Part II: Sparse Gaussian Processes

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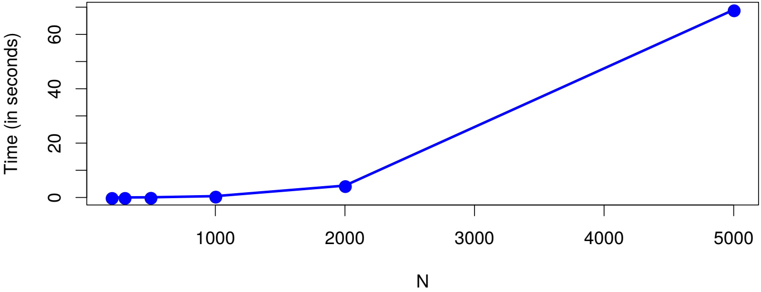

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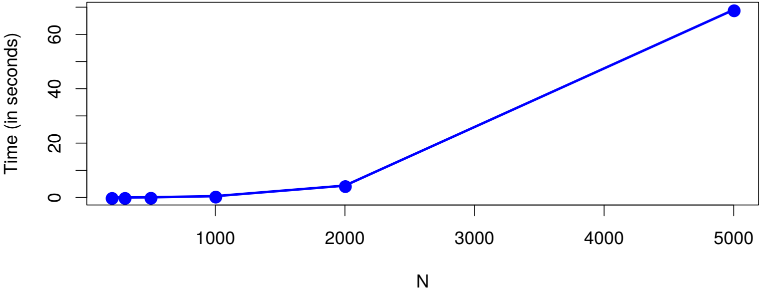

We can handle just a few thousand data instances at most!

Run the first cells of the notebook to measure GP fitting time and complete task 1!

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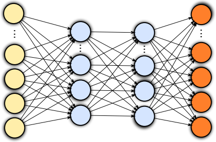

Neural Network (parametric model)

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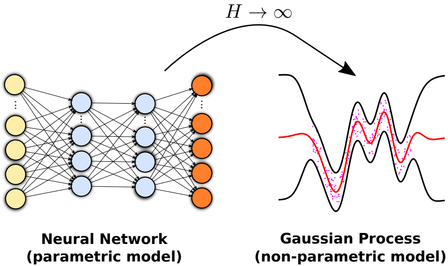

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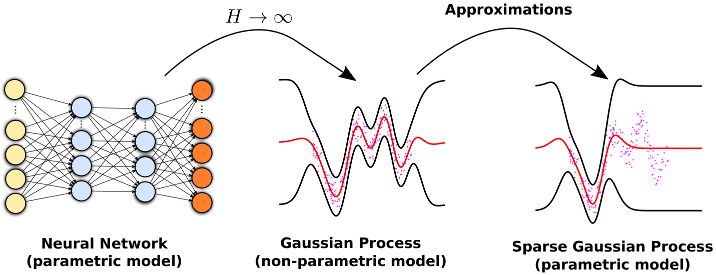

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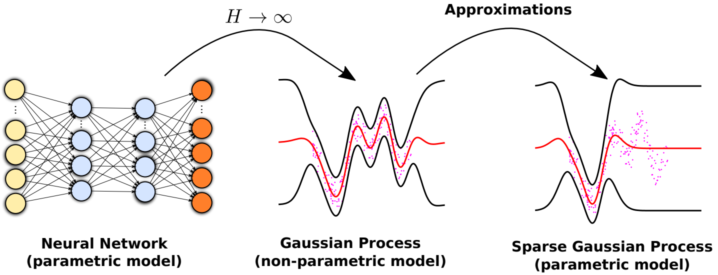

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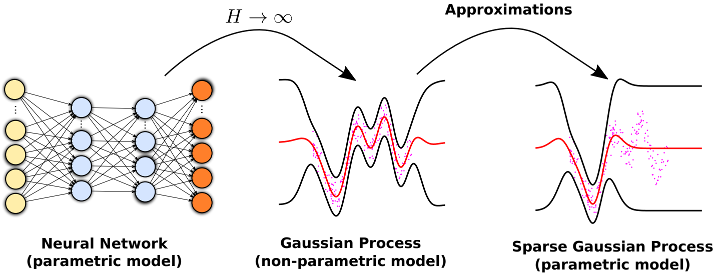

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- **VFE**: does approximate inference with a simplified distribution q.

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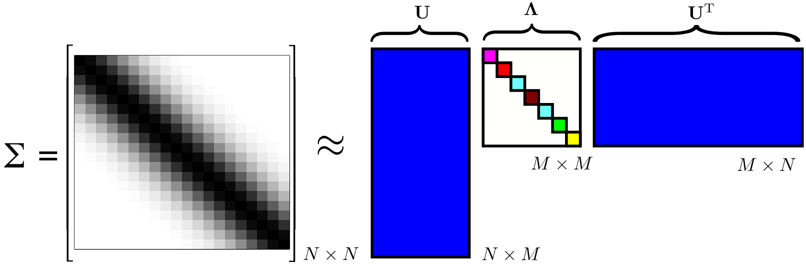

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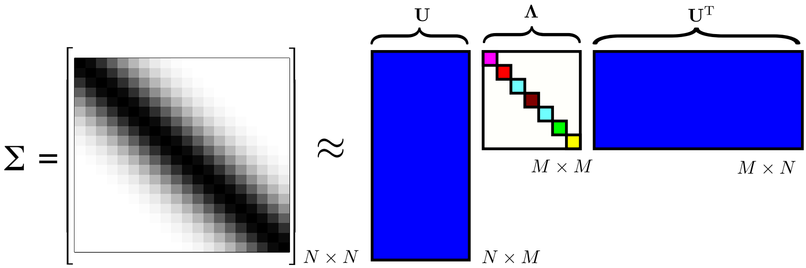

The Woodbury formula gives $(\mathbf{I}\sigma^2 + \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\mathsf{T})^{-1}$ with cost $\mathcal{O}(M^2 N)$!

Woodbury Formula

$$(\mathbf{A} + \mathbf{PCQ})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{P}\left(\mathbf{C}^{-1} + \mathbf{QA}^{-1}\mathbf{P}\right)^{-1}\mathbf{QA}^{-1}$$

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Computing the whole expression has cost $\mathcal{O}(NM^2)$!

