A tutorial on Gaussian Processes

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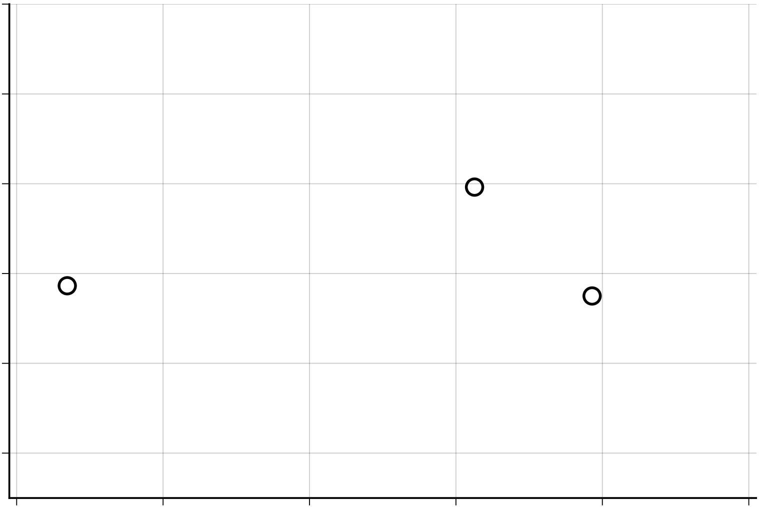
Motivation: Non-linear Regression



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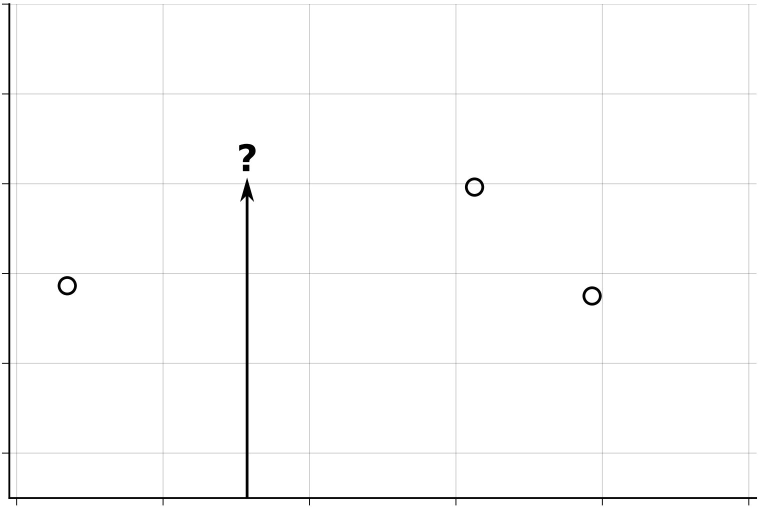

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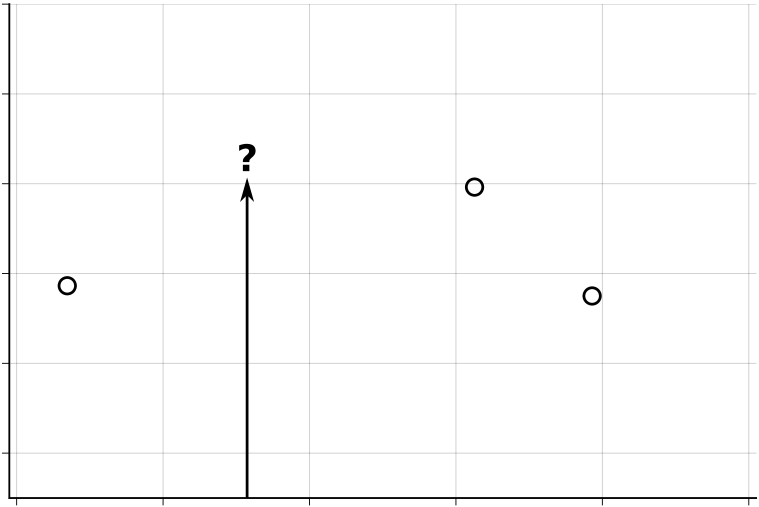

We have to specify a model that may depend on parameters W.

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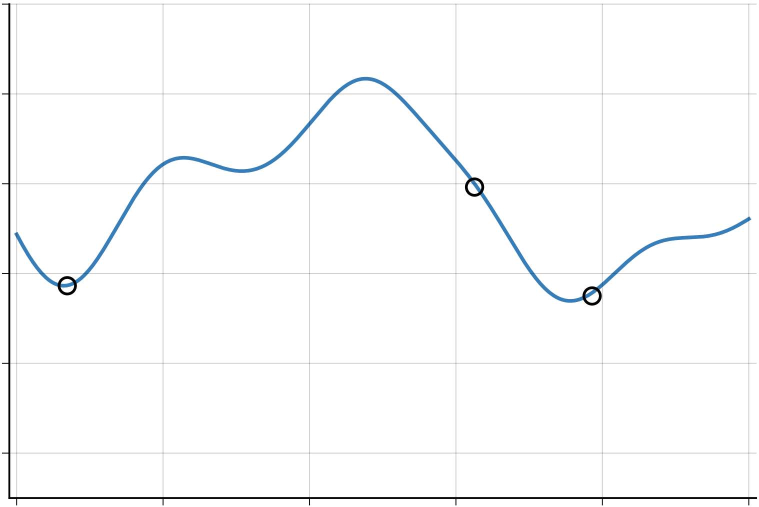

Given W the model will output a prediction.

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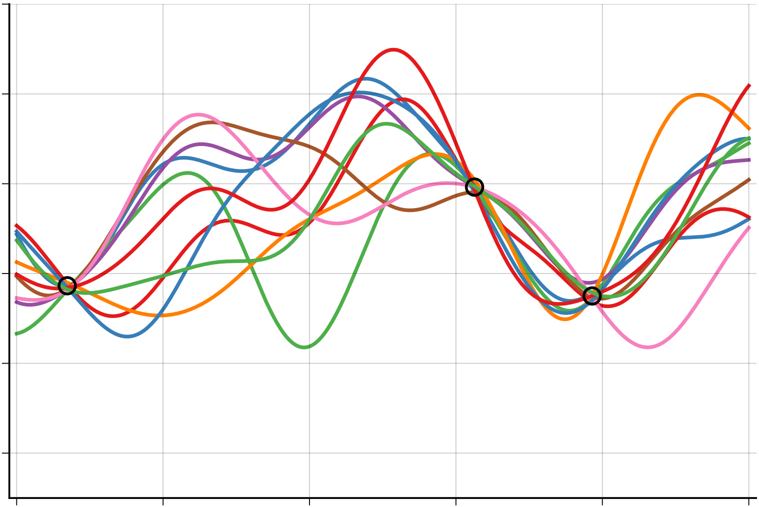

Many values for W can be compatible with the data!

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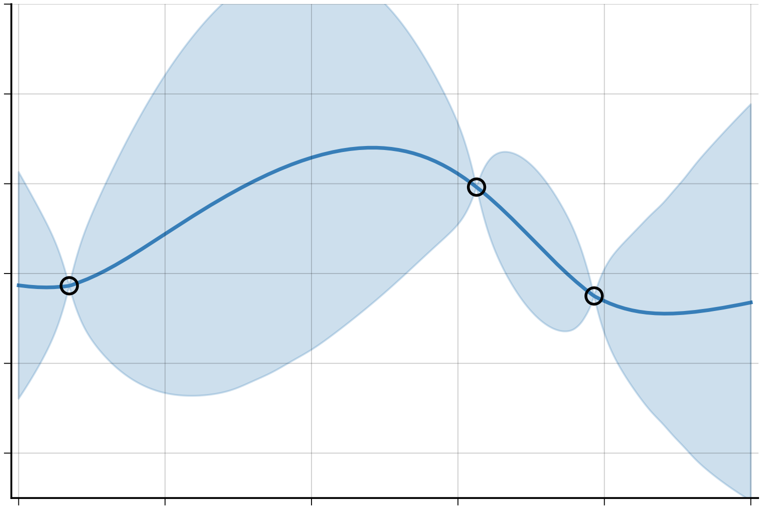
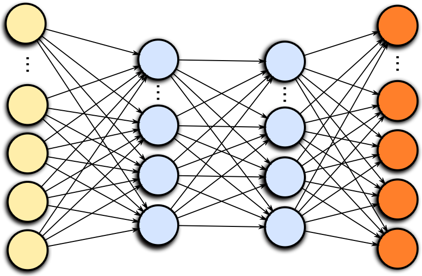


We are interested in a predictive distribution!

Computation of the Posterior Distribution



$$h_j(\mathbf{x}) = \tanh\left(\sum_{i=1}^{I} x_i w_{ji}\right)$$

$$f(\mathbf{x}) = \sum_{j=1}^{H} v_j h_j(\mathbf{x})$$

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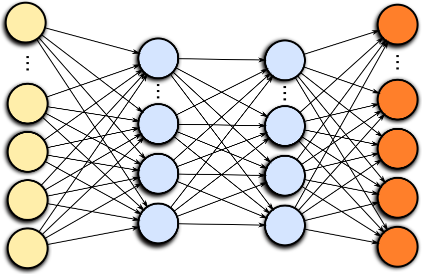

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The posterior distribution of **W** is:

$$p(\mathbf{W}|\mathbf{y}, \mathbf{X}) = \frac{p(\mathbf{y}|\mathbf{W}, \mathbf{X})p(\mathbf{W})}{p(\mathbf{y}|\mathbf{X})}\,, \qquad p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|\mathbf{W}, \mathbf{X})p(\mathbf{W})d\mathbf{W}\,,$$

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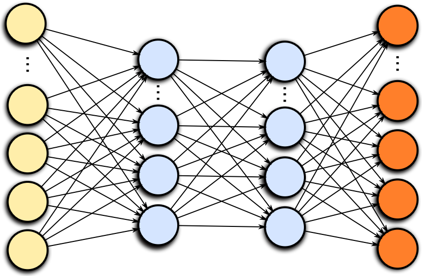

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The posterior captures the values of W compatible with y and X.

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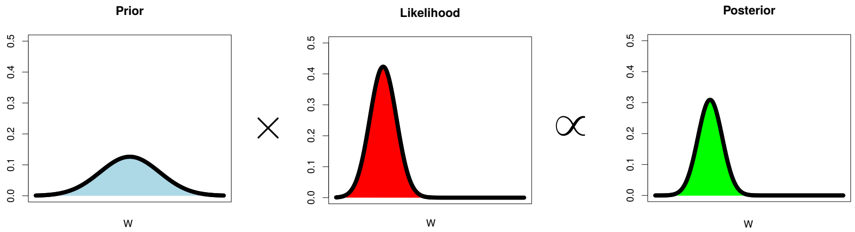

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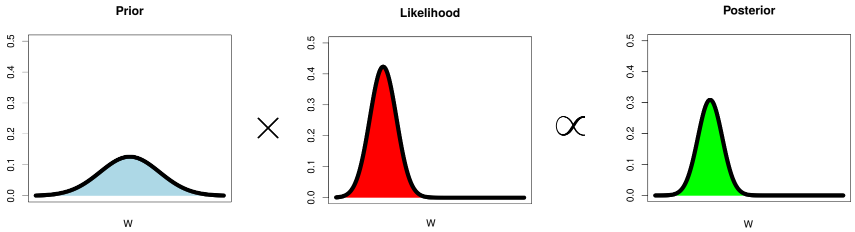

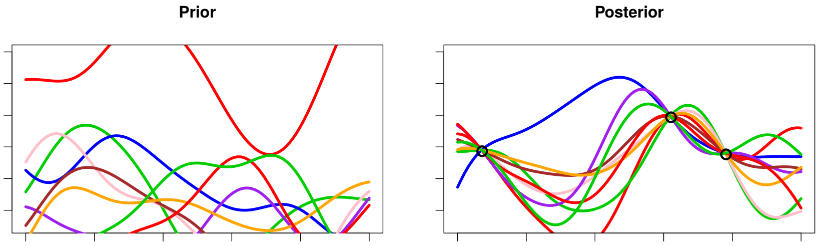

Computation of the Predictive Distribution

The predictive distribution $y^\star$ is computed using the posterior:

$$p(y^\star|\mathbf{y}, \mathbf{X}) = \int p(y^\star|\mathbf{W}, \mathbf{x}^\star) p(\mathbf{W}|\mathbf{y}, \mathbf{X}) d\mathbf{W} \, .$$

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Takes into account all potential values for W!

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Challenges:

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- $p(\mathbf{y}|\mathbf{X})$ cannot be computed!

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Challenges:

- $p(\mathbf{y}|\mathbf{X})$ cannot be computed!
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Solved by setting $p(\mathbf{W}) = \prod_{ij} \mathcal{N}(w_{ji}|0, \sigma^2 H^{-1})$ **and letting** $H \to \infty$**!**

Gaussian Processes

Distribution over functions $f(\cdot)$ so that for any finite $\{\mathbf{x}_i\}_{i=1}^N$, $(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N))^\mathsf{T}$ follows an N-dimensional Gaussian distribution.

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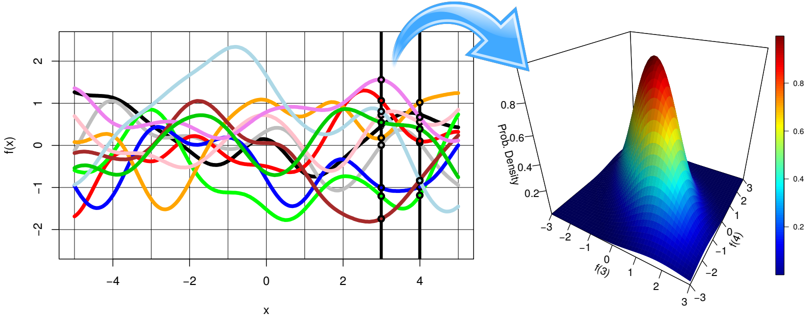

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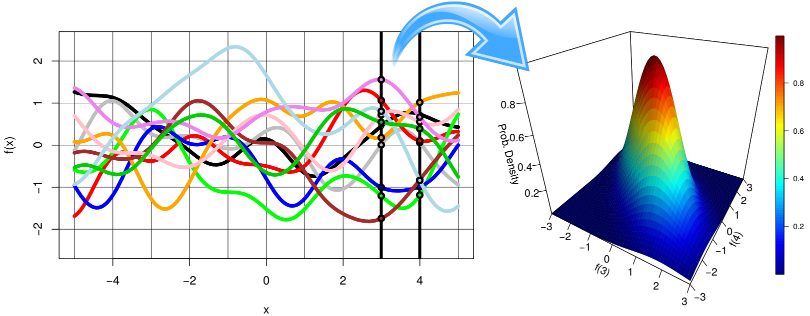

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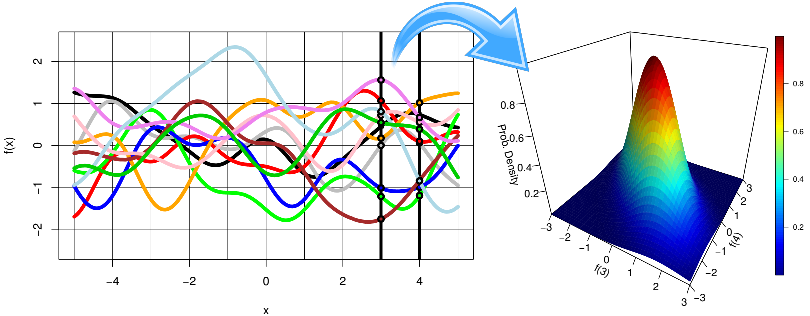

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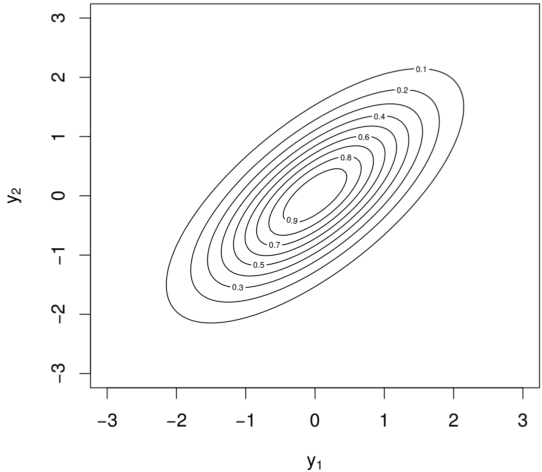
Due to Gaussian form, there are closed-form solutions for many useful questions about finite data.

