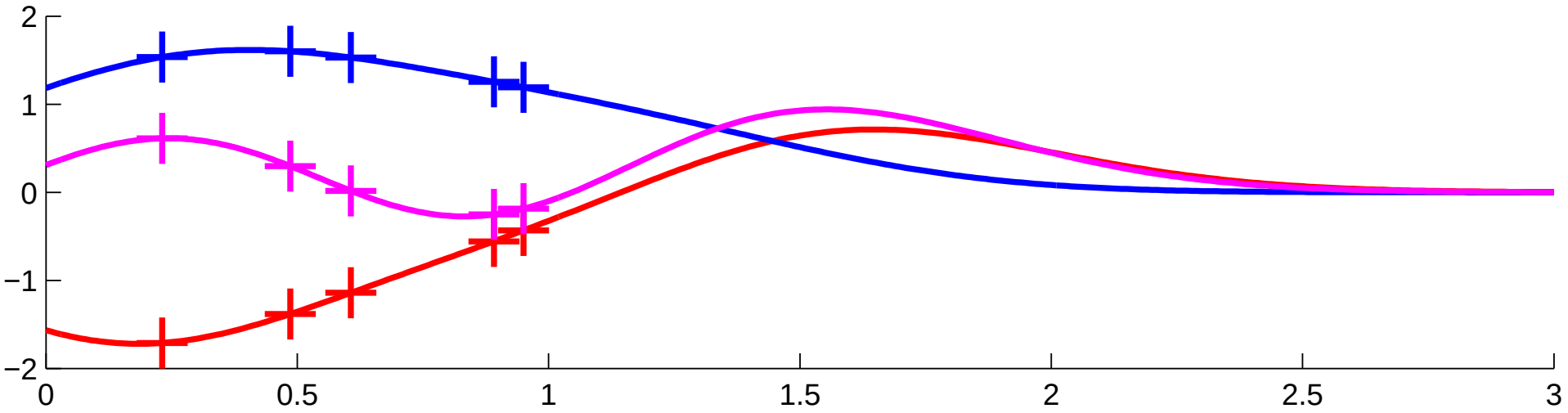
$\mathcal{O}(mn)$ covariances

$\mathcal{O}(m)$ mean prediction

$\mathcal{O}(m^2)$ error bars

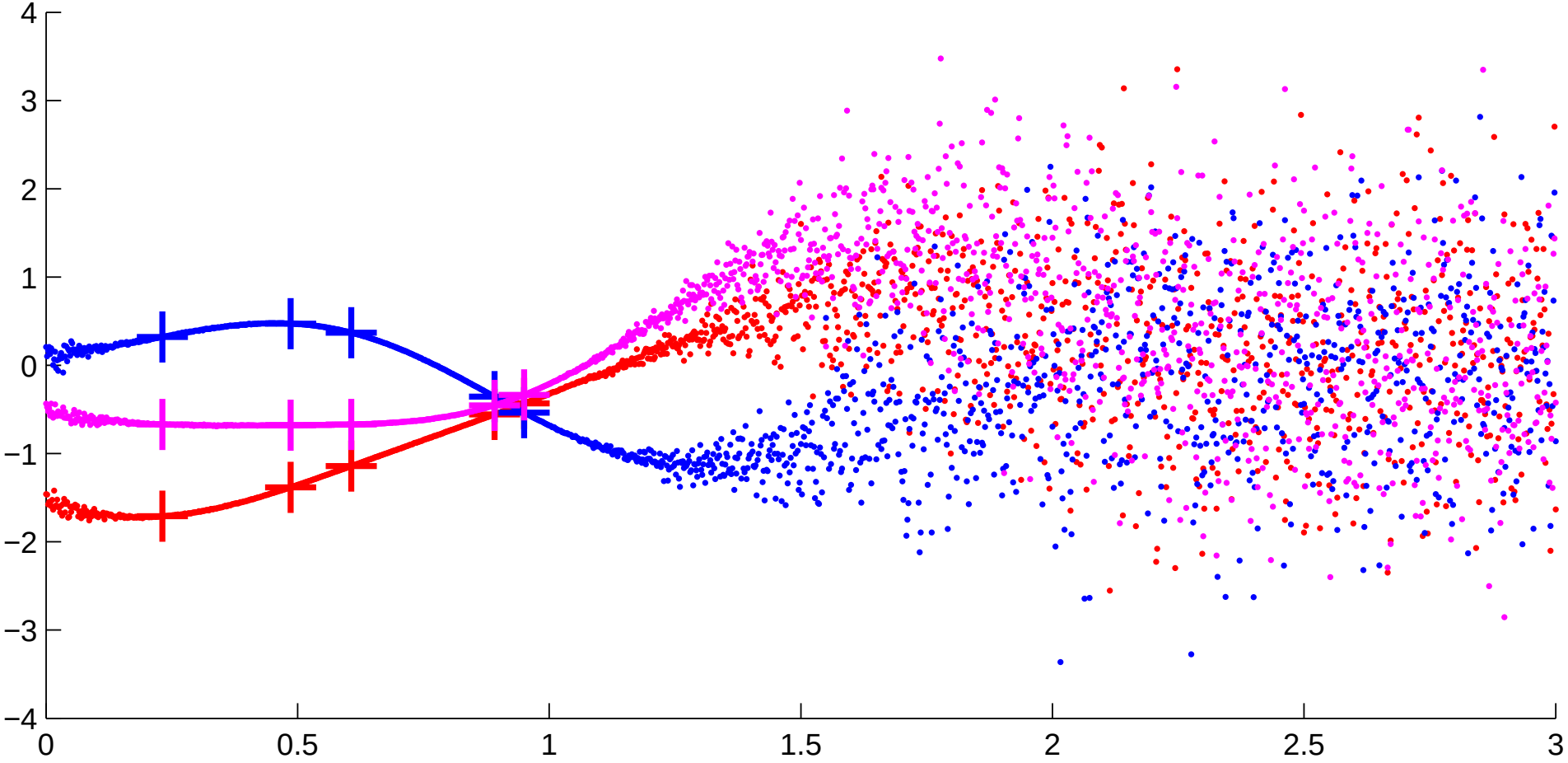
Limited fitting power

Those SoR prior draws again:



FIC / SPGP