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Extended input space: A function $\phi(\cdot)$ that obeys

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Mercer's theorem:

$$C(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{\infty} \lambda_i \phi_i(\mathbf{x})\phi_i(\mathbf{x}')\,.$$

An Analytic Example

Consider:

$$p(x) = \mathcal{N}(x|0, \sigma^2)\,, \qquad C(x, x') = \exp\left\{-\frac{1}{2\ell^2}(x - x')^2\right\}\,.$$

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Then,

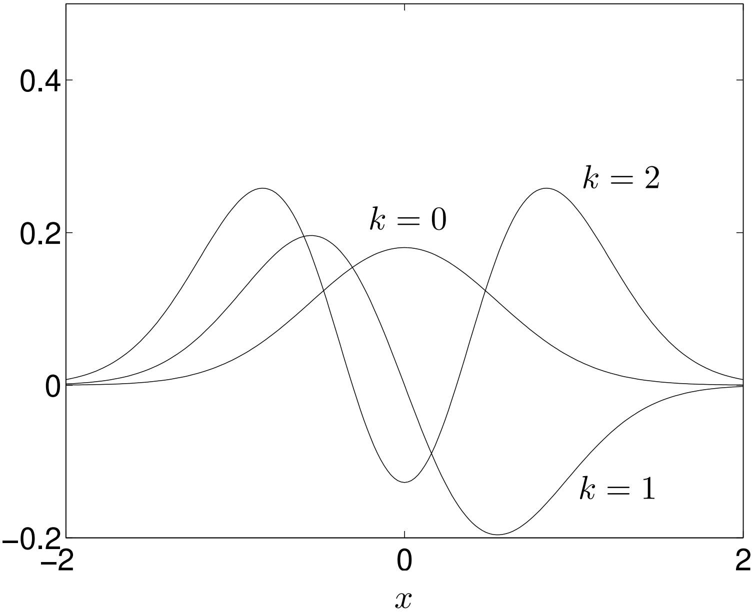
$$\lambda_k = \sqrt{\frac{2a}{A}} B^k\,, \qquad \phi_k(x) = \exp\left\{-(c - a)x^2\right\} H_k(\sqrt{2c}x)\,,$$

for $k = 0, 1, 2, \ldots$, with

$$a^{-1} = 4\sigma^2\,, \quad b^{-1} = 2\ell^2\,, \quad c = \sqrt{a^2 + 2ab}\,, \quad A = a + b + c\,, \quad B = b/a\,,$$

and $H_k(\cdot)$, the k-th order Hermite polynomial.

Hermite Polynomials



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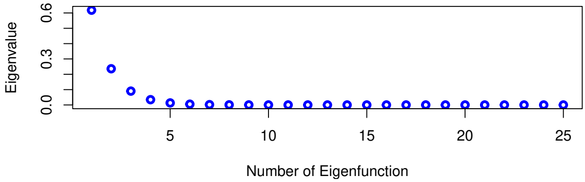

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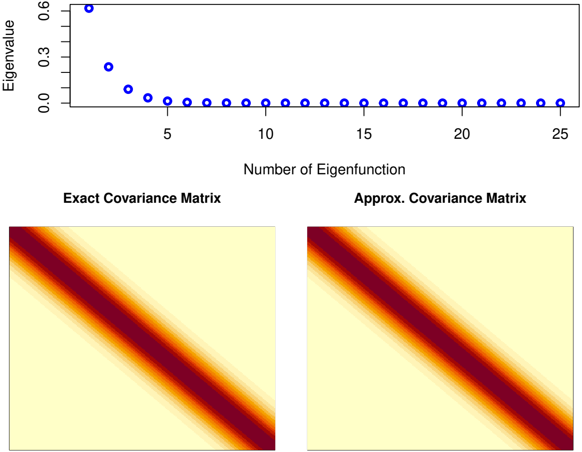

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$$\lambda_i \phi_i(\mathbf{x}') = \int C(\mathbf{x}, \mathbf{x}') \phi_i(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \approx \frac{1}{N} \sum_{n=1}^{N} C(\mathbf{x}_n, \mathbf{x}') \phi_i(\mathbf{x}_n) \,.$$

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For $\mathbf{x}'$ in the training set, this motivates the following eigenvalue problem:

$$\lambda_i^{\mathrm{mat}} \mathbf{u}_i = \mathbf{\Sigma} \mathbf{u}_i \,,$$

with $\Sigma_{i,j} = C(\mathbf{x}_i, \mathbf{x}_j)$. Then, we approximate $\phi_i(\mathbf{x}_j) \approx \sqrt{N}(\mathbf{u}_i)_j = \tilde{\phi}_i(\mathbf{x}_j)$, and $\lambda_i \approx \lambda_i^{\mathrm{mat}}/N = \tilde{\lambda}_i$, which guarantees that $\mathbf{\Sigma} = \tilde{\mathbf{\Phi}} \tilde{\mathbf{\Lambda}} \tilde{\mathbf{\Phi}}^{\mathsf{T}}$, with $j = 1, \ldots, N$.

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For an arbitrary $\mathbf{x}'$ not in the training set, then:

$$\tilde{\phi}_i(\mathbf{x}') = \frac{1}{N\lambda_i}\sum_{n=1}^{N} C(\mathbf{x}', \mathbf{x}_n)\phi_i(\mathbf{x}_n) \approx \frac{\sqrt{N}}{\lambda_i^{\text{mat}}}\sum_{n=1}^{N} C(\mathbf{x}', \mathbf{x}_n)(\mathbf{u}_i)_n = \frac{\sqrt{N}}{\lambda_i^{\text{mat}}}\mathbf{\Sigma}(\mathbf{x}')^{\text{T}}\mathbf{u}_i\,.$$

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The inverse of $\mathbf{I}\sigma^2 + \tilde{\mathbf{\Sigma}}$ can be efficiently computed using the Woodbury formula with cost $\mathcal{O}(NM^2)$!

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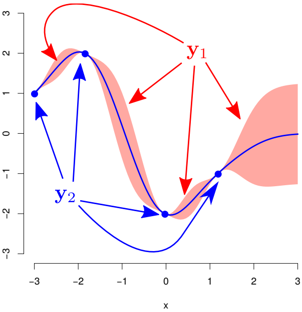

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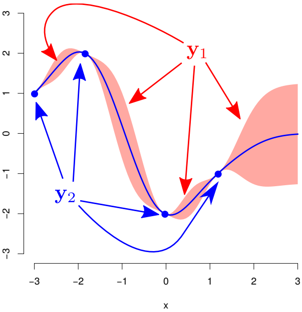

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\top & \mathbf{B} \end{bmatrix} \right),$$

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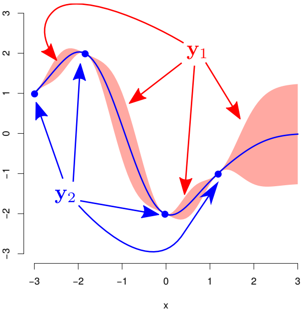