Gaussian Distribution

$$p(\mathbf{y}|\boldsymbol{\Sigma}) \propto \exp\left\{-0.5\mathbf{y}^\mathsf{T}\boldsymbol{\Sigma}^{-1}\mathbf{y}\right\} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}.$$



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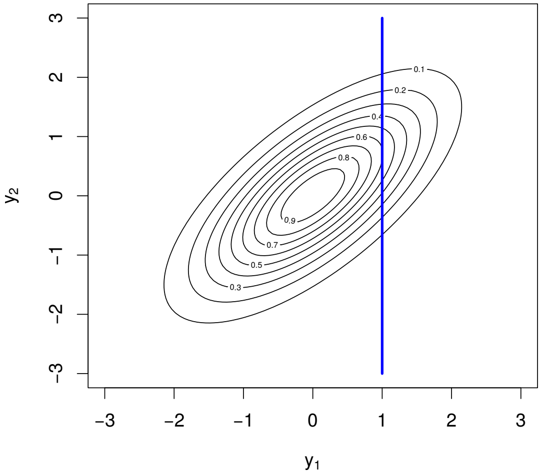

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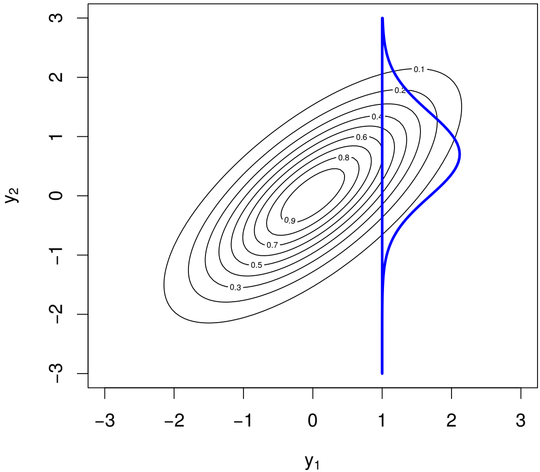

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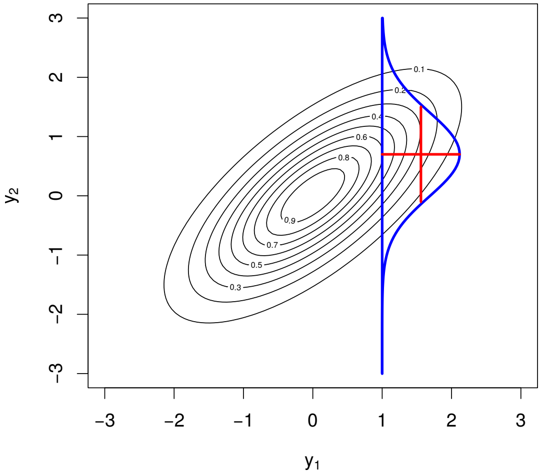

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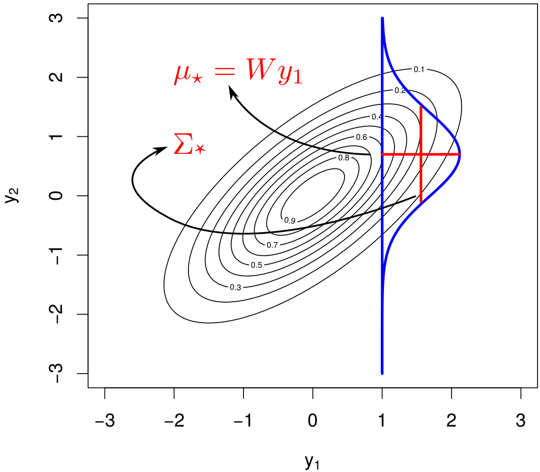
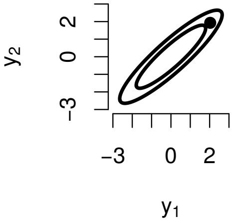


Two Dimensional Example



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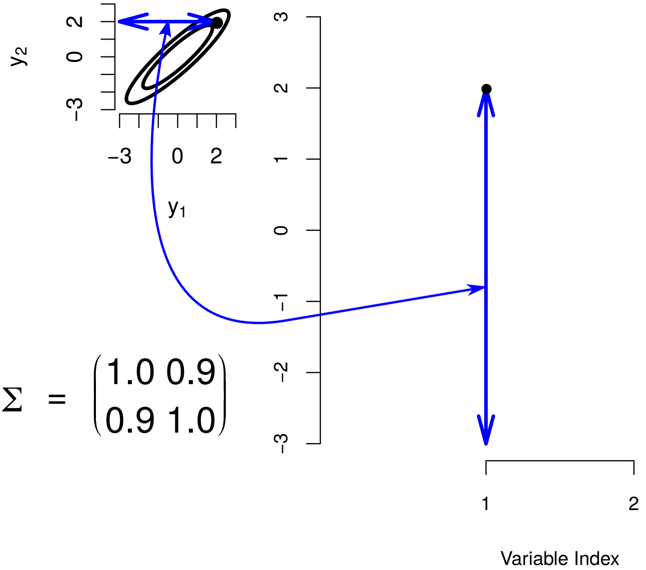

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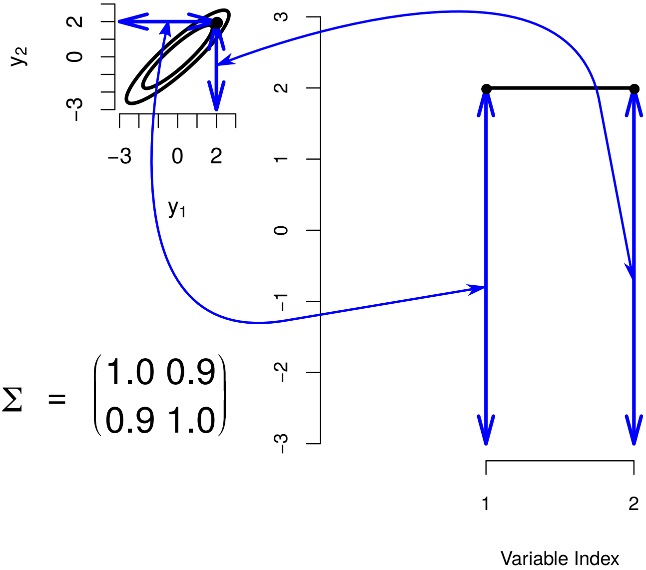

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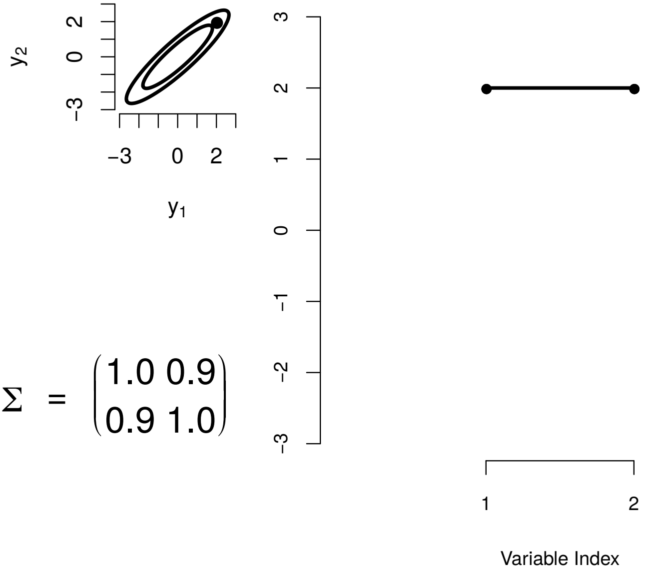

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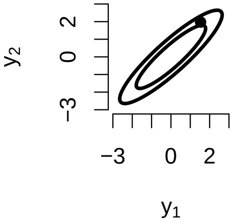

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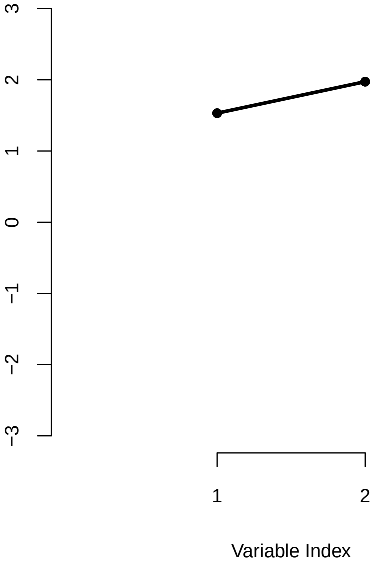

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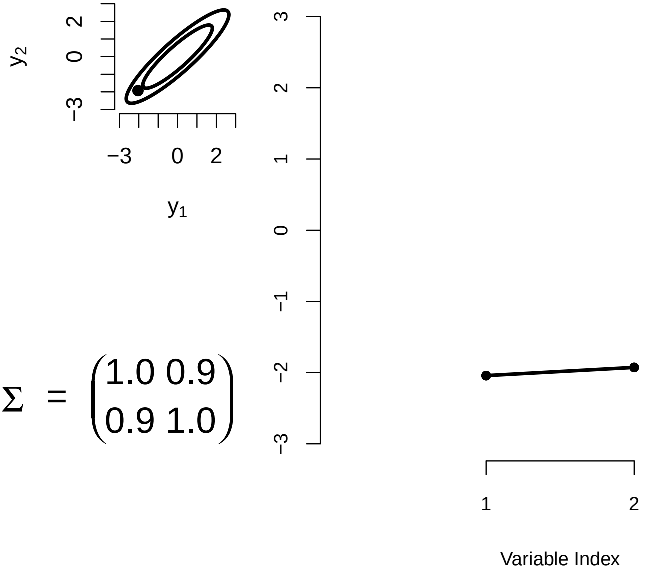

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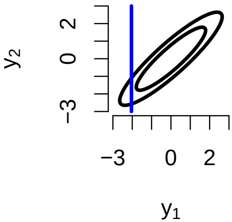

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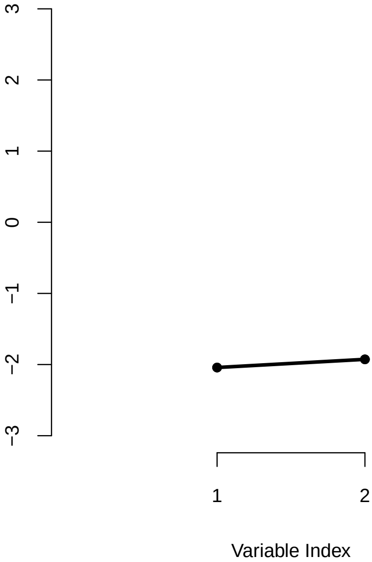

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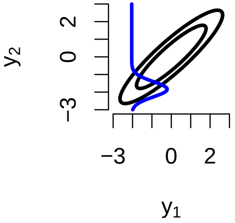

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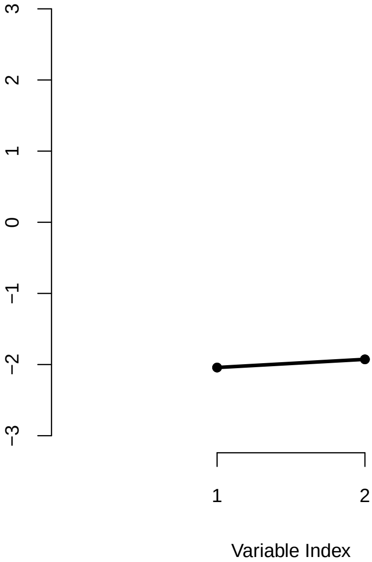

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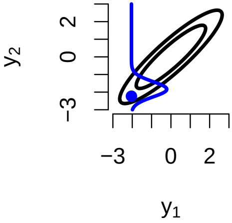

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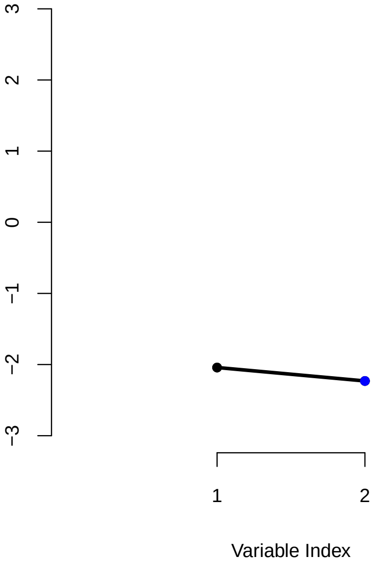
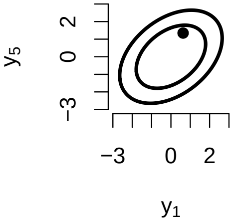
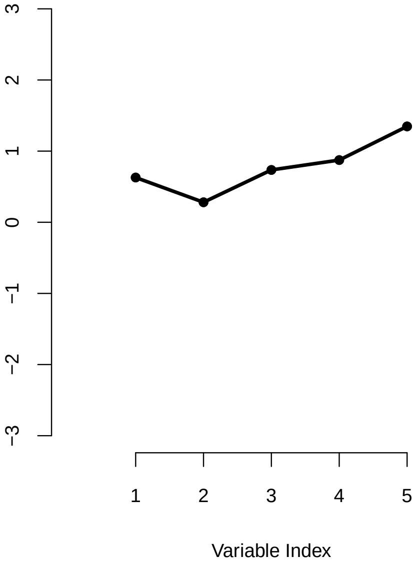


Five Dimensional Example



$$\Sigma = \begin{bmatrix} 1.0 & .9 & .8 & .6 & .4 \\ .9 & 1.0 & .9 & .8 & .6 \\ .8 & .9 & 1.0 & .9 & .8 \\ .6 & .8 & .9 & 1.0 & .9 \\ .4 & .6 & .8 & .9 & 1.0 \end{bmatrix}$$



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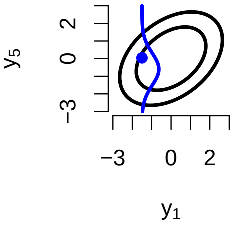

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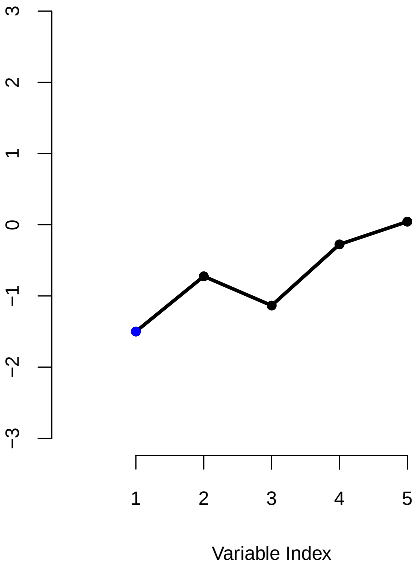
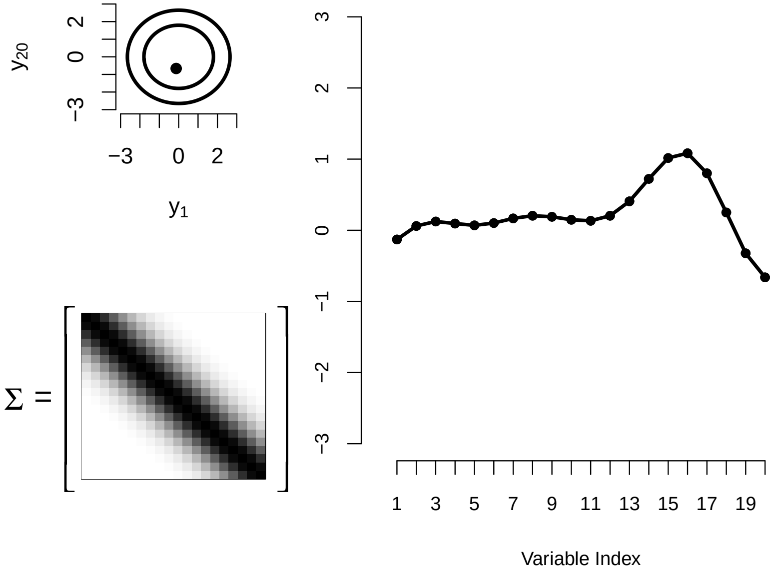


Twenty Dimensional Example



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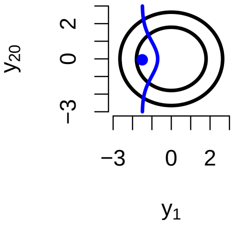
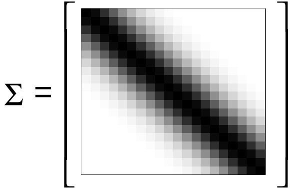
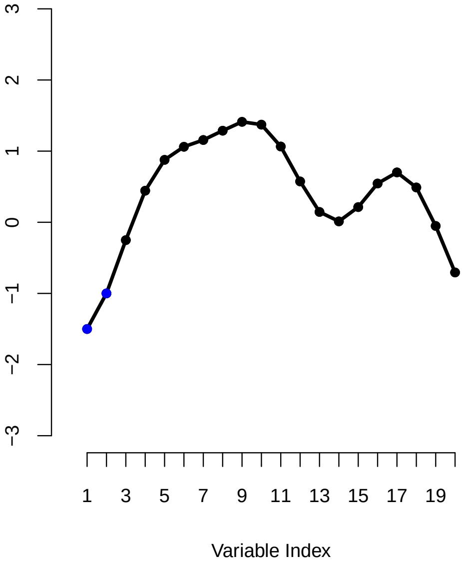
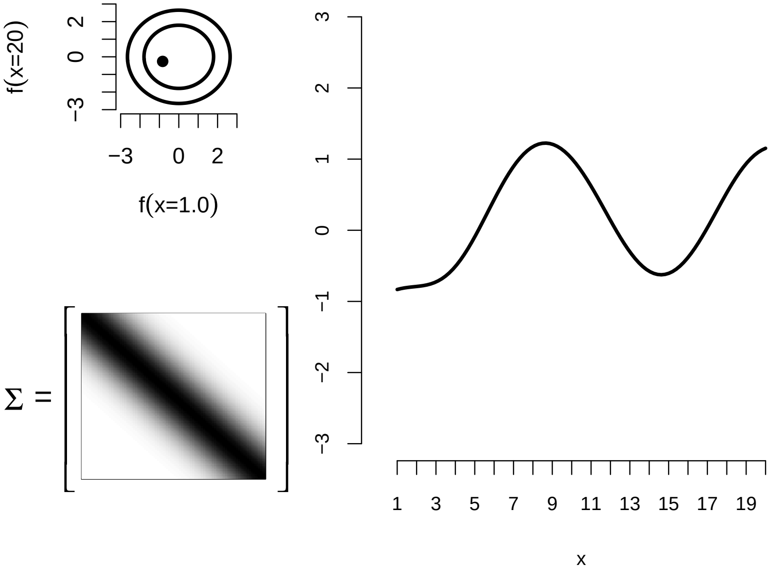






Infinite Dimensional Example



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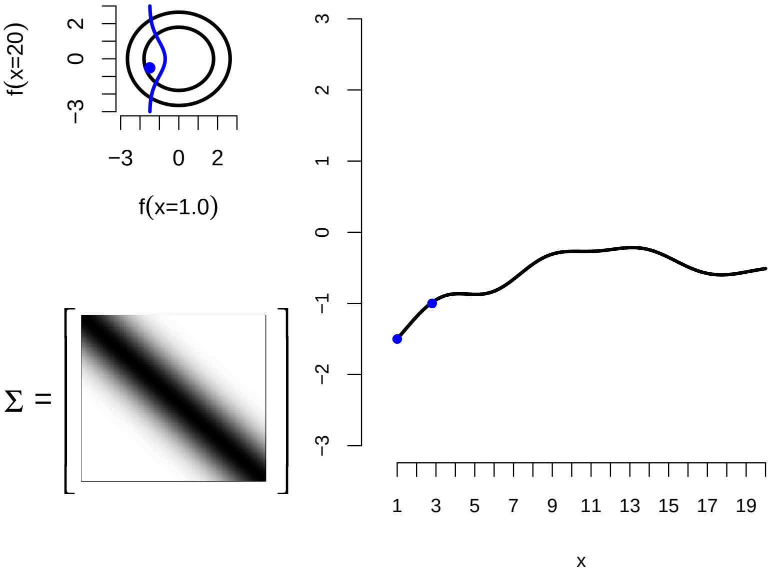
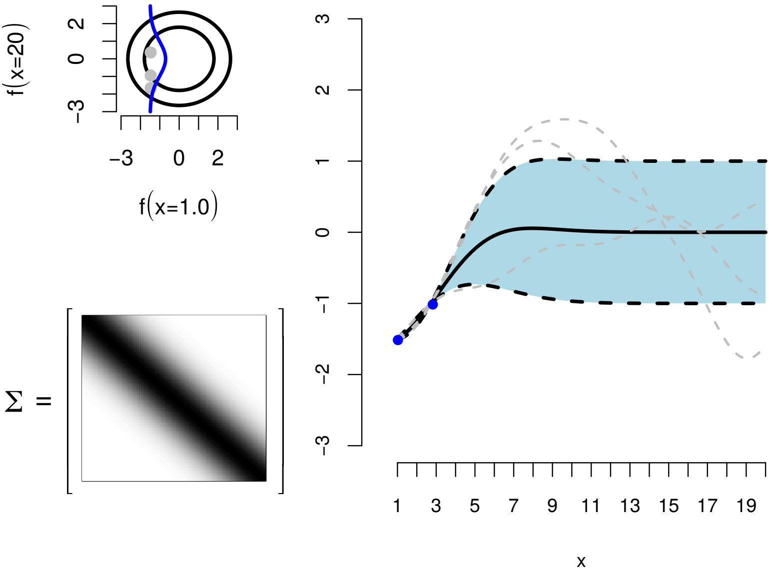