$$q(\mathbf{f} \,|\, \mathbf{u}) \;=\; \prod_i p_{\mathcal{GP}}(f_i \,|\, \mathbf{u})$$



$\mathcal{O}(\cdot)$ costs are the same as SoR

[If time or at end: discuss low noise behaviours]

Training and Test times

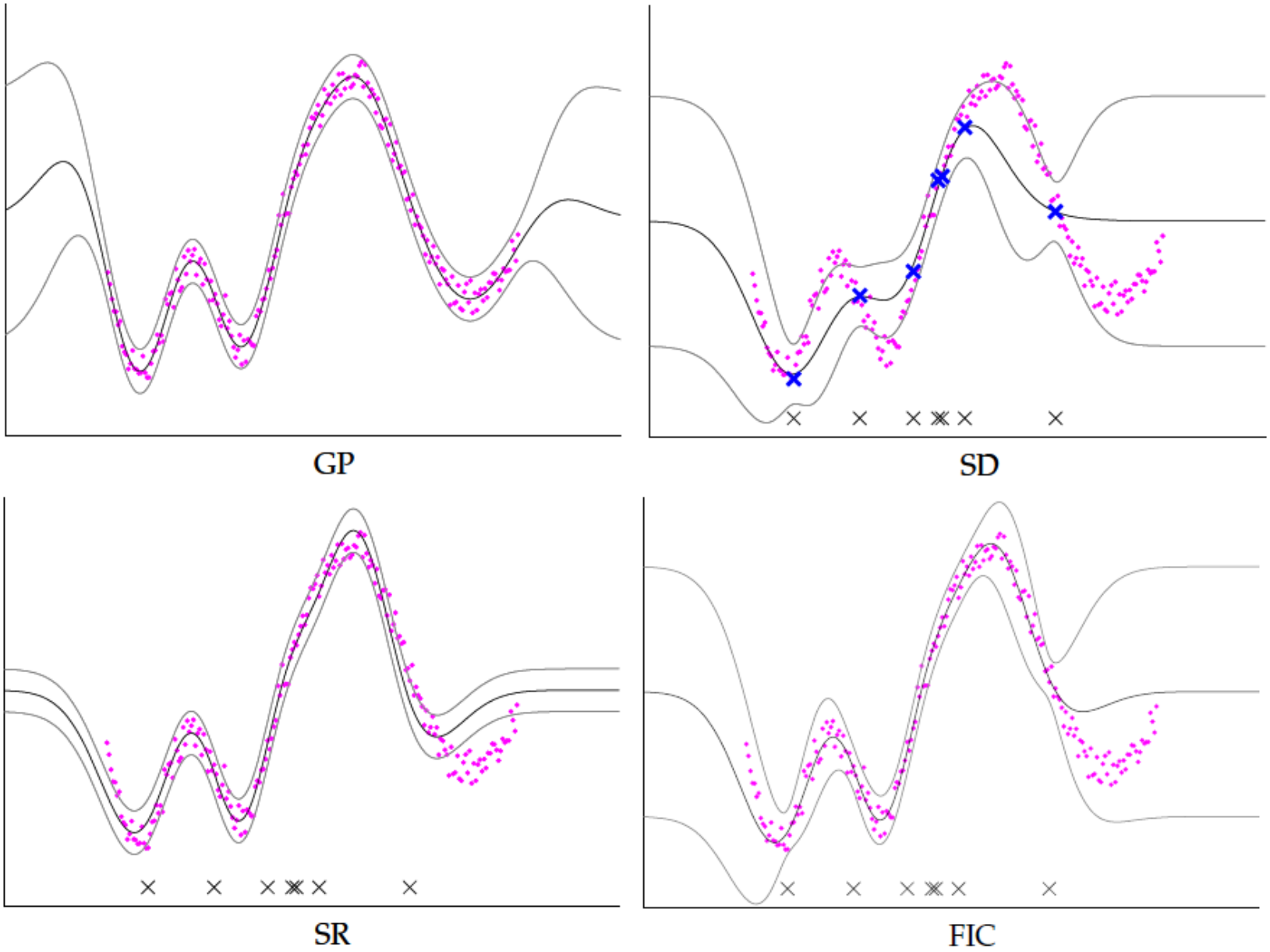
Training time: before looking at the test set