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$$p(\mathbf{y}_1|\mathbf{y}_2) = \mathcal{N}\left(\mathbf{y}_1\middle|\mathbf{a}+\mathbf{C}\mathbf{B}^{-1}(\mathbf{y}_2-\mathbf{b}),\mathbf{A}-\mathbf{C}\mathbf{B}^{-1}\mathbf{C}^\top\right)$$

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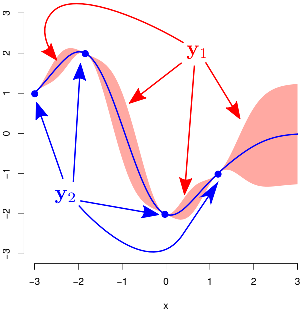

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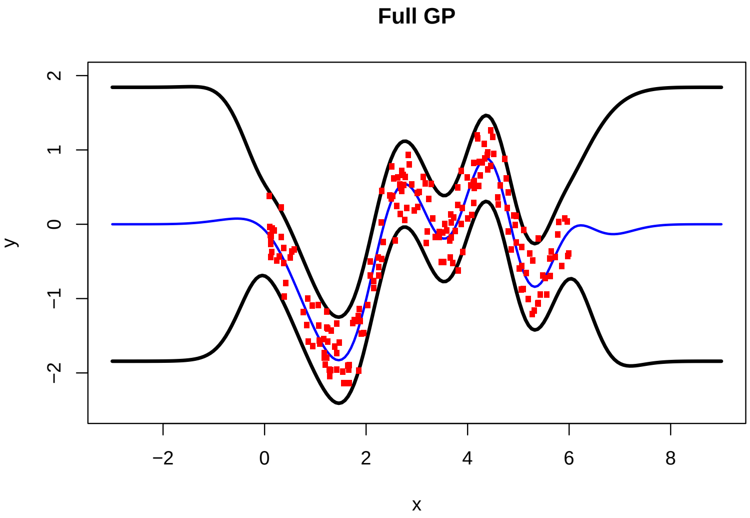
$$p(\mathbf{f}^\star | \mathbf{f}) = \mathcal{N}\left(\mathbf{f}^\star \middle| \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}} \tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}}^{-1} \mathbf{f}, \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}^\star} - \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}} \tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}}^{-1} \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}}^\top\right)$$

Nyström Approximation: Illustrative Example



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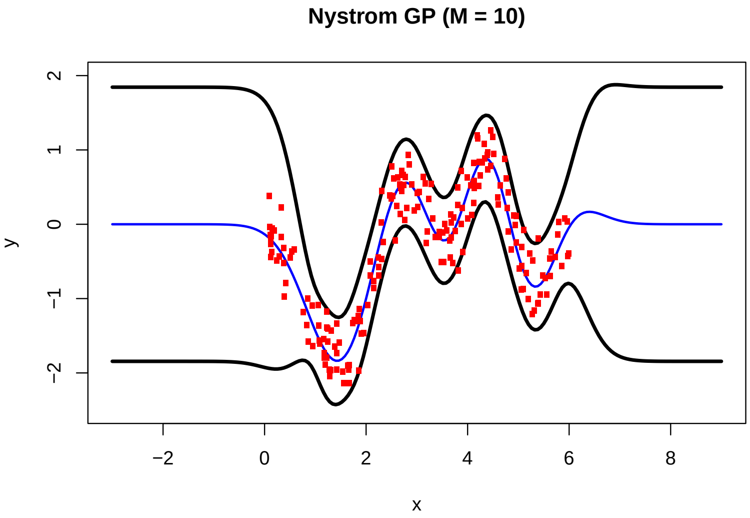

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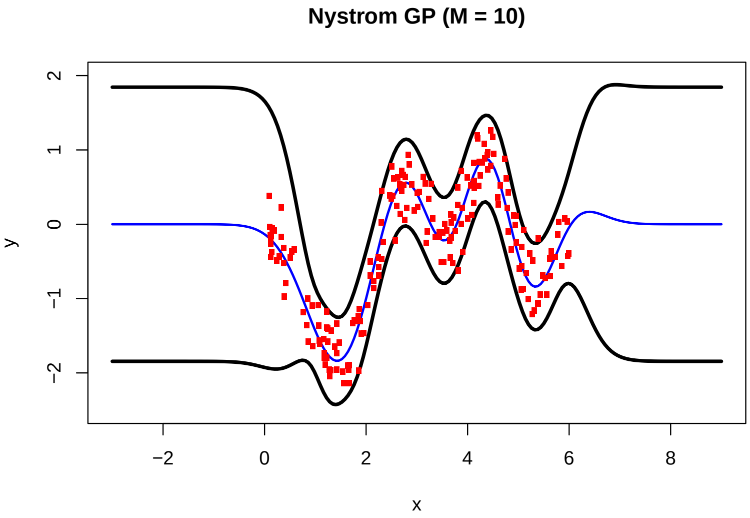

The approximation is similar to the full GP in some regions!

Summary of Nyström Approximation

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- It can perform well if $\boldsymbol{\Sigma}$ is dominated by a few eigenvalues.
- As the M points are chosen at random it may give different results.
- Since the approximation is done only over the covariance matrix of the training data, negative predictive variances are possible, but rare.

Run the cells of the notebook to fit a sparse GP using the Nyström approximation and complete task 2!

Run the cells of the notebook compare the exact and approximate predictive distribution and complete task 3!

Random Features Approximations

They can be used to approximate any stationary covariance function (only depends on the distance between points).

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A covariance function $C(\mathbf{x}, \mathbf{x}') = C(\mathbf{x} - \mathbf{x}')$ on $\mathbb{R}^D$ is positive definite if and only if $C(\mathbf{x} - \mathbf{x}')$ is the Fourier transform of a distribution $s(\mathbf{w})$.

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$s(\mathbf{w})$ is called the spectral density of the covariance function.

Covariances as Expectations of Cosines

Due to Bochner's theorem, the covariance can be written as:

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$$C(\mathbf{x}, \mathbf{x}') \approx \frac{2}{M}\sum_{m=1}^{M} cos\left(\mathbf{w}_m^{\mathsf{T}}\mathbf{x} + b_m\right)\cos\left(\mathbf{w}_m^{\mathsf{T}}\mathbf{x}' + b_m\right) = \phi(\mathbf{x})^{\mathsf{T}}\phi(\mathbf{x}')$$

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For the squared exponential covariance function $s(\mathbf{w})$ is Gaussian!

Approximate Covariance Function

The covariance matrix can be simply approximated as:

$$\boldsymbol{\Sigma} \approx \tilde{\boldsymbol{\Sigma}} = \boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathsf{T}}$$

and hence $\mathbf{I}\sigma^2 + \tilde{\boldsymbol{\Sigma}}$ can be inverted with cost $\mathcal{O}(NM^2)$.