Predictive Distribution



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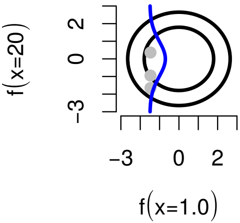

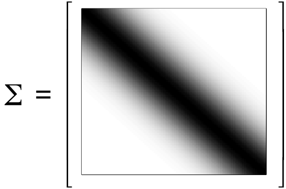

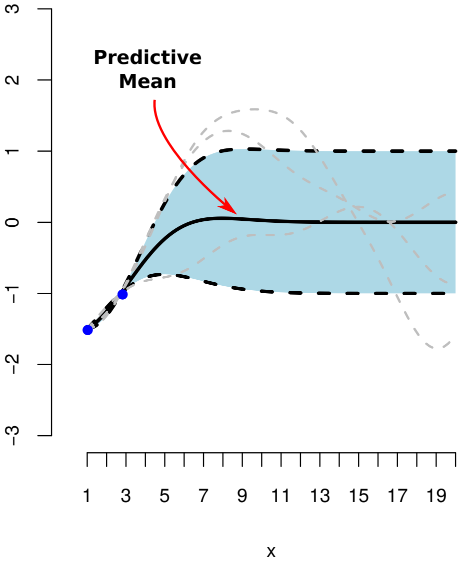

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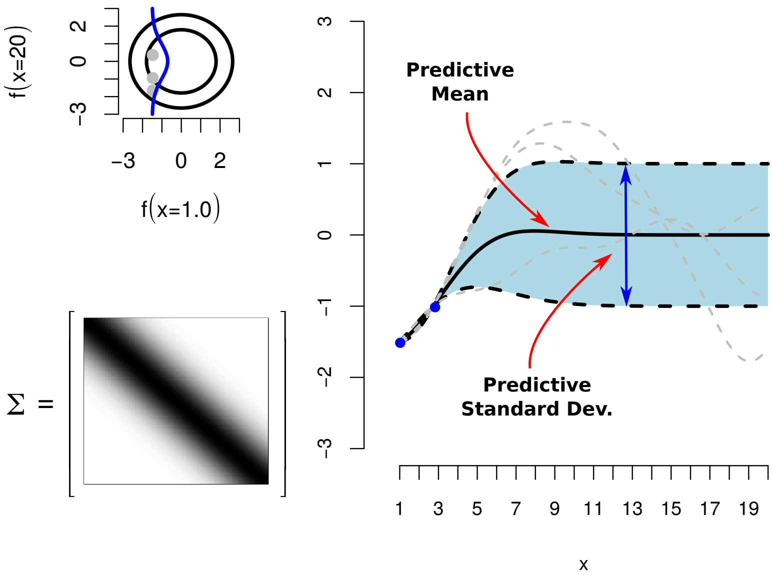

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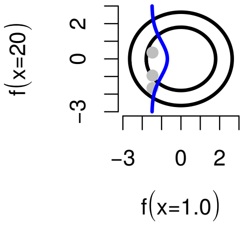

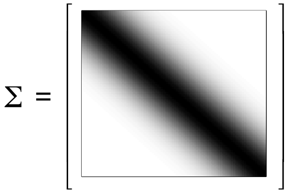

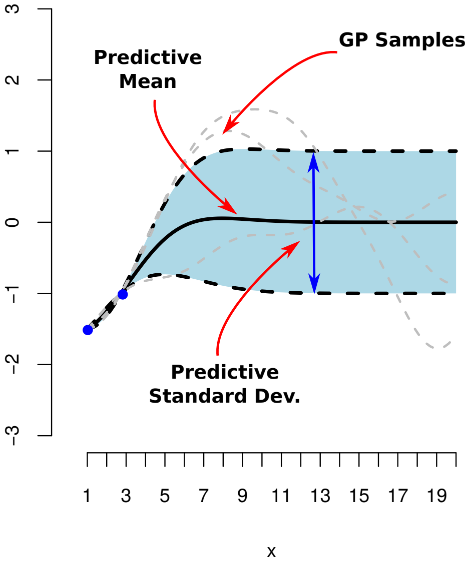

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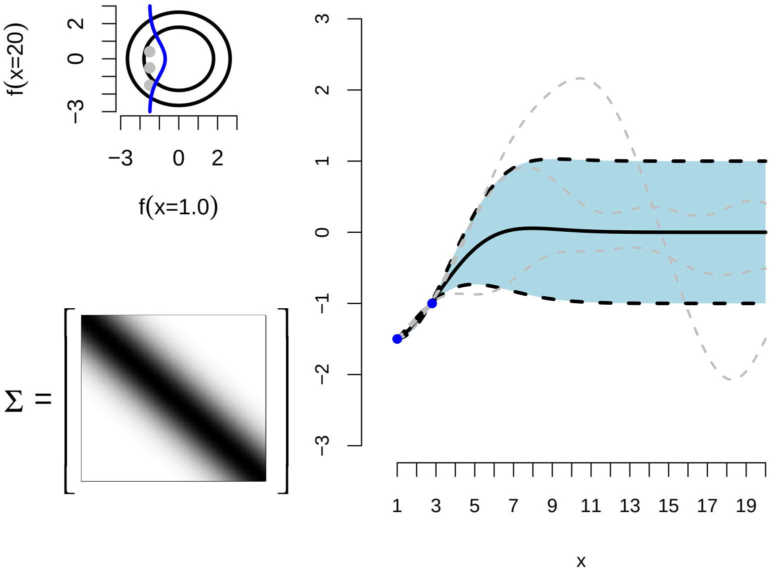

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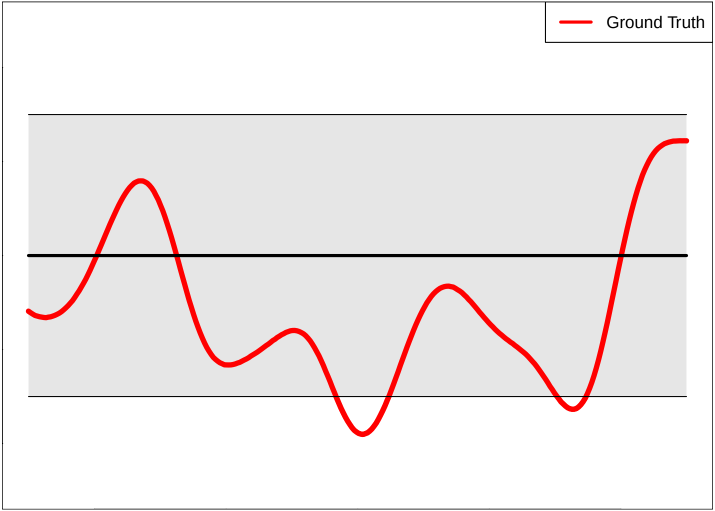

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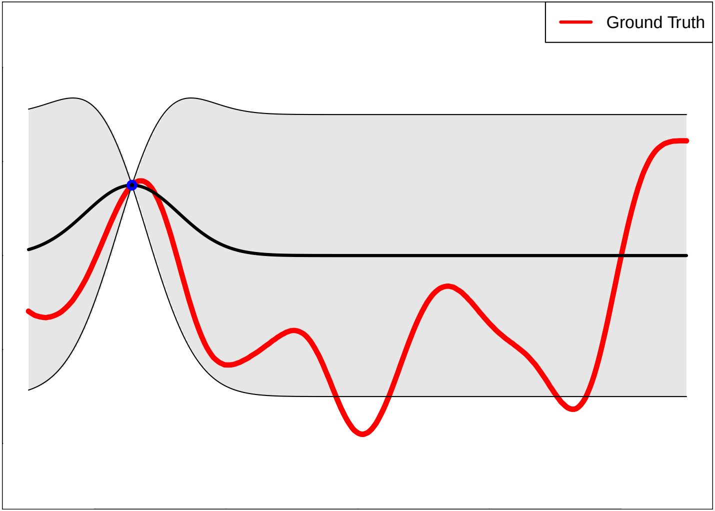

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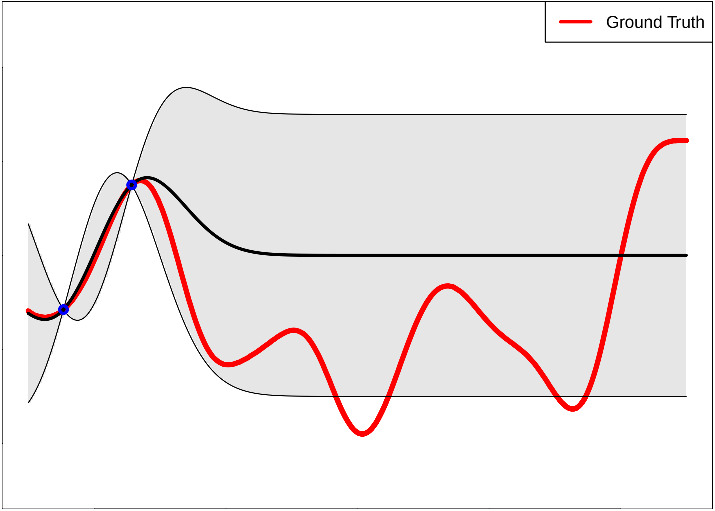

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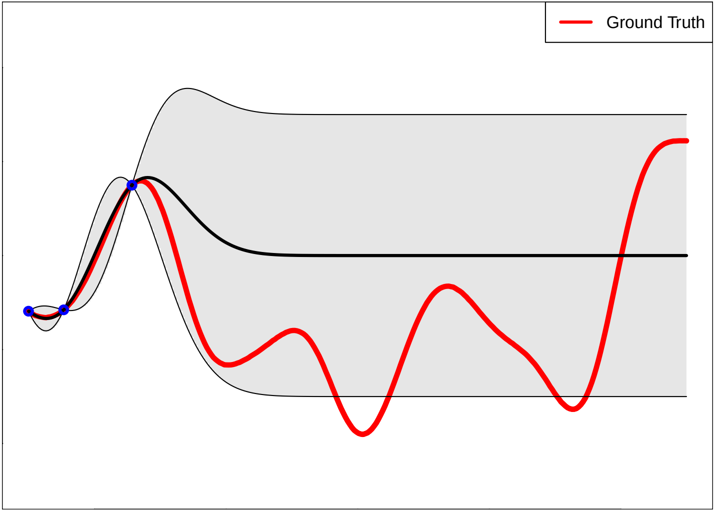

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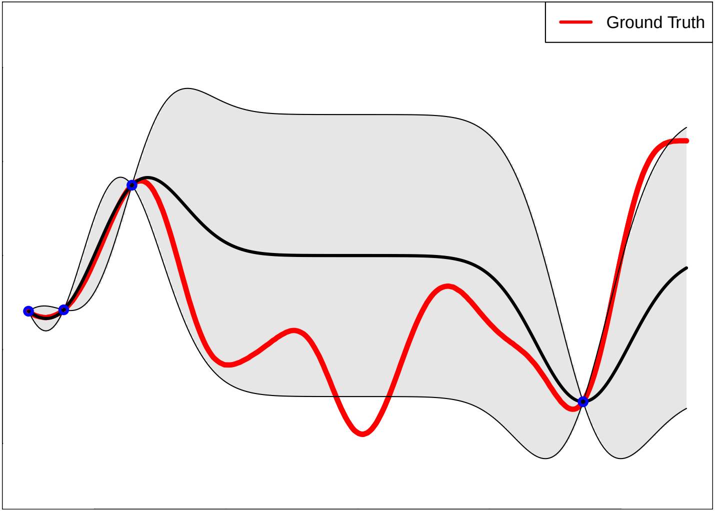

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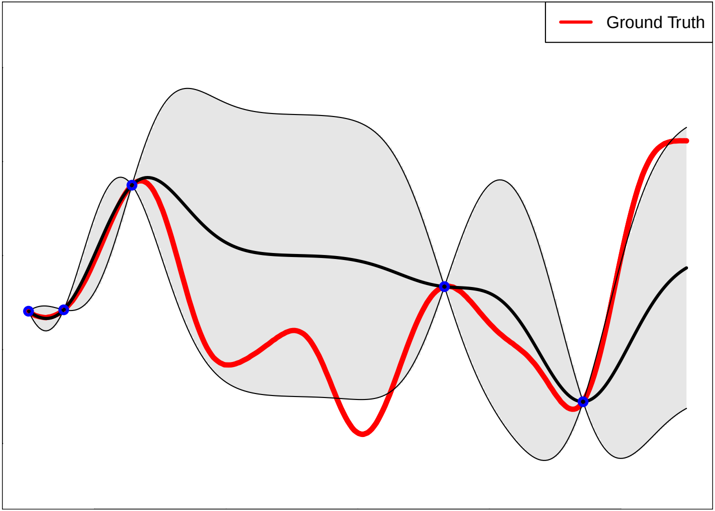

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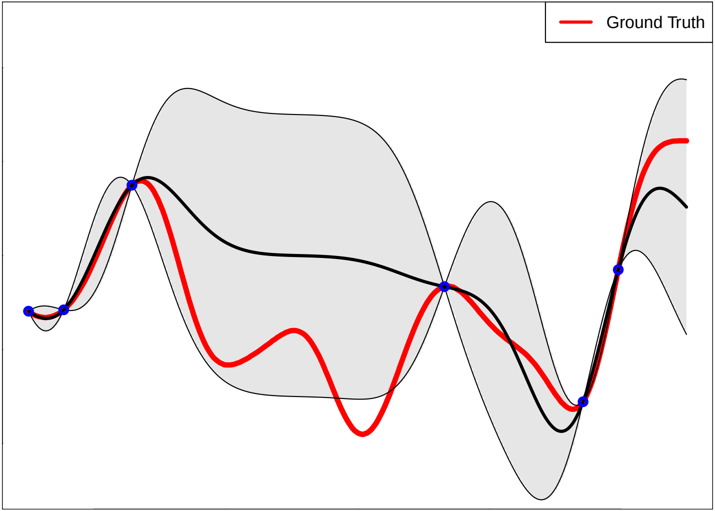

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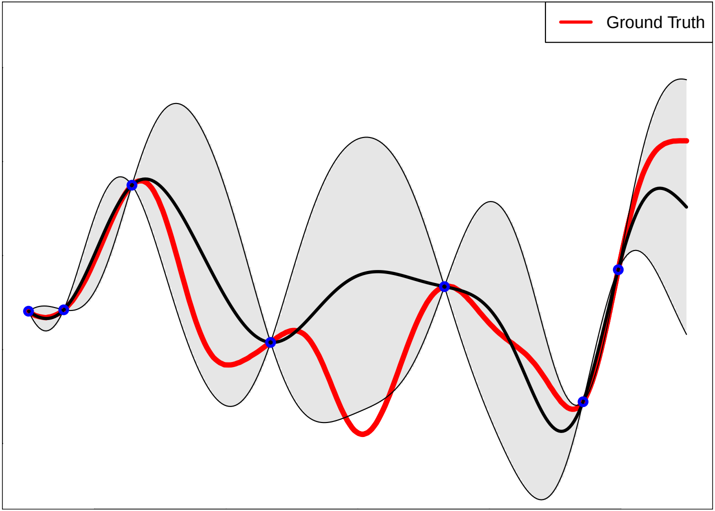

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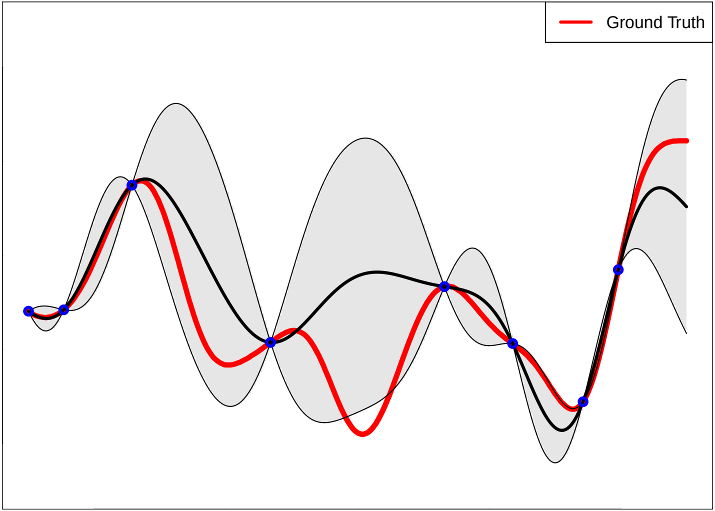

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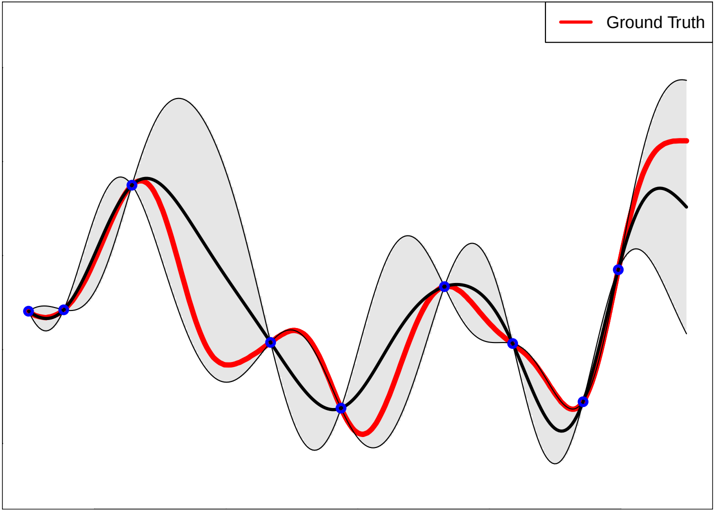