Method	Covariance	Inversion
Full GP	$\mathcal{O}(n^2)$	$\mathcal{O}(n^3)$
SoD	$\mathcal{O}(m^2)$	$\mathcal{O}(m^3)$
Sparse	$\mathcal{O}(mn)$	$\mathcal{O}(mn^2)$

Test time: spent making predictions

Method	Mean	Error bar
Full GP	$\mathcal{O}(n)$	$\mathcal{O}(n^2)$
SoD	$\mathcal{O}(m)$	$\mathcal{O}(m^2)$
Sparse	$\mathcal{O}(m)$	$\mathcal{O}(m^2)$

Sparse behaviour

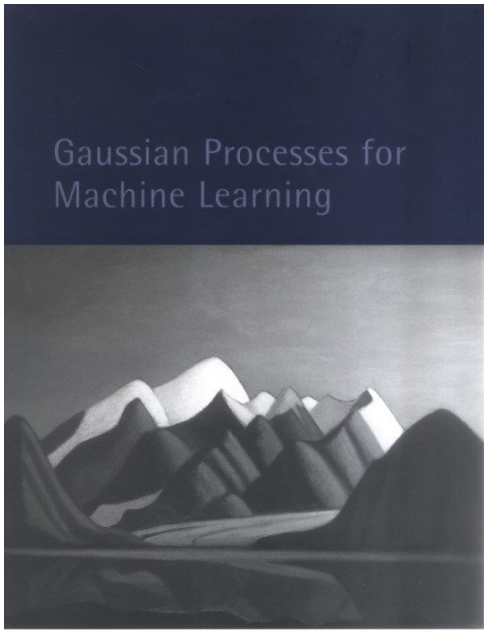


from Edward Snelson's thesis

Take-home messages

- **Simple to use:**
  - Just matrix operations (if likelihoods are Gaussian)
  - Few parameters: *relatively* easy to set or sample over
  - Predictions are often very good
- **No magic bullet:** best results need (at least) careful data scaling, which could be modelled or done by hand.
- **The need for approximate inference:**
  - Sometimes Gaussian likelihoods aren't enough
  - $\mathcal{O}(n^3)$ and $\mathcal{O}(n^2)$ costs are bad news for big problems

Further reading



Many more topics and code:
`http://www.gaussianprocess.org/gpml/`

More software:
`http://becs.aalto.fi/en/research/bayes/gpstuff/`

Gaussian processes for ordinal regression, Chu and Ghahramani, $JMLR$, 6:1019–1041, 2005.

Flexible and efficient Gaussian process models for machine learning, Edward L. Snelson, PhD thesis, UCL, 2007.