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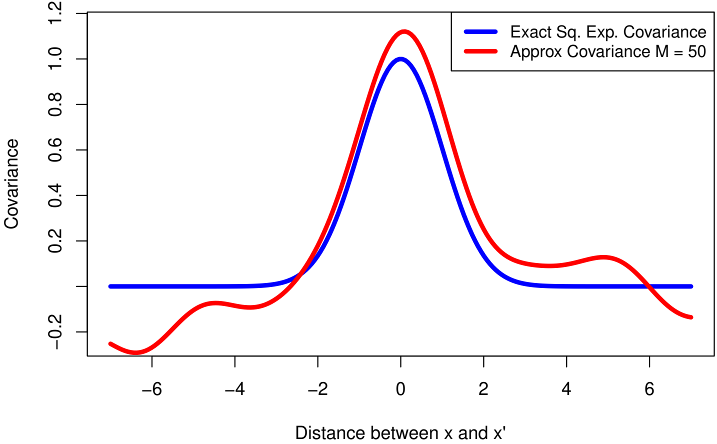

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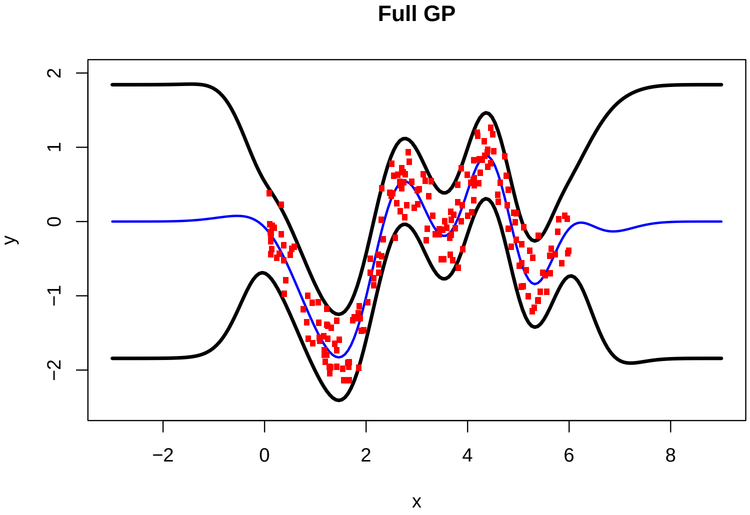
The computational cost is $\mathcal{O}(NM^2)$!

Random Features: Illustrative Example



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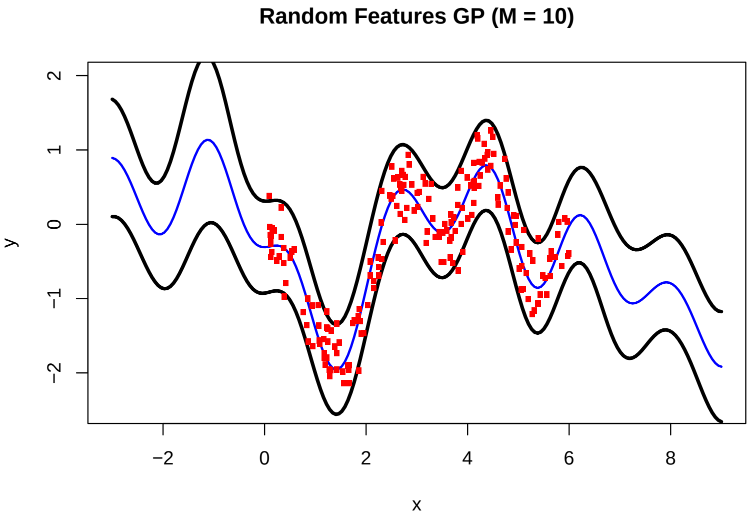

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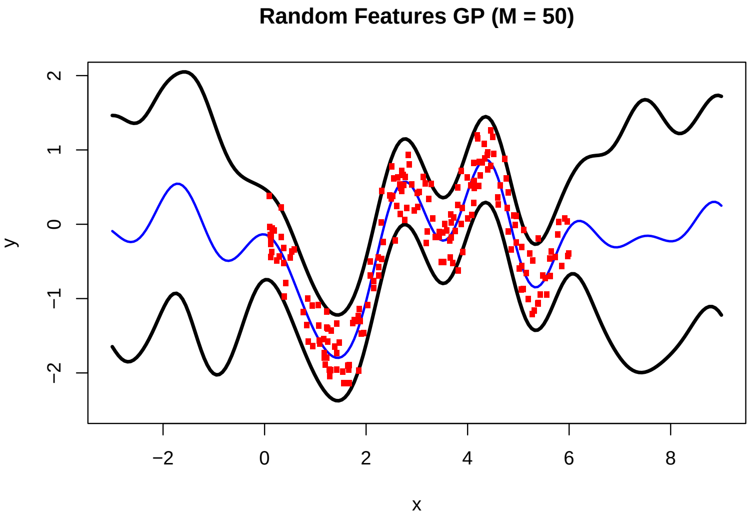

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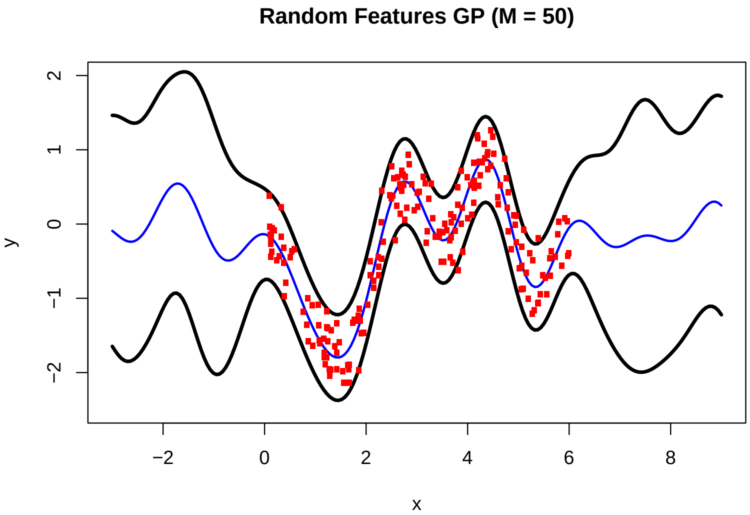

In regions with no data the approximation may be wiggling a lot!

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- Very simple to implement!
- Equivalent to a neural network with a hidden layer with M units and cosine activations, and a Bayesian linear model in the last layer!