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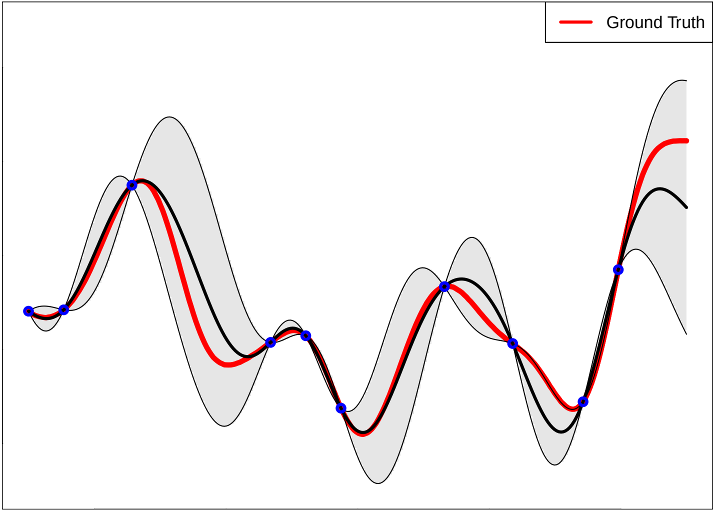

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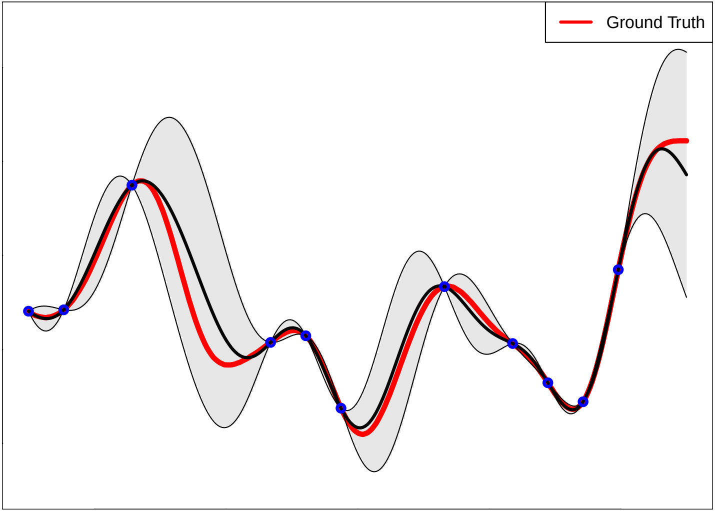

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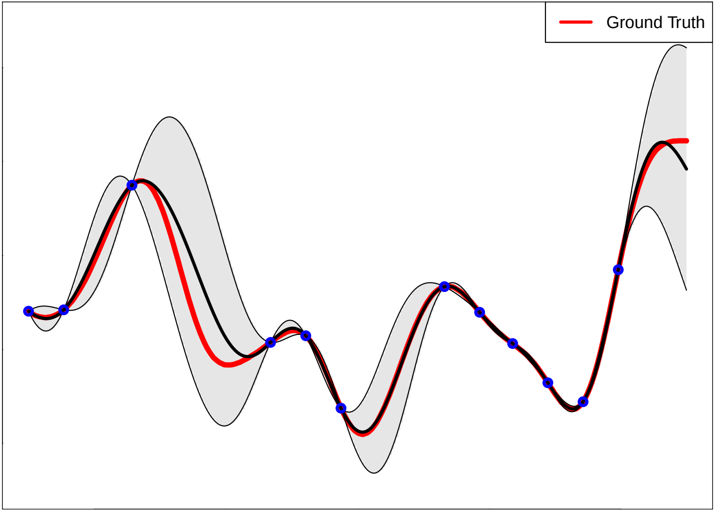

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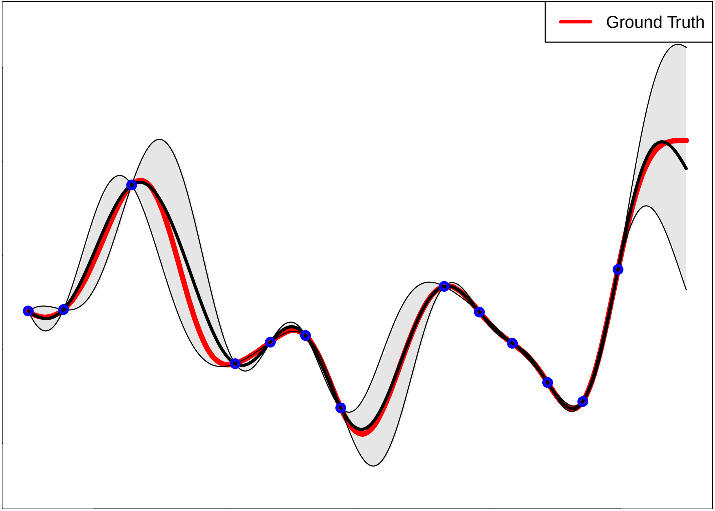

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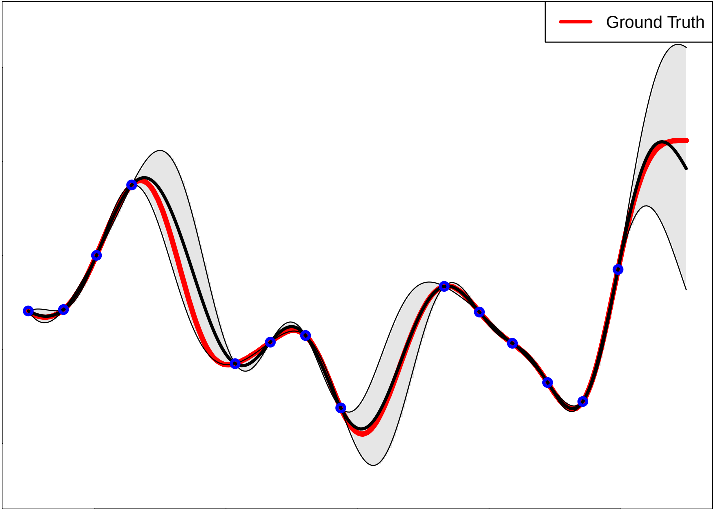

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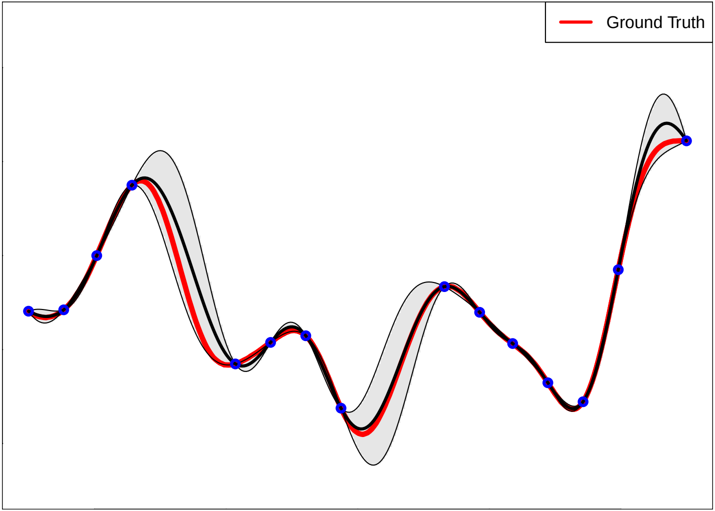

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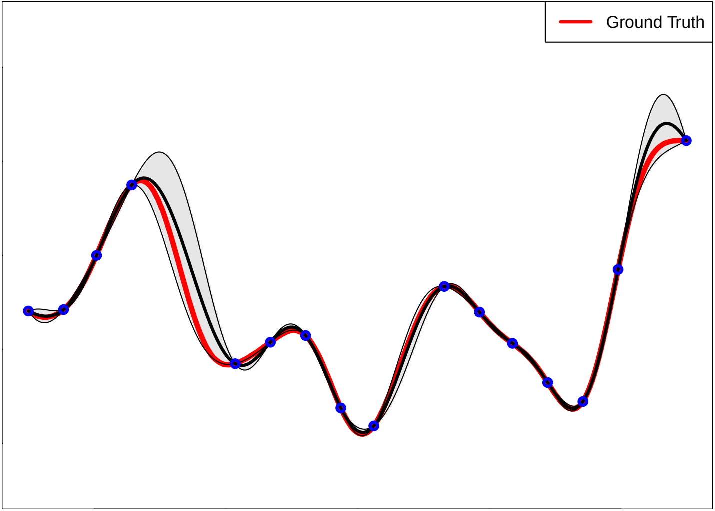

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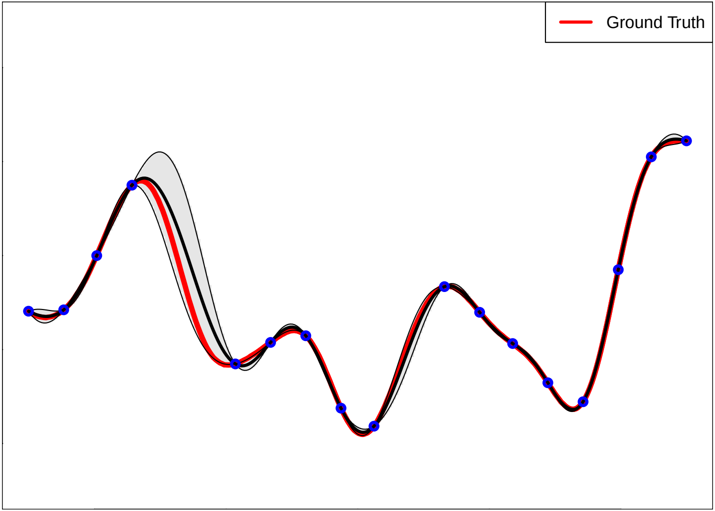

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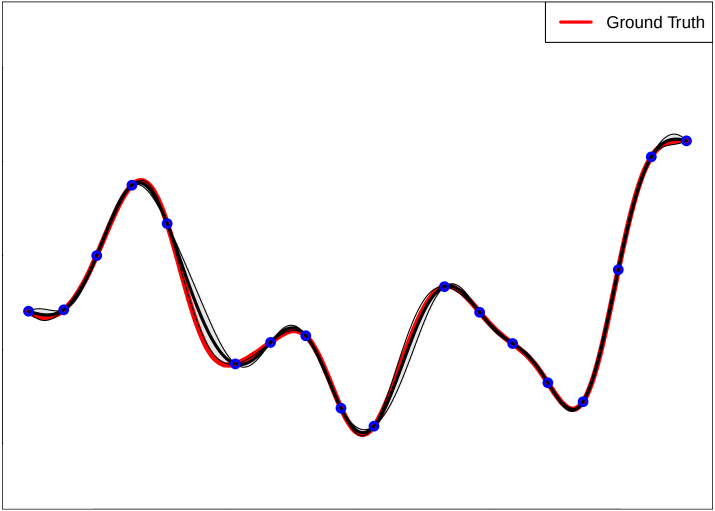

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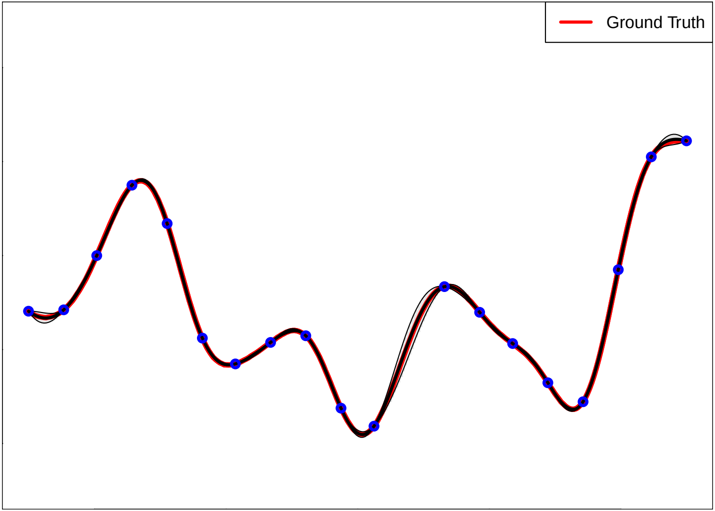

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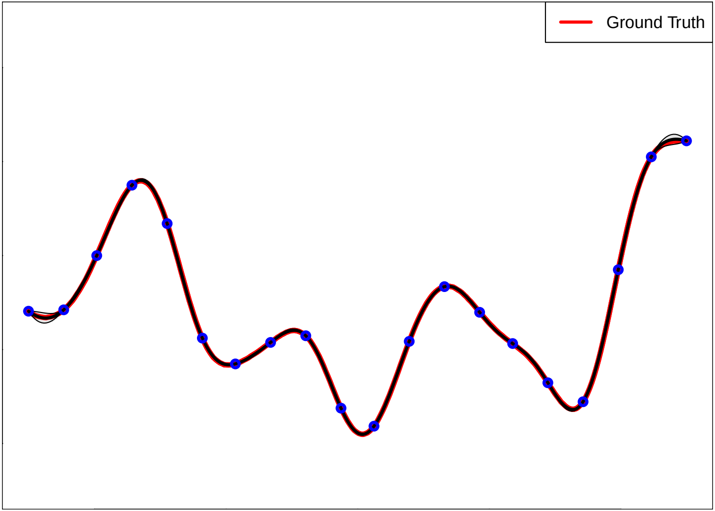

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- GPs are **non-parametric models** and become more expressive the more data we have.

Definition

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A Gaussian process is fully specified by a mean function $m(\mathbf{x})$ and covariance function $C(\mathbf{x}, \mathbf{x}')$:

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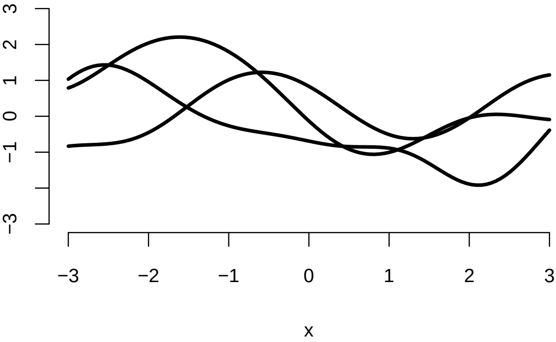

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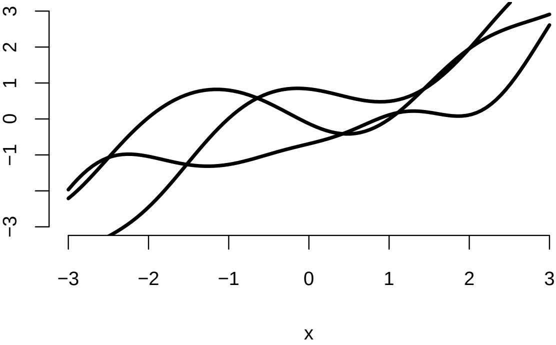

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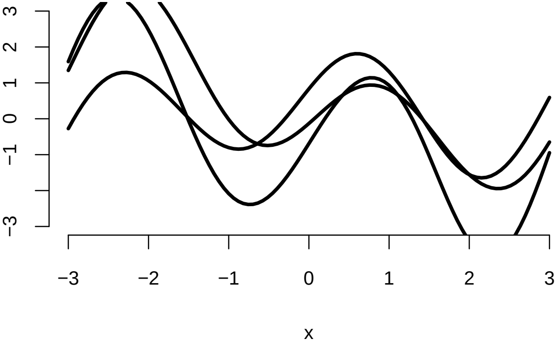

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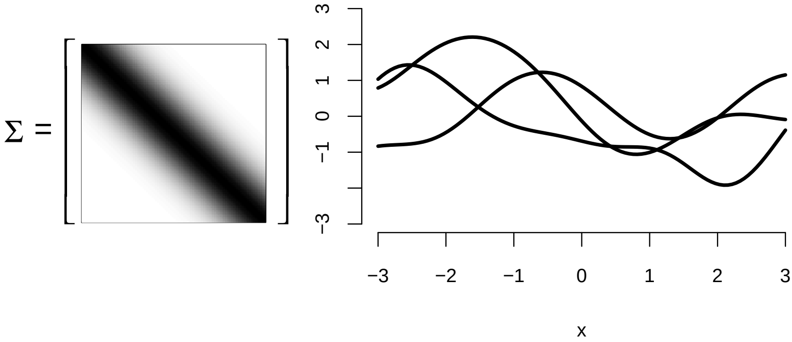

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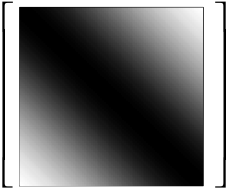
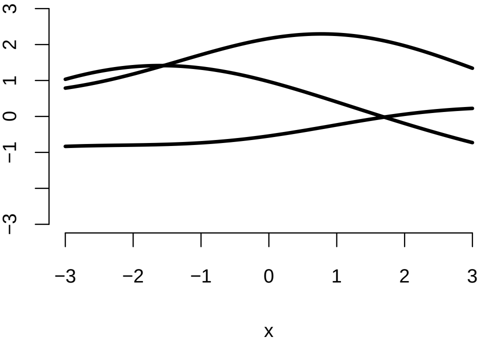
$\Sigma =$ 



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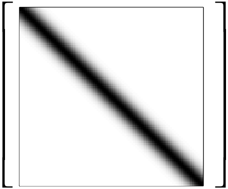
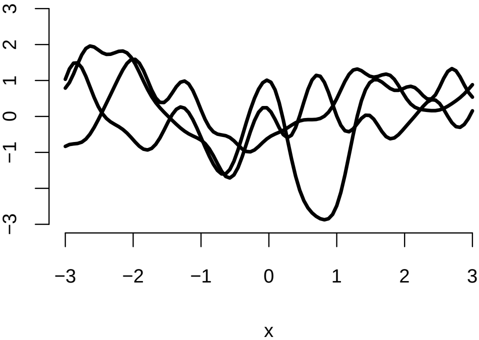
$\Sigma =$ 



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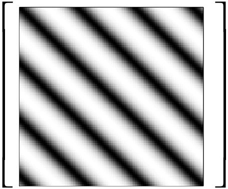

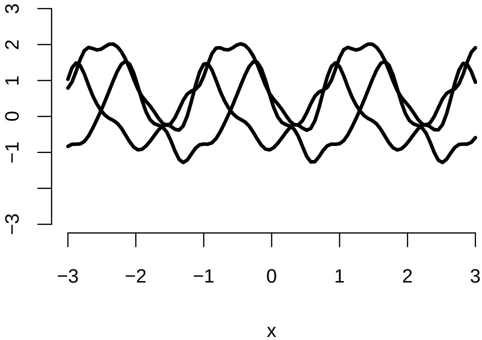

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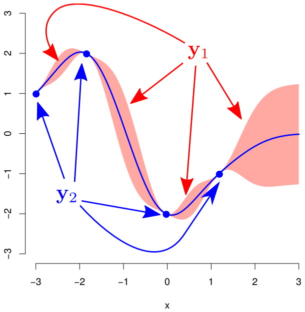
We only need to work with finite sets of random variables!