Run the cells of the notebook to fit a sparse GP using the Random Features approximation and complete task 4!

Full Independent Training Conditional (FITC)

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

$$p(\mathbf{f}, \mathbf{u}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix} \middle| \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} \mathbf{\Sigma_{ff}} & \mathbf{\Sigma_{fu}} \\ \mathbf{\Sigma_{uf}} & \mathbf{\Sigma_{uu}} \end{bmatrix}\right)$$

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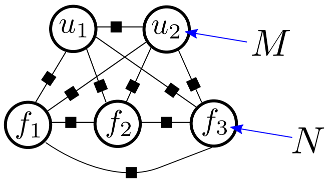

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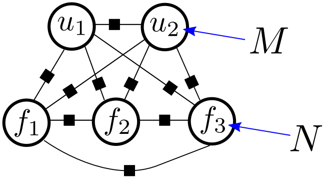

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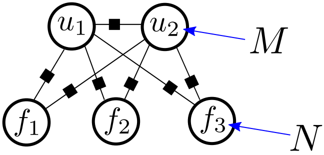

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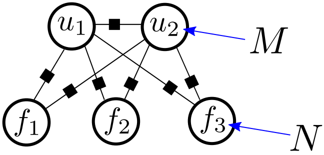

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3. Marginalize $\mathbf{u}$ to obtain an approximate GP prior for $\mathbf{f}$.

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

where $\tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}} = \mathbf{D} + \mathbf{Q}_{\mathbf{ff}}$ with $\mathbf{D}$ diagonal and $\mathbf{Q}_{\mathbf{ff}} = \boldsymbol{\Sigma}_{\mathbf{fu}}\boldsymbol{\Sigma}_{\mathbf{uu}}^{-1}\boldsymbol{\Sigma}_{\mathbf{uf}}$ 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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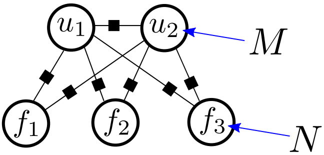

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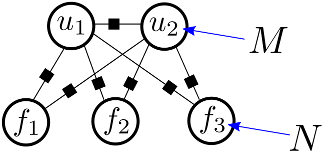

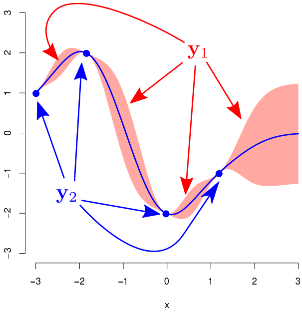

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\mathsf{T} & \mathbf{B} \end{bmatrix} \right),$$

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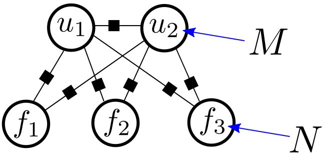

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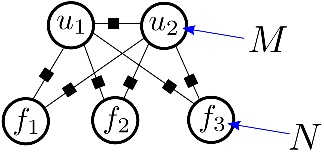

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Due to the structure in $\tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}}$ all computations have cost in $\mathcal{O}(NM^2)$.

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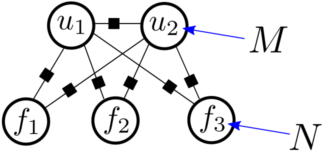

$$p(\mathbf{f}^\star|\mathbf{f}) = \mathcal{N}\left(\mathbf{f}^\star \middle| \mathbf{Q}_{\mathbf{f}^\star\mathbf{f}} \tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}}^{-1} \mathbf{f}, \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}^\star} - \mathbf{Q}_{\mathbf{f}^\star\mathbf{f}} \tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}}^{-1} \mathbf{Q}_{\mathbf{f}^\star\mathbf{f}}^\mathsf{T}\right)$$

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

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

Full Independent Training Conditional (FITC)

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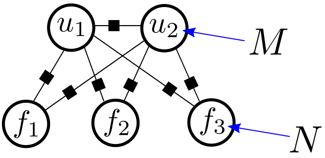

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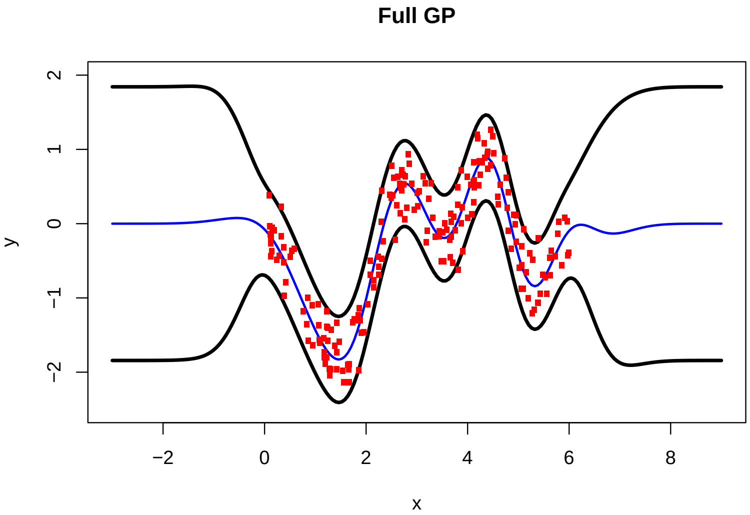
Due to the structure in $\tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}}$ all computations have cost in $\mathcal{O}(NM^2)$.

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

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

FITC: Illustrative Example



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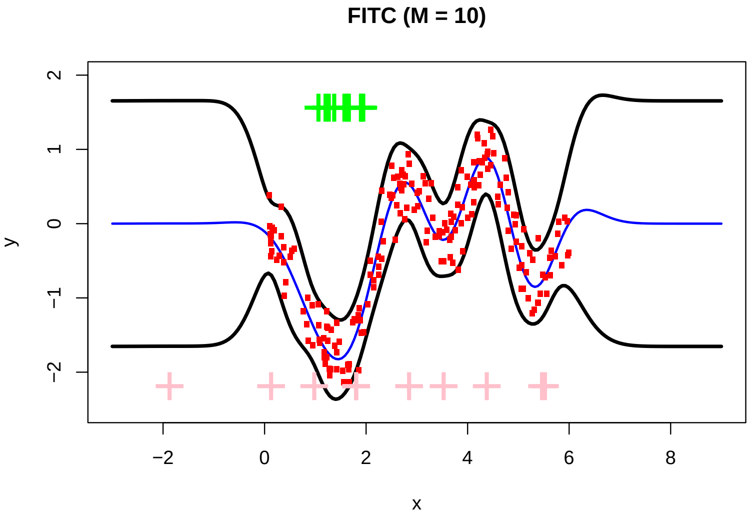