Computing the Predictive Distribution



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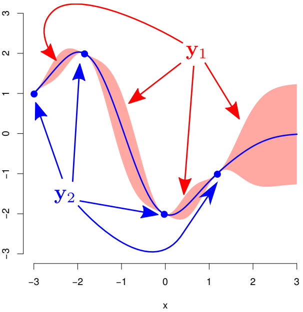

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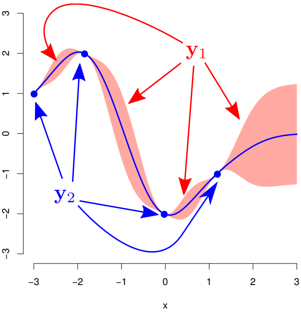

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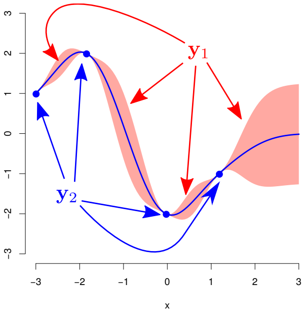

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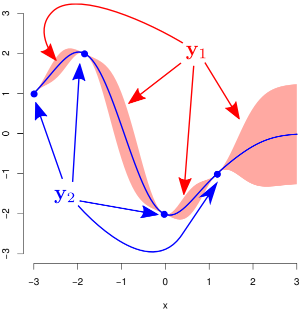

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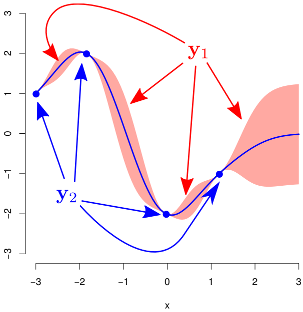

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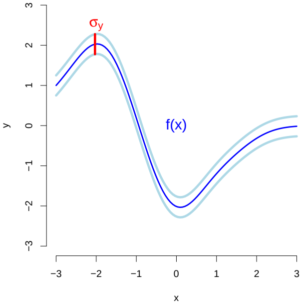
- The predictive mean is linear in $\mathbf{y}_2$.
- The predictive covariance is **more confident** than the prior!.

Considering Additive Noise



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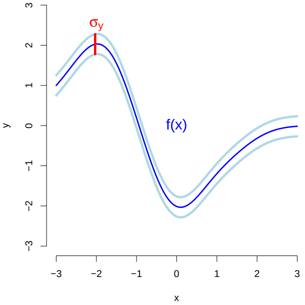

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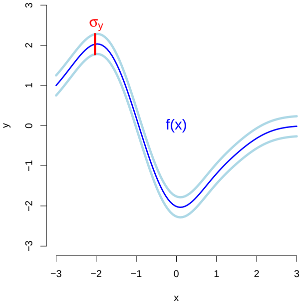

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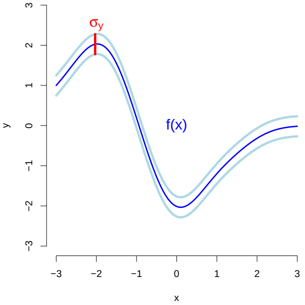
Considering Additive Noise



$$y(\mathbf{x}) = f(\mathbf{x}) + \epsilon\sigma_y ,$$
$$p(\epsilon) = \mathcal{N}(\epsilon|0, 1) .$$

Since $f(\mathbf{x})$ follows a GP and ϵ is Gaussian $y(\mathbf{x})$ is another GP!

$$y(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), C(\mathbf{x}, \mathbf{x}') + \mathbb{I}(\mathbf{x} = \mathbf{x}')\sigma_y^2)$$

The predictive distribution is:

$$p(\mathbf{y}_1|\mathbf{y}_2) = \mathcal{N}\left(\mathbf{y}_1 \middle| \mathbf{a} + \mathbf{C}(\mathbf{B} + \mathbf{I}\sigma_y^2)^{-1}(\mathbf{y}_2 - \mathbf{b}), \mathbf{A} - \mathbf{C}(\mathbf{B} + \mathbf{I}\sigma_y^2)^{-1}\mathbf{C}^\mathsf{T}\right)$$

An Example of a Covariance Function

Squared Exponential: $$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left\{ -\frac{1}{2} \sum_{j=1}^{d} \left(\frac{x_j - x'_j}{l_j} \right)^2 \right\}$$

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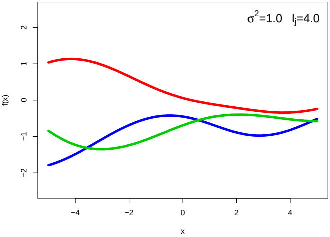

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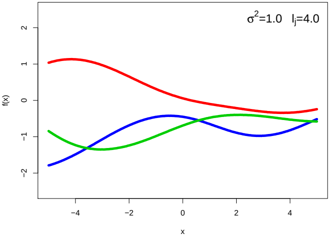

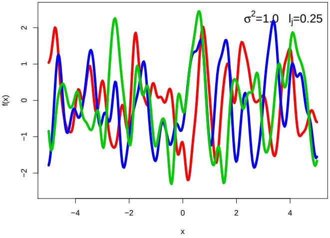

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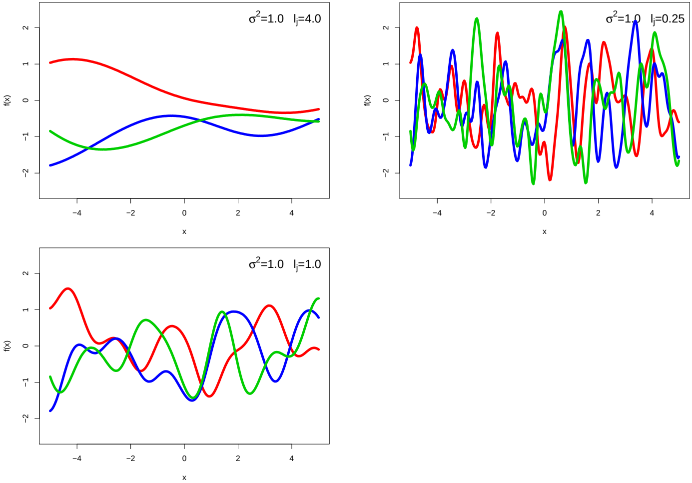

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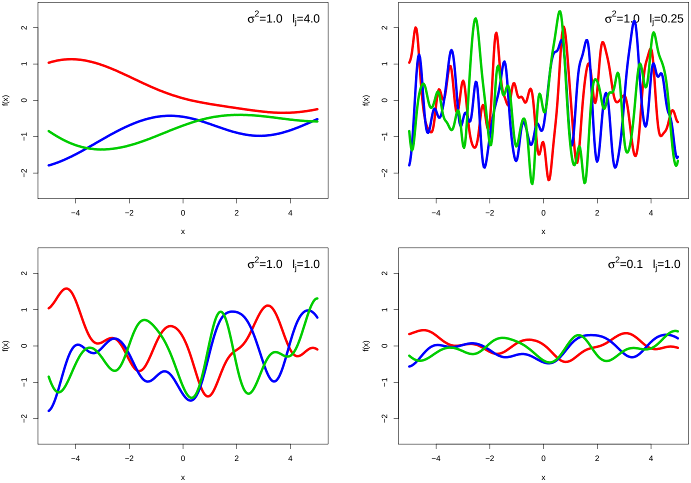

How do we choose the hyper-parameters?

Intuition: find parameters θ that are compatible with the observed data.

$$p(\theta|\mathbf{y}) = \frac{p(\mathbf{y}|\theta)p(\theta)}{p(\mathbf{y})}$$

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Often, with a reasonable amount of data, maximizing $p(\mathbf{y}|\theta)$ w.r.t. θ gives good results as it favors the right model!

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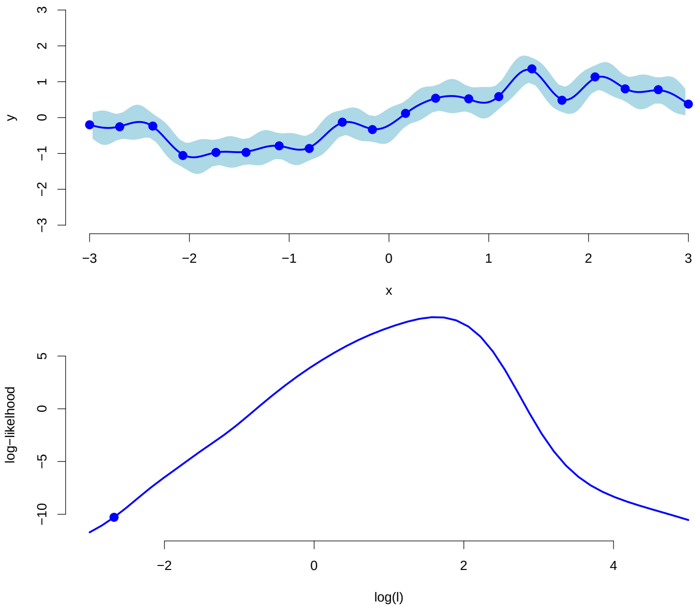
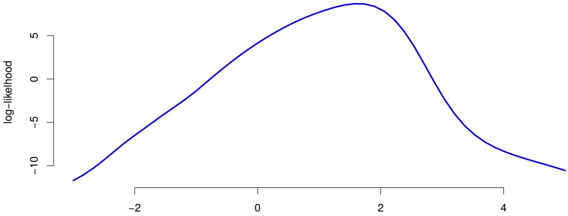


Why maximizing the likelihood is robust?



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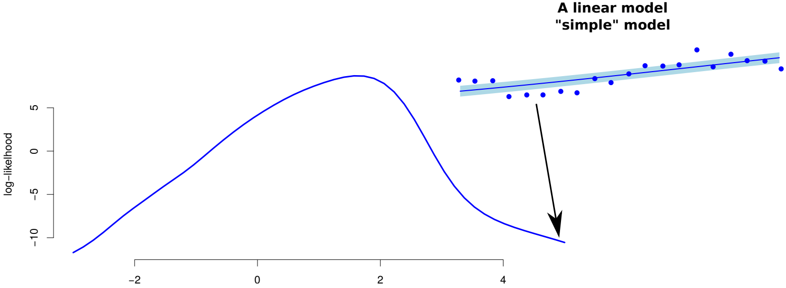

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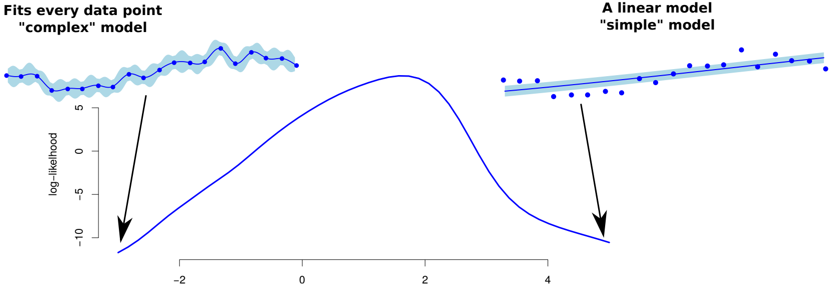

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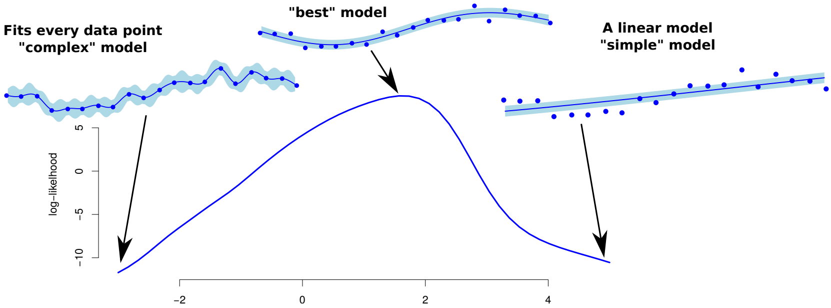

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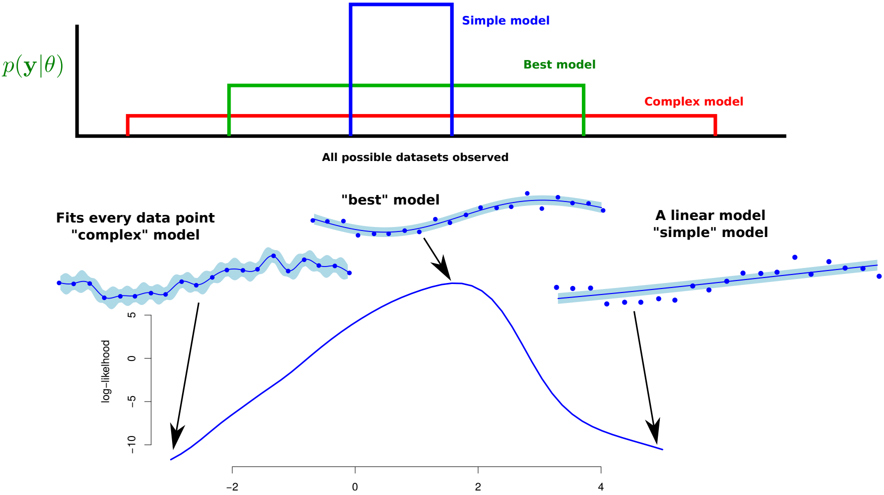

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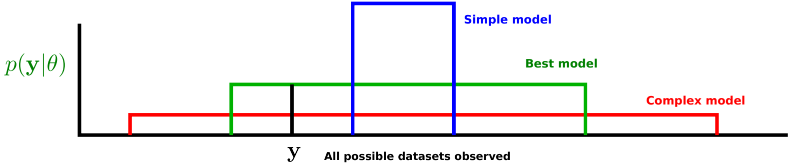

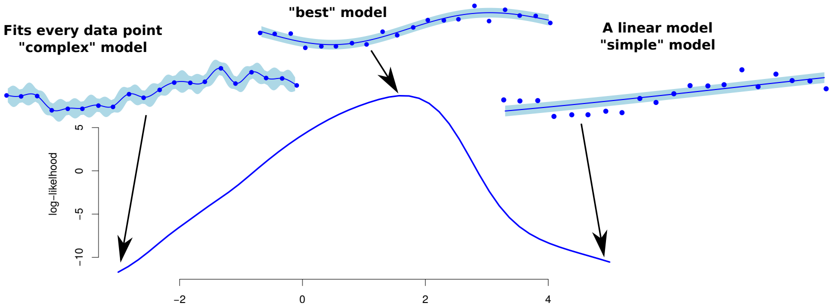

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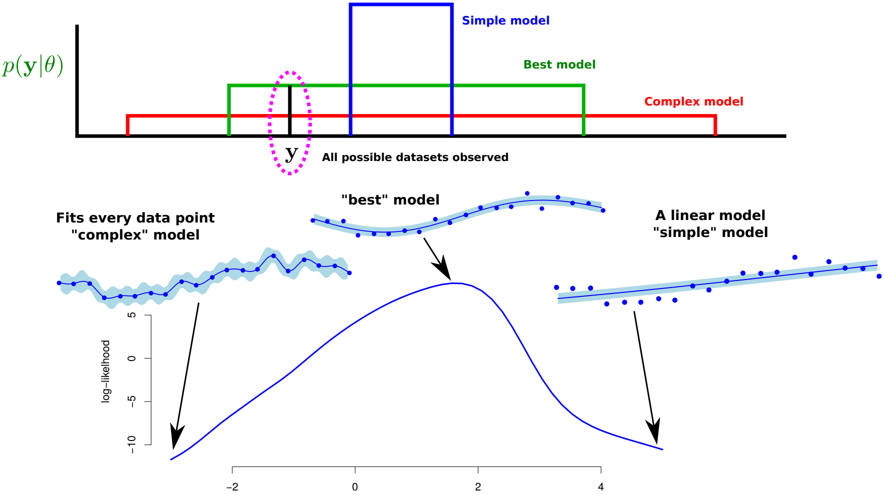

Covariance Functions: Matérn

$$C(\mathbf{x}, \mathbf{x}') = \sigma^2 \frac{2^{1-\nu)}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu r}}{l} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu} r}{l} \right)$$

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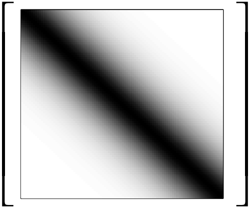
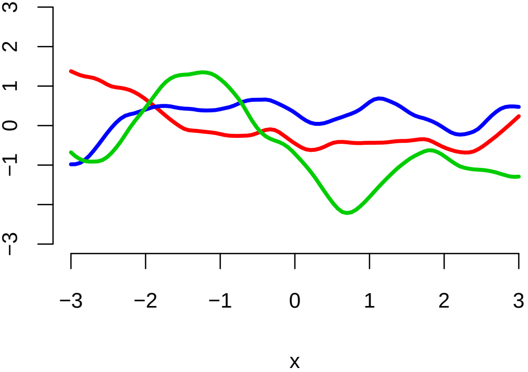
$\Sigma =$ 



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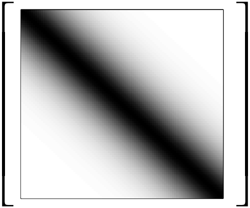
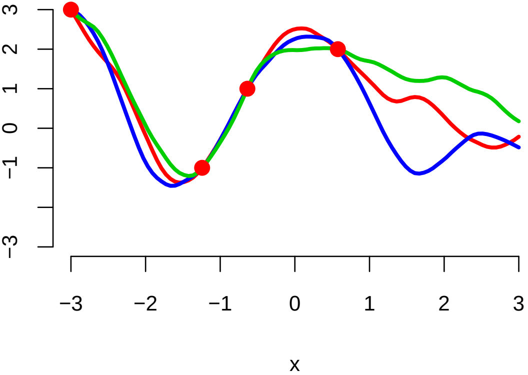
$\Sigma =$ 