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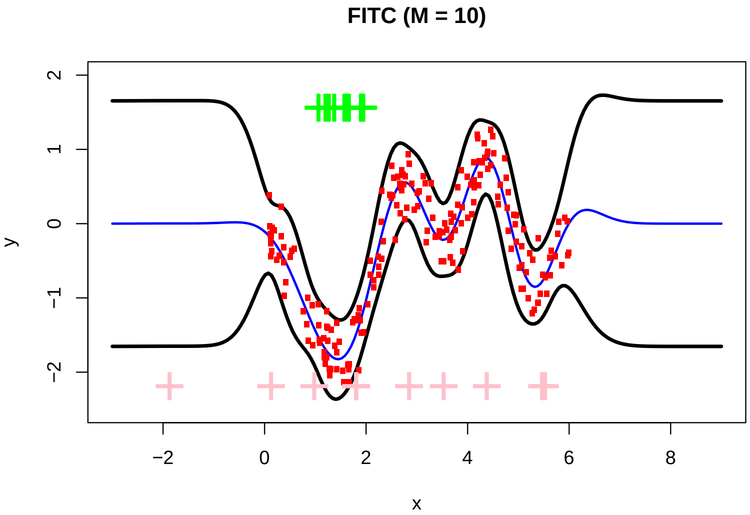

The inducing points cover the regions where the function changes!

Summary of FITC

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- The optimized inducing points spread over the input space where the latent function changes.
- Guaranteed to be exact if $M = N$ and the inducing points are not optimized and located at the training points.
- It can be understood as considering heteroscedastic (input dependent) noise!

Run the cells of the notebook to fit a sparse GP using the FITC approximation and complete task 5!

Generalized FITC

Combines FITC with the use of Expectation Propagation to address binary classification problems!

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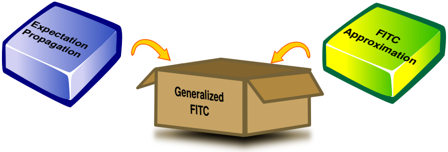

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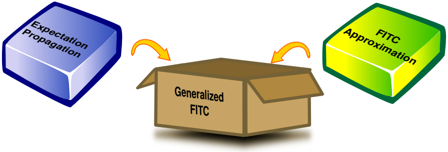

Assumes $y_i \in \{-1, 1\}$ and a probit likelihood:

$$p(y_i|f(\mathbf{x}_i)) = \phi(y_i f(\mathbf{x}_i)) \,, \quad \phi(\cdot) \equiv \text{The c.d.f. of a standard Gaussian.}$$

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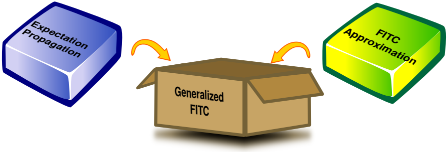

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Approximates with a **Gaussian distribution** the intractable posterior:

$$p(\mathbf{f}|\mathbf{y}) = \frac{\prod_{i=1}^{N} \phi(y_i f(\mathbf{x}_i))\mathcal{N}(\mathbf{f}|\mathbf{0}, \tilde{\boldsymbol{\Sigma}})}{p(\mathbf{y})},$$

where $\tilde{\boldsymbol{\Sigma}}$ is the **approximate FITC covariance matrix**.

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The exponential family:

$$q(\mathbf{x}) = \exp\left(\boldsymbol{\eta}^\mathsf{T}\mathbf{u}(\mathbf{x}) - g(\boldsymbol{\eta})\right) \,, \qquad g(\boldsymbol{\eta}) = \log \int \exp\left(\boldsymbol{\eta}^\mathsf{T}\mathbf{u}(\mathbf{x})\right) d\mathbf{x}$$

where $\boldsymbol{\eta}$ is a vector of natural parameters of q, $\mathbf{u}(\mathbf{x})$ are the sufficient statistics and $g(\boldsymbol{\eta})$ is a **log partition function**.

Examples of Distributions in the Exponential Family

Gaussian:

$$\mathcal{N}(x|\mu, \sigma^2) = 1/\sqrt{2\pi\sigma^2} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

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Most parametric distributions belong to the exponential family!

Product and Ratio of Gaussians

Consider these two Gaussian distributions:

$$p_1(x) = \frac{1}{\sqrt{2\pi\sigma_1^2}} \exp\left\{ -\frac{1}{2}\sigma_1^2 (x - \mu_1)^2 \right\} ,$$

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Consider the KL-divergence between p and q (q in the exponential family):

$$\mathrm{KL}(p||q) = -\int p(\mathbf{x}) \log \left\{ \frac{q(\mathbf{x})}{p(\mathbf{x})} \right\} d\mathbf{x} = g(\boldsymbol{\eta}) - \boldsymbol{\eta}^{\mathsf{T}} \mathbb{E}_p[\mathbf{u}(\mathbf{x})] + \mathrm{Const}\,.$$

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If q is Gaussian, then we have to match $\mathbb{E}_q[\mathbf{x}] = \mathbb{E}_p[\mathbf{x}]$ and $\mathbb{E}_q[\mathbf{x}\mathbf{x}^{\mathrm{T}}] = \mathbb{E}_p[\mathbf{x}\mathbf{x}^{\mathrm{T}}]$.

Joint Approximation

EP approximates this joint distribution by **a product of simpler factors**:

$$p(\mathbf{f}, \mathbf{y}) = \prod_{i=1}^{N} \phi_i(y_i f(\mathbf{x}_i) \mathcal{N}(\mathbf{f}|\mathbf{0}, \tilde{\mathbf{\Sigma}}) = \prod_i t_i(\mathbf{f}) \approx \prod_i \tilde{t}_i(\mathbf{f}) \,,$$

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The exponential family is closed under the product and $\prod_i \tilde{t}_i$ can be easily normalized to compute an approximate distribution:

$$p(\mathbf{f}|\mathbf{y}) = \frac{1}{p(\mathbf{y})} \prod_i t_i(\mathbf{f}) \approx \frac{1}{Z} \prod_i \tilde{t}_i(\mathbf{f}) = q(\mathbf{f}),$$

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Therefore q has the same form as the approximate factors!

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Then, $\tilde{t}_j$ is updated to minimize the KL-divergence between:

$$q_{\text{new}}(\mathbf{f}) \propto \tilde{t}_j(\mathbf{f}) q^{\setminus j}(\mathbf{f}) \,, \quad \hat{p}_j(\mathbf{f}) = \frac{1}{Z_j} t_j(\mathbf{f}) q^{\setminus j}(\mathbf{f}) \,, \quad Z_j = \int t_j(\mathbf{f}) q^{\setminus j}(\mathbf{f}) d\mathbf{f} \,,$$

where $q^{\setminus j}$ is fixed. This ensures that $\tilde{t}_j$ is accurate where $q^{\setminus j}$ is high.