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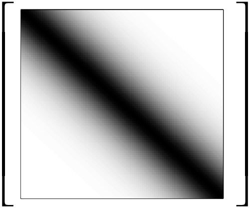
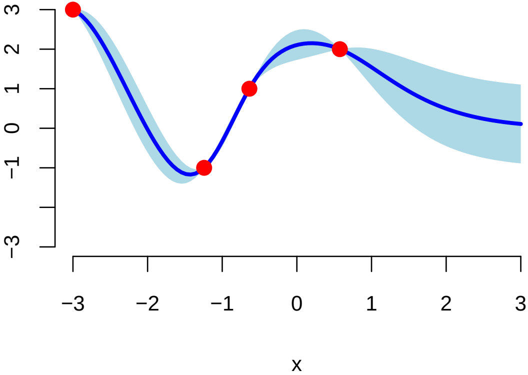
$\Sigma =$ 



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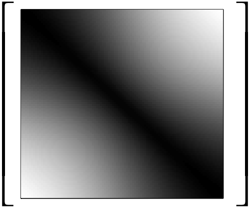
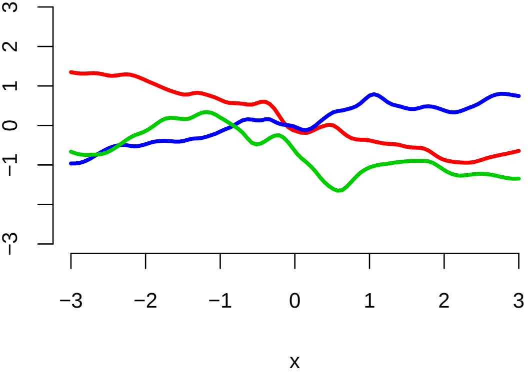
$\Sigma =$ 



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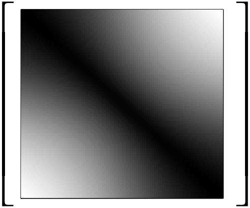
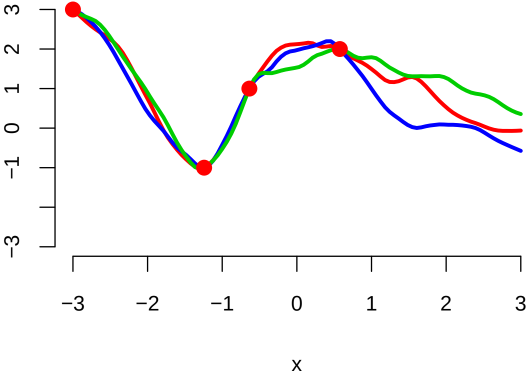
$\boldsymbol{\Sigma} =$ 



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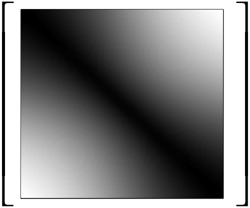

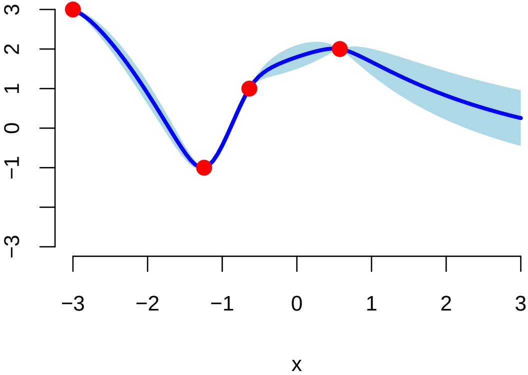

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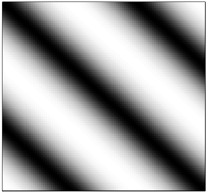

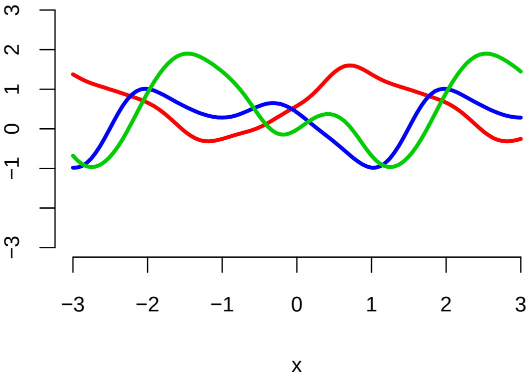

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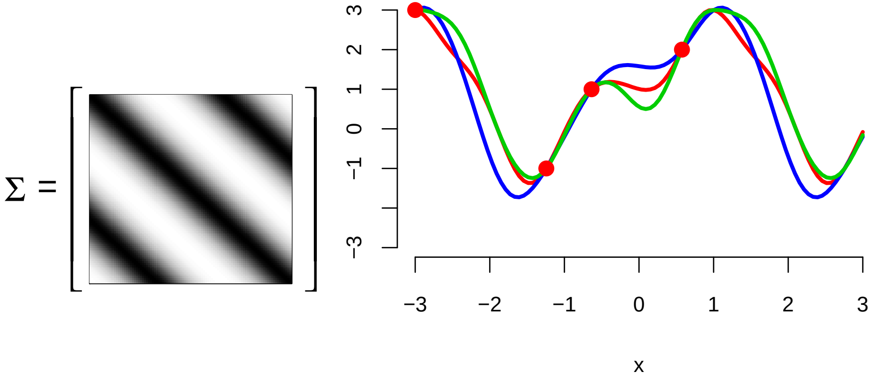

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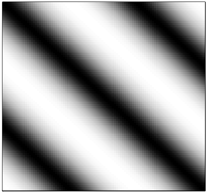
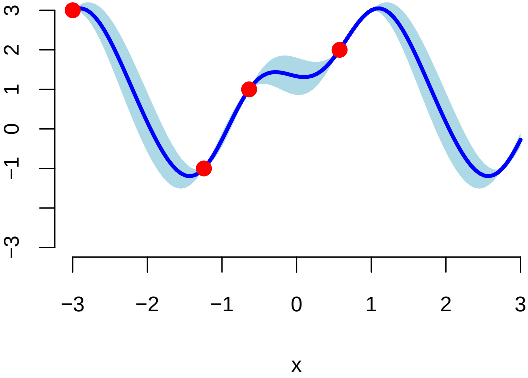
$\Sigma =$ 



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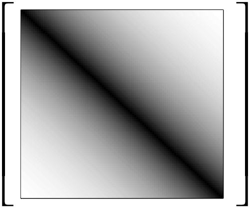
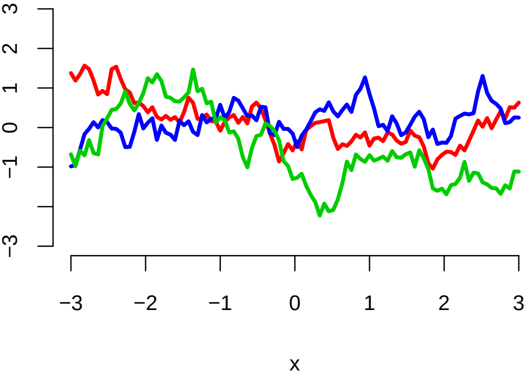
$\Sigma =$ 



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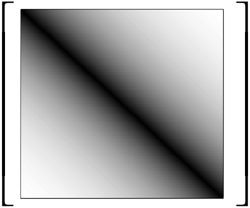
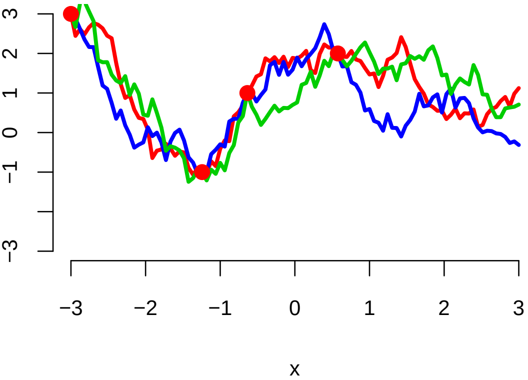
$\Sigma =$ 



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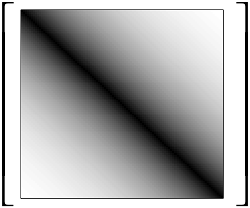
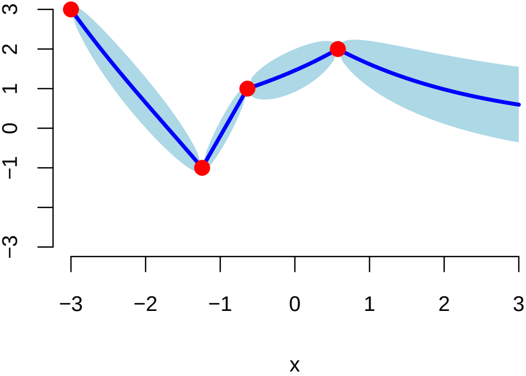
$\Sigma =$ 



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- Covariance functions can be combined (sum $+$ and product $\times$).
- The likelihood $p(\mathbf{y})$ can *discriminate* among them (use with care).

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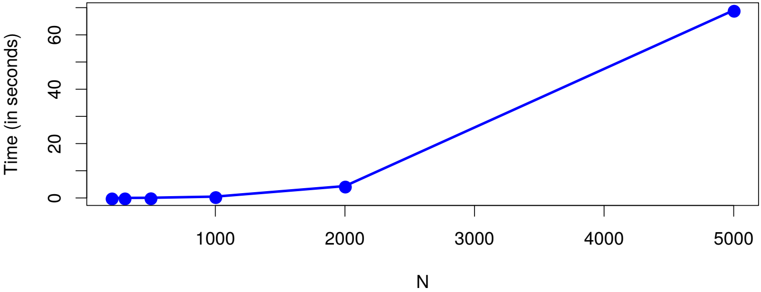

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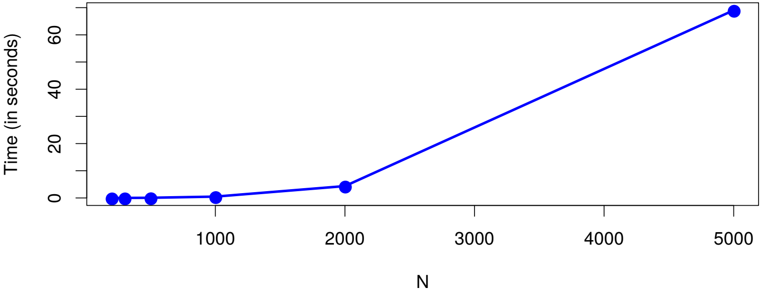

We can handle just a few thousand data instances at most!

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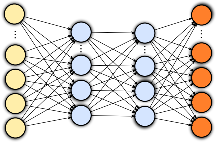

Neural Network
(parametric model)

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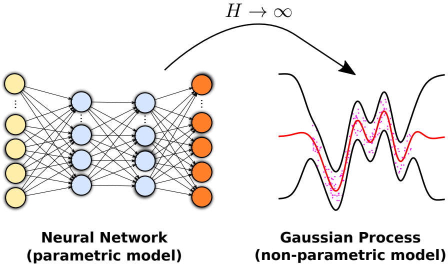

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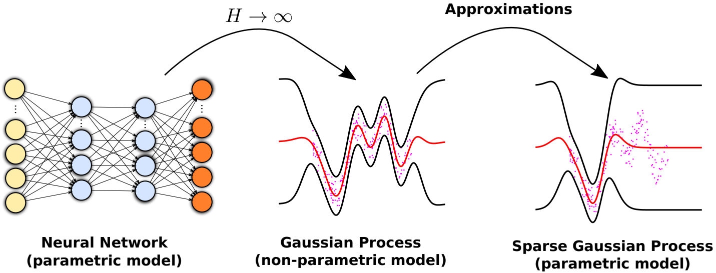

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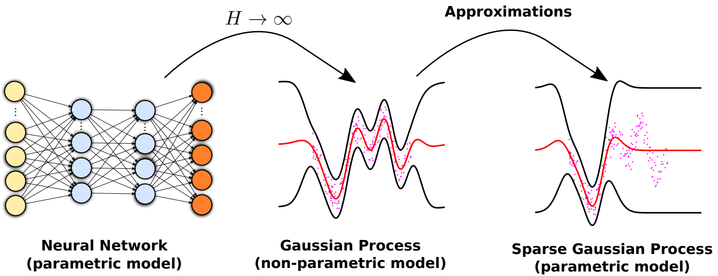

Approximations based on inducing points:

Improving the Cost of Gaussian Processes

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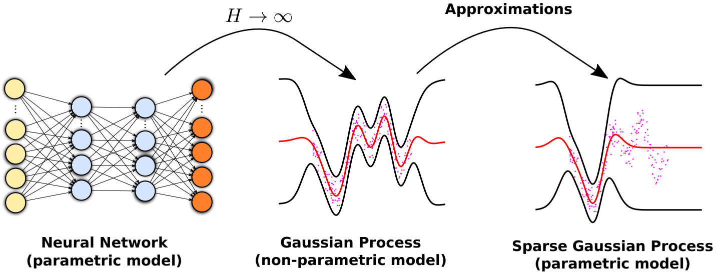

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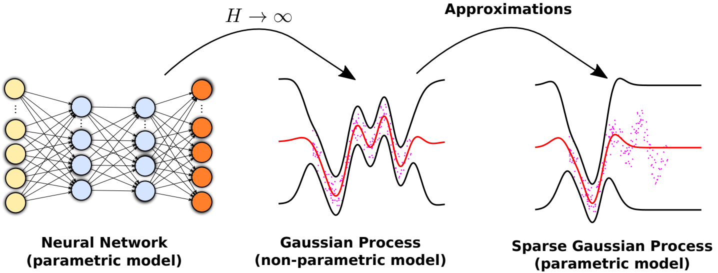

Approximations based on inducing points:

- **FITC**: changes the GP model to remove some dependencies!
- **VFE**: does approximate inference with a simplified distribution q.

Full Independent Training Conditional (FITC)

1. Extend model with $M \ll N$ inducing points and outputs at $\overline{\mathbf{X}}$.

$$p(\mathbf{f}, \mathbf{u}) = \mathcal{N}\left(\left[\begin{array}{c} \mathbf{f} \\ \mathbf{u} \end{array}\right] \middle| \left[\begin{array}{c} \mathbf{0} \\ \mathbf{0} \end{array}\right], \left[\begin{array}{cc} \mathbf{K_{ff}} & \mathbf{K_{fu}} \\ \mathbf{K_{uf}} & \mathbf{K_{uu}} \end{array}\right]\right)$$

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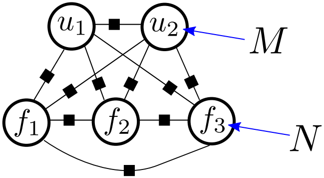

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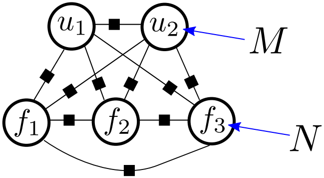

2. Introduce conditional independences:

$$p(\mathbf{f}|\mathbf{u}) = \prod_{i=1}^{N} p(f_i|\mathbf{u})$$

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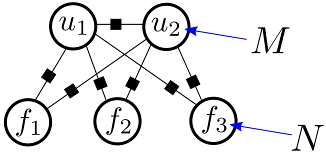

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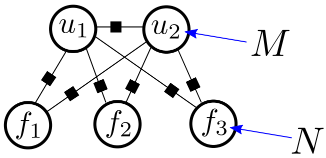

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3. Marginalize $\mathbf{u}$ to obtain an approximate GP prior for $\mathbf{f}$.

$$p(\mathbf{f}) = \int p(\mathbf{f}|\mathbf{u})p(\mathbf{u})d\mathbf{u} = \prod_{i=1}^{N} p(f_i|\mathbf{u})p(\mathbf{u})d\mathbf{u} = \mathcal{N}(\mathbf{f}|0, \tilde{\mathbf{K}}_{\mathbf{ff}})$$

where $\tilde{\mathbf{K}}_{\mathbf{ff}} = \mathbf{D} + \mathbf{Q_{ff}}$ with $\mathbf{D}$ diagonal and $\mathbf{Q_{ff}} = \mathbf{K_{fu}}\mathbf{K_{uu}}^{-1}\mathbf{K_{uf}}$ of rank M.

Full Independent Training Conditional (FITC)

5. We make the prediction of $f^\star$ at $\mathbf{x}^\star$ by considering the approximate GP prior:

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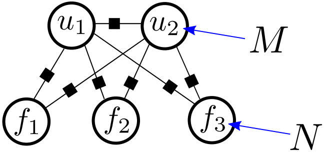

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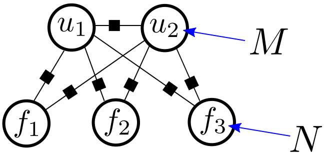

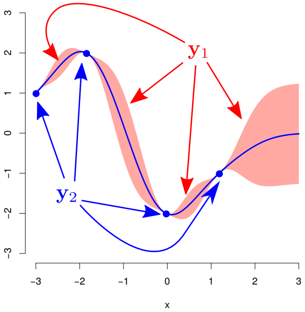

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\mathsf{T} & \mathbf{B} \end{bmatrix} \right),$$

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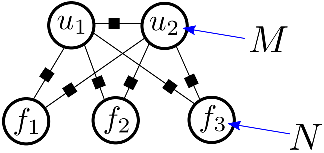

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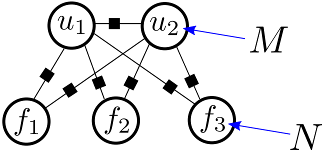

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Due to the structure in $\tilde{\mathbf{K}}_{\mathbf{ff}}$ all computations have cost in $\mathcal{O}(NM^2)$.

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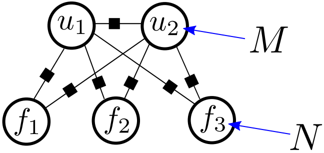

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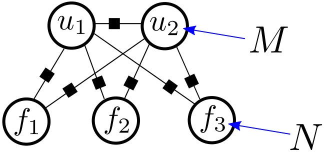

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6. How do we find the location of the inducing points $\overline{\mathbf{X}}$?

Simply treat them as prior parameters and maximize the approximate likelihood $p(\mathbf{f}|\mathbf{0}, \tilde{\mathbf{K}}_{\mathbf{ff}})$!