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In practice, $\tilde{t}_j$ is found by first **minimizing** with respect to q_{new}:

$$\mathrm{KL}\left(\frac{t_j(\mathbf{f}) q^{\setminus j}(\mathbf{f})}{Z_j} \middle| \, q_{\text{new}}(\mathbf{f}) \right) .$$

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The refined factor $\tilde{t}_j$ is set in practice to be:

$$\tilde{t}_j(\mathbf{f}) = Z_j \frac{q_{\text{new}}(\mathbf{f})}{q^{\setminus j}(\mathbf{f})} , \qquad \text{with} \quad \tilde{t}_j(\mathbf{f}) q^{\setminus j}(\mathbf{f}) \propto q_{\text{new}} ,$$

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Several passes are made trough the factors until they **converge**. The **model evidence** is approximated by the **normalizing constant** of q.

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The FITC prior results in a total cost of $\mathcal{O}(NM^2)$!

Graphical Illustration

Approximates $p(\mathbf{f}|\mathbf{y}) \propto t_0(\mathbf{f}) \prod_{j=1}^{N} t_j(\mathbf{f})$ with $q(\mathbf{f}) \propto t_0(\mathbf{f}) \prod_{j=1}^{N} \tilde{t}_j(\mathbf{t})$

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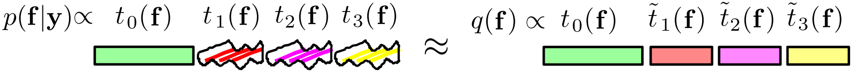

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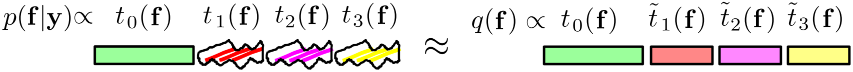

The $\tilde{t}_j$ are tuned by minimizing the KL-divergence

$$\mathrm{KL}[\hat{p}_j || q] \quad \text{for } j = 1, \ldots, N, \quad \text{where} \quad \begin{array}{rcl} \hat{p}_j(\mathbf{f}) & \propto & t_j(\mathbf{f}) \prod_{i \neq j} \tilde{t}_i(\mathbf{f}) \\ q(\mathbf{f}) & \propto & \tilde{t}_j(\mathbf{f}) \prod_{i \neq j} \tilde{t}_i(\mathbf{f}) \end{array}.$$

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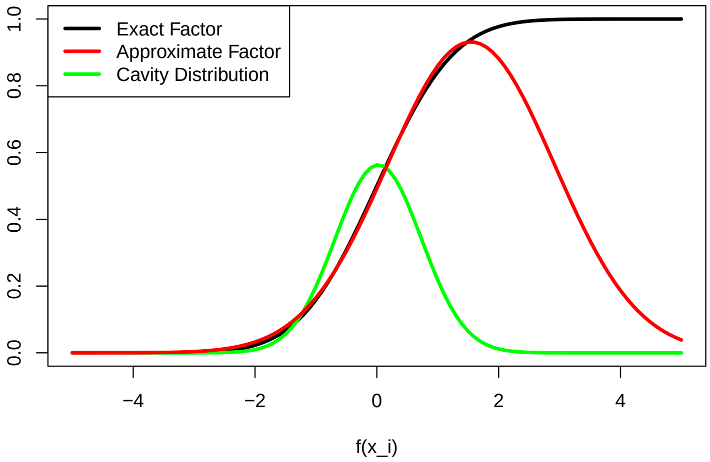
If the exact factor already belongs to the exponential family it needs not be approximated!

GFITC: Factor Approximation



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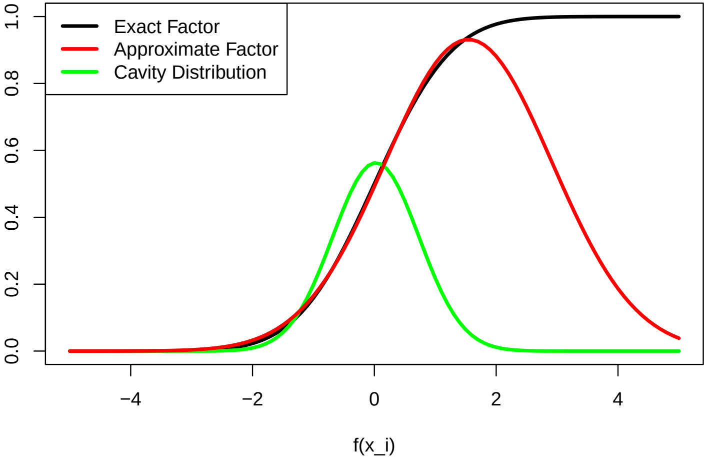

The approximate factor is accurate in regions of high posterior probability as indicated by the cavity distribution!

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If EP converges the gradient of $\log Z$ w.r.t. each θ_i is zero, which allows to easily compute the gradients of $\log Z$!

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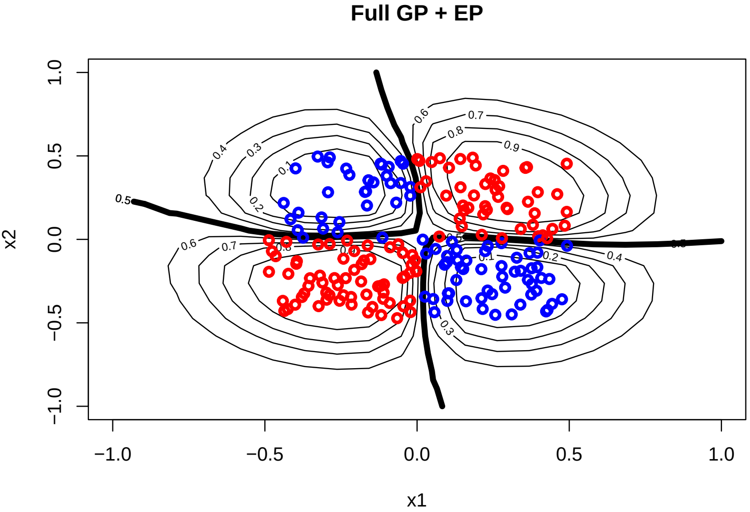
After marginalizing $\mathbf{f}$ w.r.t. $q(\mathbf{f})$, we obtain the predictive distribution:

$$\begin{aligned} p(\mathbf{f}^\star|\mathbf{y}) &= \int p(\mathbf{f}^\star|\mathbf{f}) q(\mathbf{f}) d\mathbf{f} \\ &= \mathcal{N}\left(\mathbf{f}^\star \middle| \, \mathbf{Q}_{\mathbf{f}^\star\mathbf{f}} \left(\tilde{\boldsymbol{\Sigma}}_{\mathbf{f}\mathbf{f}} + \tilde{\boldsymbol{\Pi}} \right)^{-1} \tilde{\mathbf{y}}, \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}^\star} - \mathbf{Q}_{\mathbf{f}^\star\mathbf{f}} \left(\tilde{\boldsymbol{\Sigma}}_{\mathbf{f}\mathbf{f}} + \tilde{\boldsymbol{\Pi}} \right)^{-1} \mathbf{Q}_{\mathbf{f}\mathbf{f}^\star} \right) \end{aligned}$$