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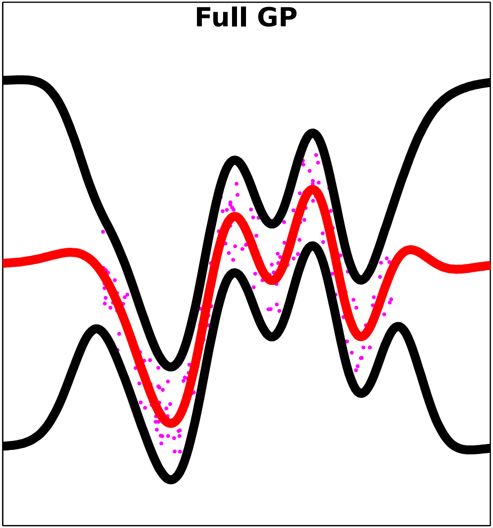

(Snelson & Gahramani, 2006)

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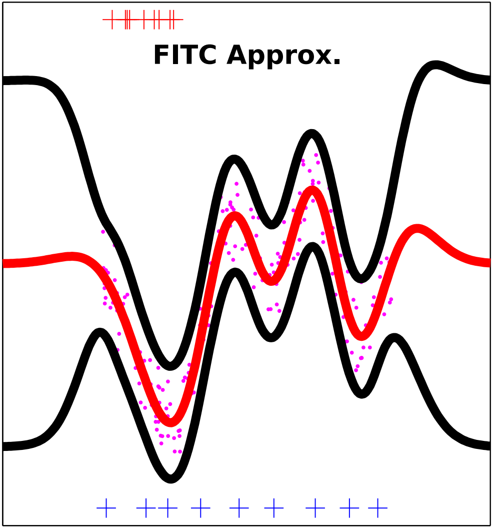

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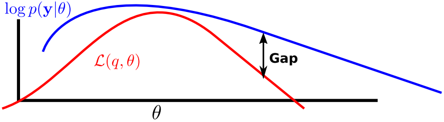
Variational Free Energy (VFE)

Lower bound the log-likelihood:

$$\log p(\mathbf{y}|\theta) = \log \int p(\mathbf{y}, \mathbf{f}, \mathbf{u}|\theta) d\mathbf{f} d\mathbf{u}$$



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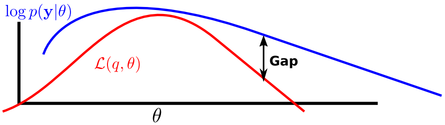

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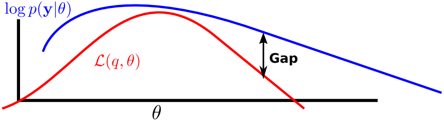

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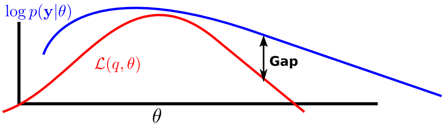

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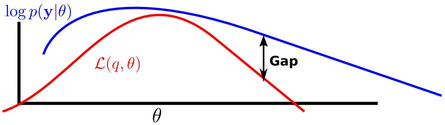

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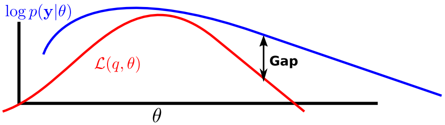

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KL $\equiv$ Kullback-Leibler divergence

By maximizing $\mathcal{L}(q,\theta)$ w.r.t q we are enforcing that $q(\mathbf{f},\mathbf{u})$ looks similar to $p(\mathbf{f},\mathbf{u}|\mathbf{y})$ in terms of the KL!

Variational Free Energy (VFE)

Consider the following approximate distribution:

$$q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f}|\mathbf{u}) \; q(\mathbf{u}) = p(\mathbf{f}|\mathbf{u}) \; \mathcal{N}(\mathbf{u}|\mathbf{m}, \mathbf{S})$$

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- Fixed
- Tunable

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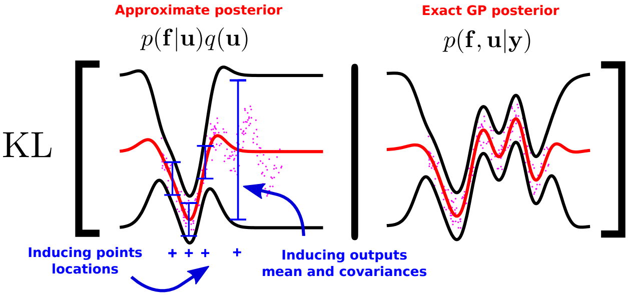

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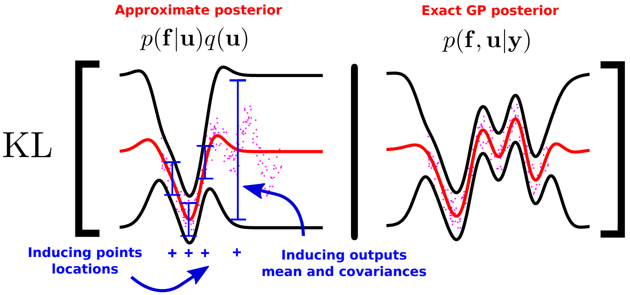

The inducing points are now parameters of the approx. dist. q!

Variational Free Energy (VFE)

Plugging $q(\mathbf{f}, \mathbf{u})$ into the lower bound we have:

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$$
\begin{aligned}
\mathcal{L}(q, \theta) &= \int q(\mathbf{f}, \mathbf{u}) \log \frac{p(\mathbf{y}, \mathbf{f}, \mathbf{u}|\theta)}{q(\mathbf{f}, \mathbf{u})} d\mathbf{f} d\mathbf{u} \\
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\end{aligned}
$$

Variational Free Energy (VFE)

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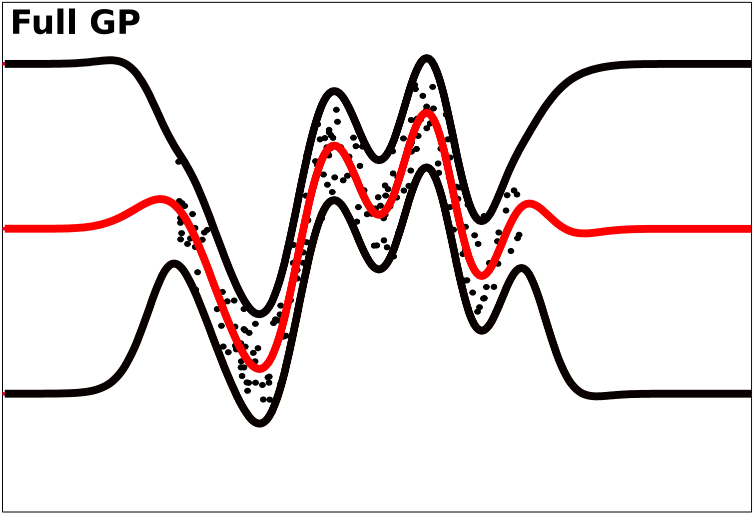
- Predictions are made using $p(\mathbf{f}^{\star}|\mathbf{u}) q(\mathbf{u})$ marginalizing out $\mathbf{u}$.

Variational Free Energy (VFE)



(Titsias, 2009)

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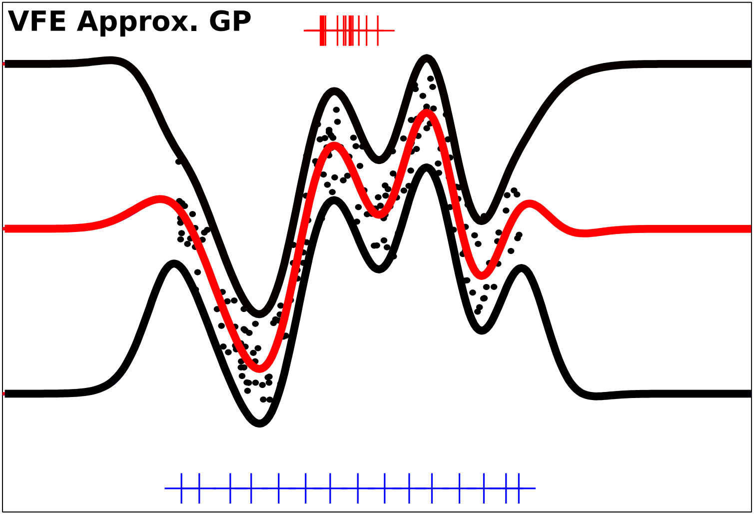

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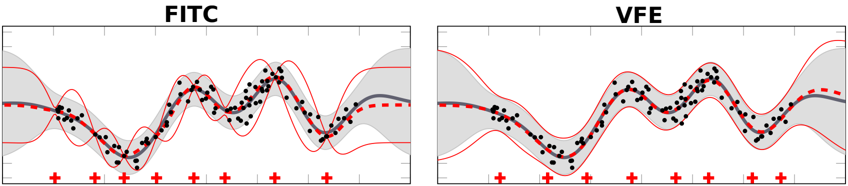

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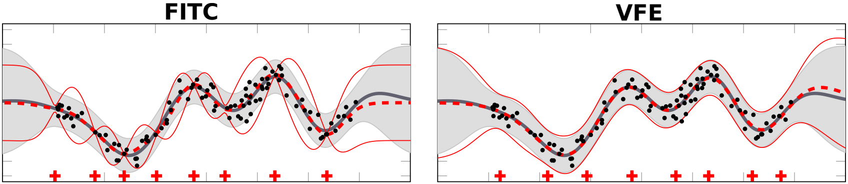

- FITC: less local optima and easier to optimize, also less accurate.
- VFE: more accurate, more local optima, more difficult to optimize.

(Bui et al., 2017) (Bauer et al., 2016)

GPs for Big Data

Can we further improve the computational cost in $\mathcal{O}(NM^2)$?

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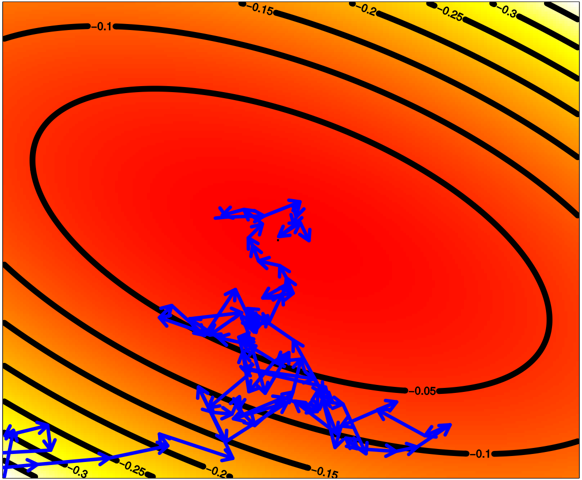
$$

The training cost goes down to $\mathcal{O}(M^3)$ which allows to address datasets with millions of instances!

(Hensman et al., 2013)

GPs for Big Data



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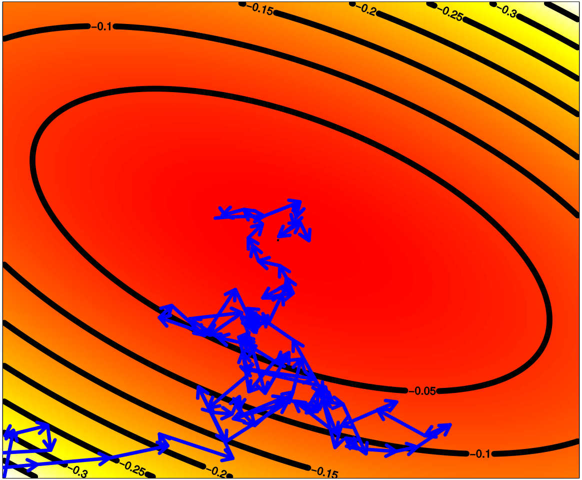
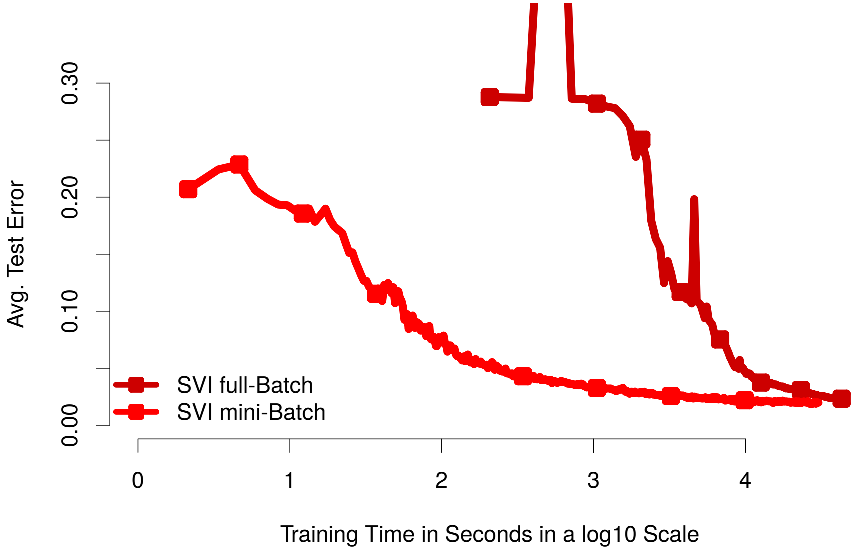


To converge to a local neighborhood of the optimum stochastic methods require an estimate of the gradient which can be very cheap!

GPs for Big Data



(Hernández-Lobato, 2015)

Summary so Far about GPs

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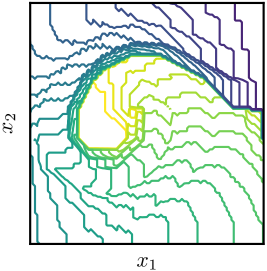
Deep GPs constitute a nice alternative to address these issues!

Motivation for Deep Gaussian Processes

Target function



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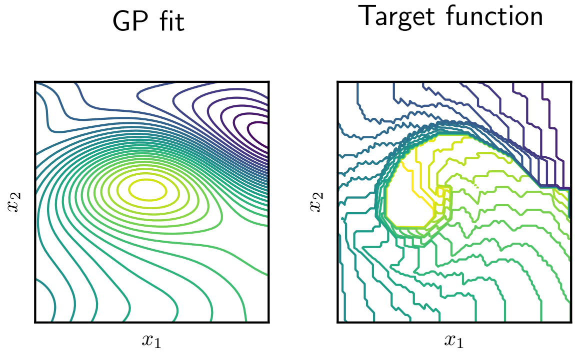

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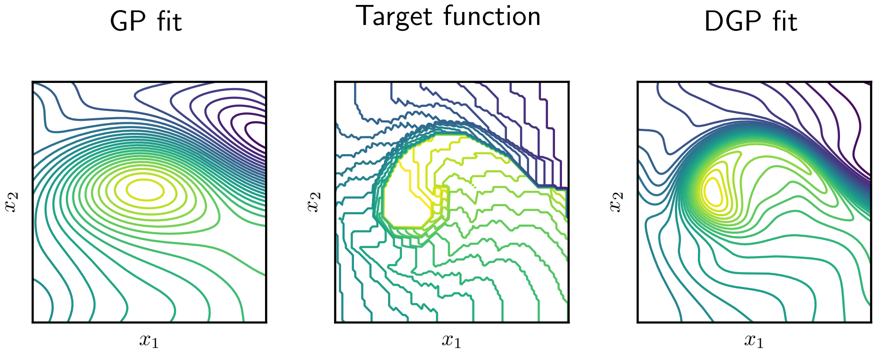

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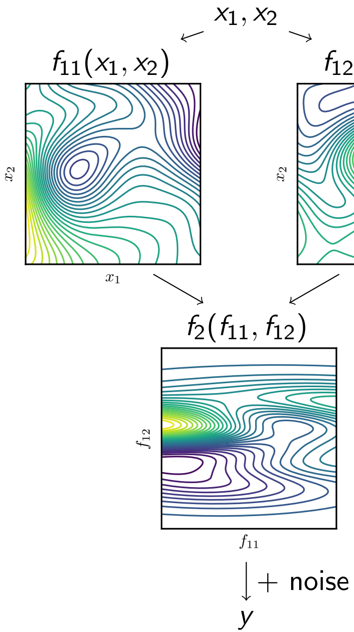

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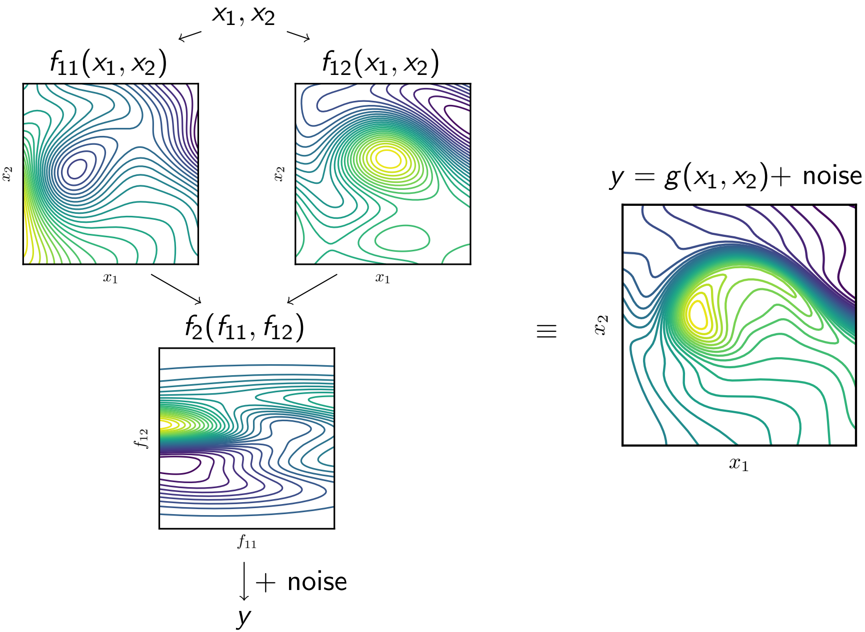

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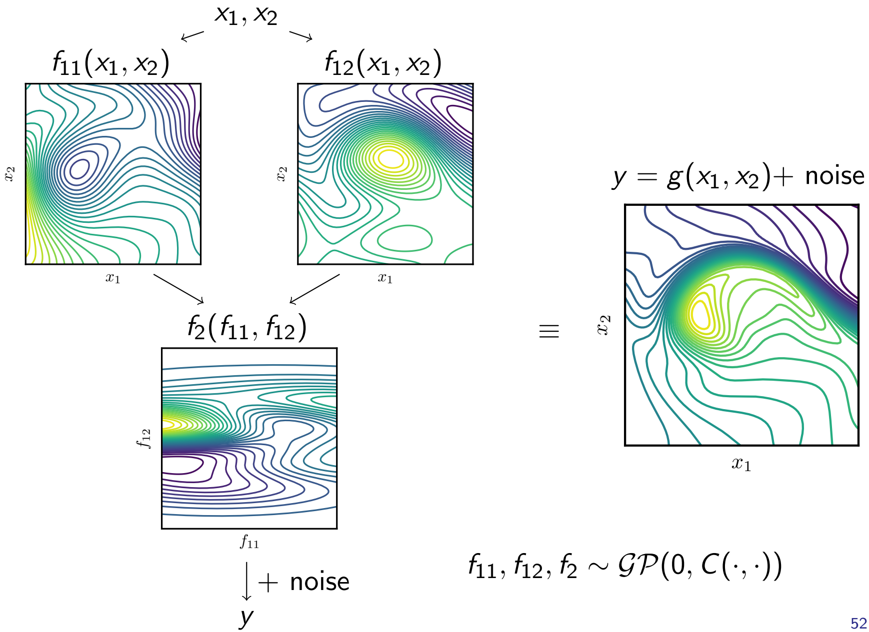
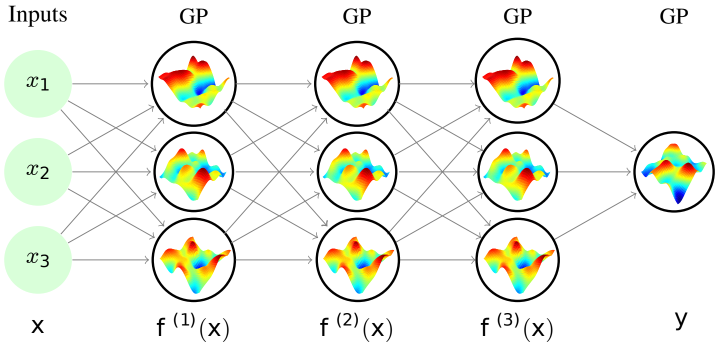


Deep GPs as Deep Neural Networks



Deep GPs: Composition of Functions

$$y = f(g(\mathbf{x}))\,, \quad f(\mathbf{x}) \sim \mathcal{GP}(0, C_f(\mathbf{x}, \mathbf{x}')) \quad g(\mathbf{x}) \sim \mathcal{GP}(0, C_g(\mathbf{x}, \mathbf{x}'))$$

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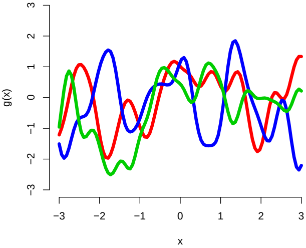

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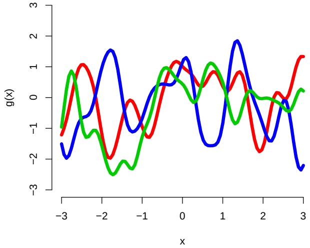

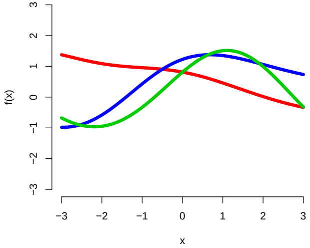

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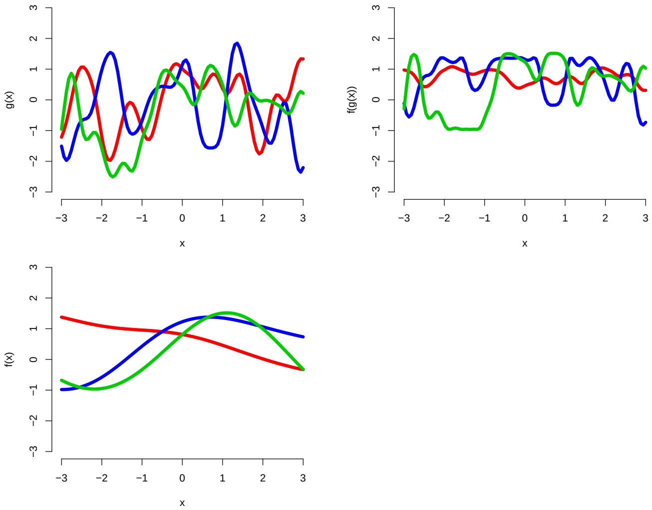

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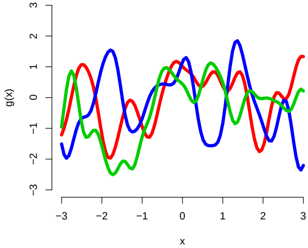
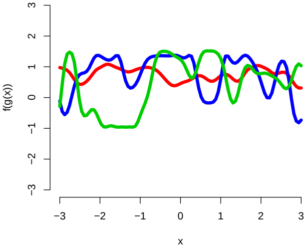
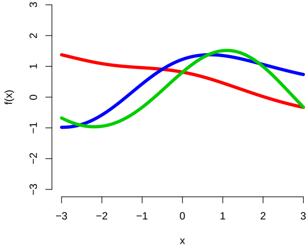
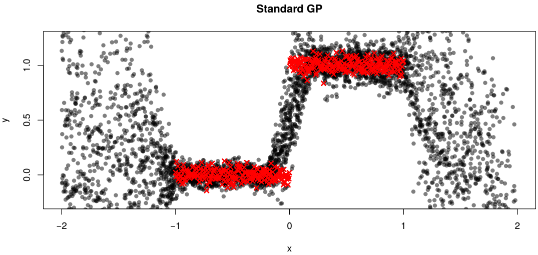






Deep GPs perform automatic covariance function design!

Deep GP Predictive Distribution



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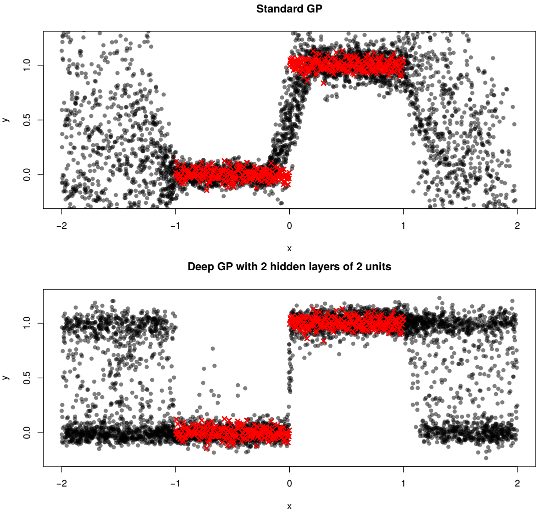

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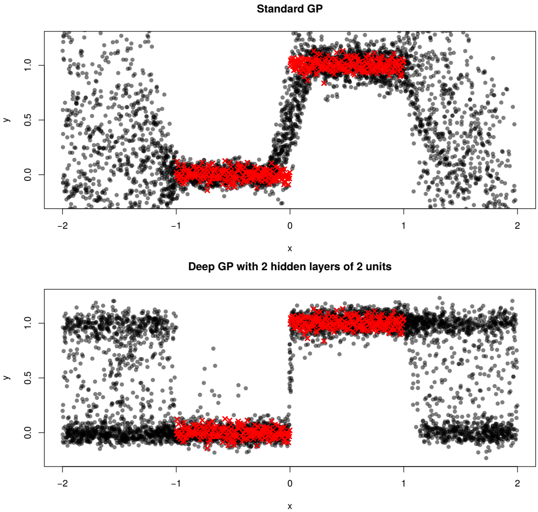

In a deep GP the predictive distribution needs not be Gaussian!

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- High computational cost.

Bayesian inference

Posterior over latent functions (typically at the observed data $\mathbf{X}$):

$$p(\mathbf{f}^1, \mathbf{f}^2, \mathbf{f}^3 | \mathbf{Y}) = \frac{p(\mathbf{f}^1)p(\mathbf{f}^2)p(\mathbf{f}^3) \; p(\mathbf{Y}|\mathbf{f}^1, \mathbf{f}^2, \mathbf{f}^3, \mathbf{X})}{p(\mathbf{Y})}$$

- GP priors
- Likelihood function
- Marginal likelihood

But the posterior $p(\mathbf{f}^1, \mathbf{f}^2, \mathbf{f}^3 | \mathbf{Y})$ is **intractable**.

Inducing Points Representation

Latent variables: from $\mathcal{O}(N)$ to $\mathcal{O}(M)$, with $M \ll N$.

Distribution on f given by GP with inducing inputs $\bar{\mathbf{X}}$ and outputs $\mathbf{u}$.

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If $p(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\mathbf{m},\mathbf{S})$, then $p(f(\mathbf{x}^\star)) = \mathcal{N}(f(\mathbf{x}^\star)|m^\star, v^\star)$, where

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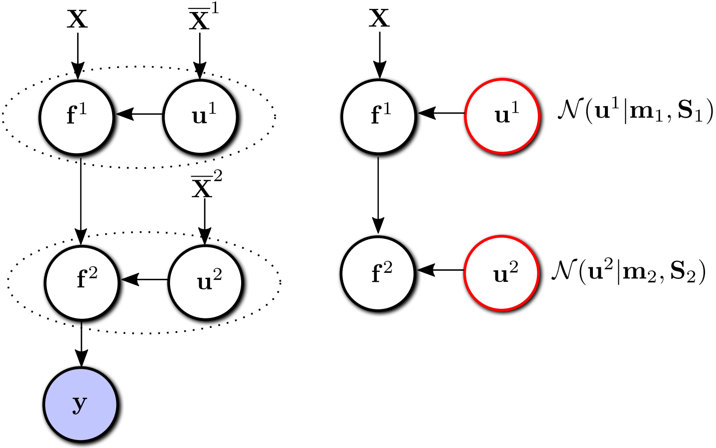
Given u or a Gaussian for u, f is fully specified!

Deep GPs Joint Distribution

$$p(\mathbf{y}, \{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^{L}) = \overbrace{\prod_{i=1}^{N} p(y_i | f_i^L)}^{\text{Likelihood}} \times \underbrace{\prod_{l=1}^{L} p(\mathbf{f}^l | \mathbf{u}^l, \overline{\mathbf{X}}^l) p(\mathbf{u}^l | \overline{\mathbf{X}}^l)}_{\text{Deep GP prior}}$$

Graphical Model and Posterior Approximation



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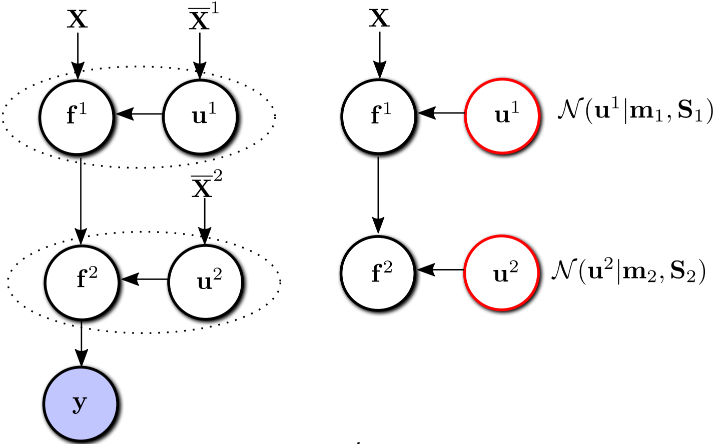

$$q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) = \prod_{l=1}^{L} p(\mathbf{f}^l|\mathbf{u}^l) \; q(\mathbf{u}^l)$$

- Fixed
- Tunable

Variational Inference for Deep GPs

Based on minimizing KL$(q(\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^{L}) | p(\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^{L} | \mathbf{y}))$

(Salimbeni, 2017)

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Equivalent to maximizing the lower bound on $\log p(\mathbf{y})$:

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$$= \sum_{i=1}^N \mathbb{E}_q[\log p(y_i|f_i^L)] - \sum_{l=1}^L \mathrm{KL}(q(\mathbf{u}^l)|p(\mathbf{u}^l)).$$

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$$= \sum_{i=1}^N \mathbb{E}_q[\log p(y_i|f_i^L)] - \sum_{l=1}^L \mathrm{KL}(q(\mathbf{u}^l)|p(\mathbf{u}^l)) .$$

- Suitable for stochastic optimization.

(Salimbeni, 2017)

Variational Inference for Deep GPs

Based on minimizing KL$(q(\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^L)|p(\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^L|\mathbf{y}))$

Equivalent to maximizing the lower bound on $\log p(\mathbf{y})$:

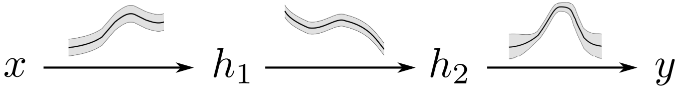
$$\mathcal{L} = \mathbb{E}_q\left[\log \frac{\prod_{i=1}^N p(y_i|f_i^L) \prod_{l=1}^L \cancel{p(\mathbf{f}^l|\mathbf{u}^l)} p(\mathbf{u}^l)}{\prod_{l=1}^L \cancel{p(\mathbf{f}^l|\mathbf{u}^l)} q(\mathbf{u}^l)}\right].$$

$$= \sum_{i=1}^N \mathbb{E}_q[\log p(y_i|f_i^L)] - \sum_{l=1}^L \mathrm{KL}(q(\mathbf{u}^l)|p(\mathbf{u}^l)).$$

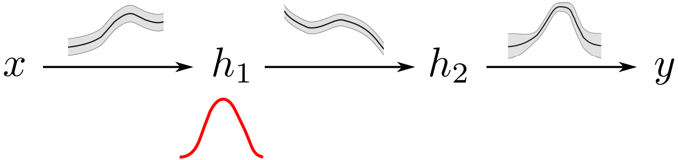
- Suitable for stochastic optimization.
- The expectations can be approximated by Monte Carlo.

(Salimbeni, 2017)

Monte Carlo Approximation



Monte Carlo Approximation



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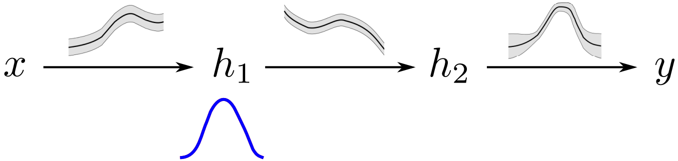

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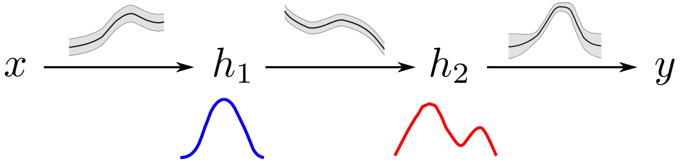

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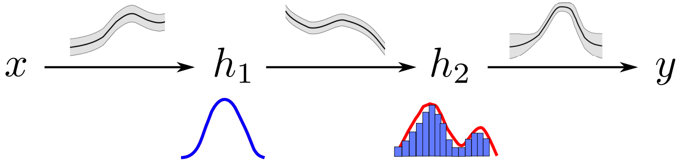

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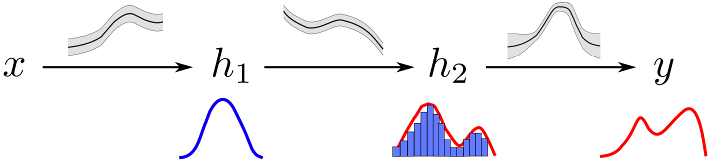

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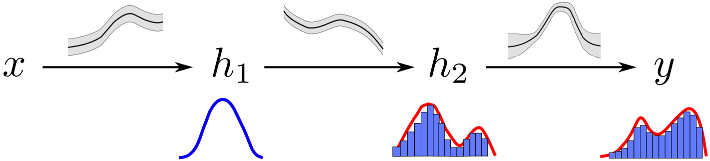
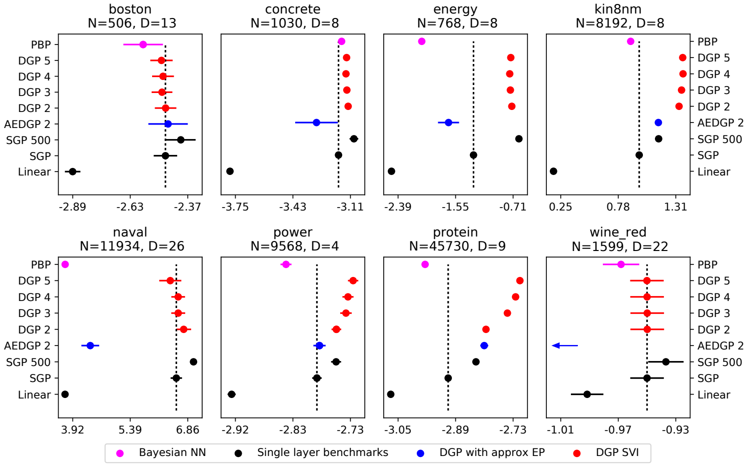


DGPs Experimental Results



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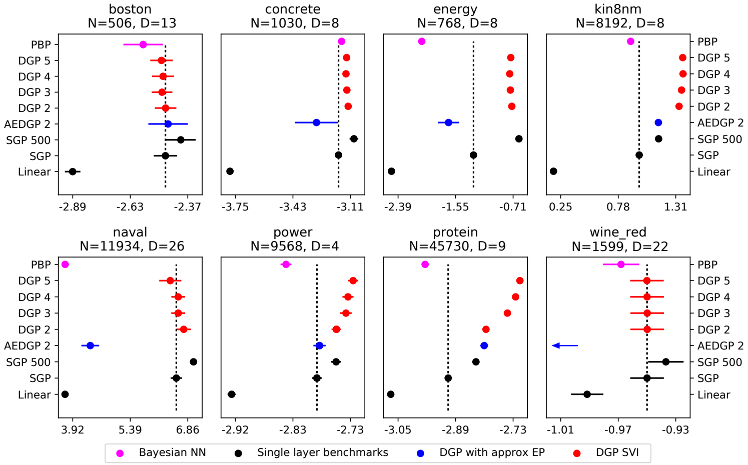

DGPs perform similar or better than the sparse GP and adding more layers does not seem to overfit!

(Salimbeni, 2017)

Software for GPs and Deep GPs

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Deep GPs: uses doubly stochastic variational inference and GPflow.

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5. **Convolutional GPs**: introduce prior knowledge about the latent function similar to that of convolutional neural networks.

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Thank you for your attention!

References

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