GFITC: Illustrative Example



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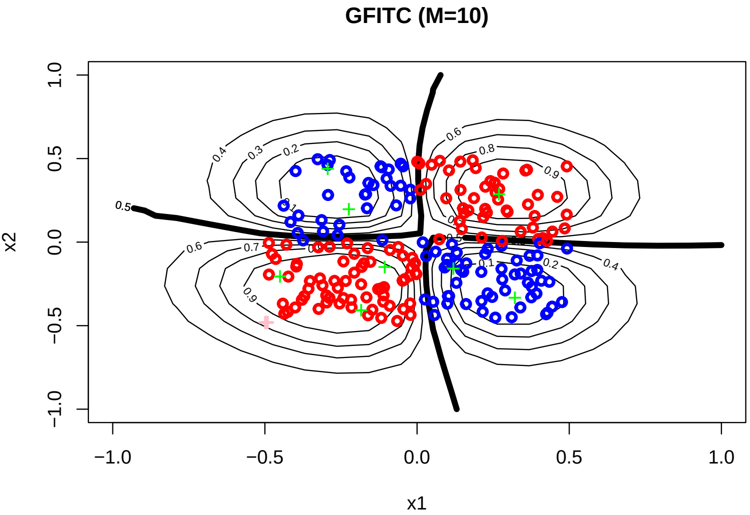

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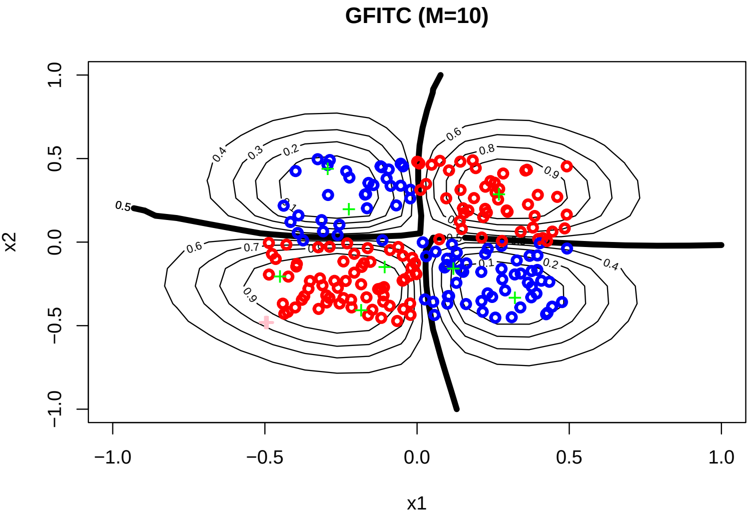

The inducing points spread across the input space!

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Since the GP prior is not changed it tends to perform better than the previous methods!

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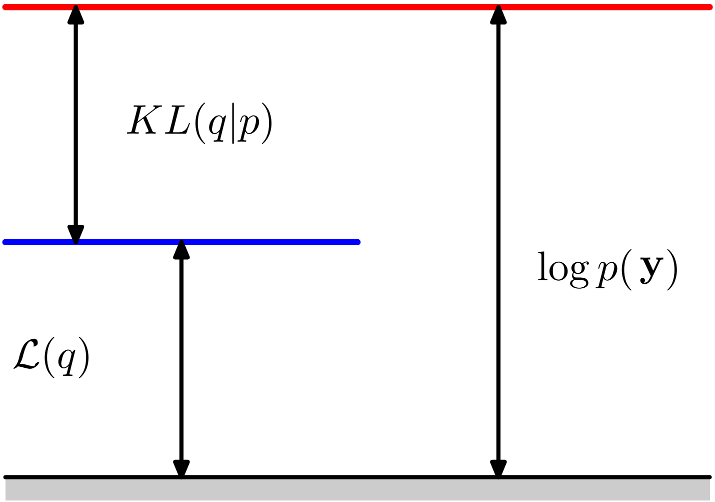
Let the target be $p(\mathbf{f}|\mathbf{y})$. Consider the decomposition of $p(\mathbf{y})$:

$$\log p(\mathbf{y}) = \mathcal{L}(q) + \mathrm{KL}(q|p)\,,$$

where

$$\mathcal{L}(q) = \int q(\mathbf{f}) \log \frac{p(\mathbf{f},\mathbf{y})}{q(\mathbf{f})} d\mathbf{f}\,, \qquad \mathrm{KL}(q|p) = \int q(\mathbf{f}) \log \frac{q(\mathbf{f})}{p(\mathbf{f}|\mathbf{y})} d\mathbf{f}\,.$$

Decomposition of the Marginal Likelihood



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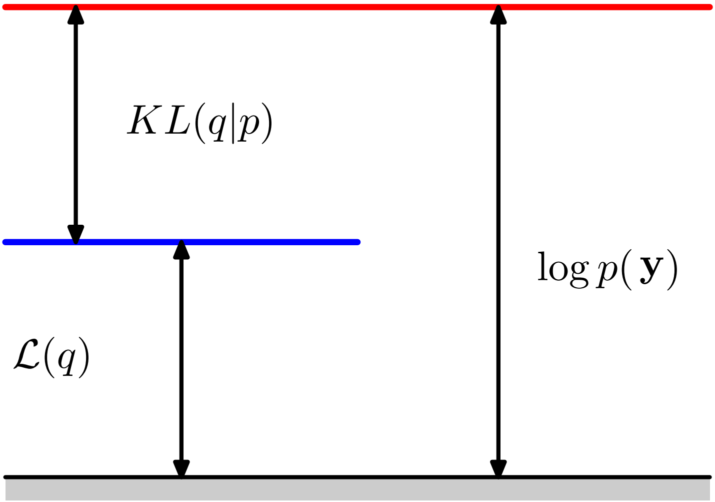
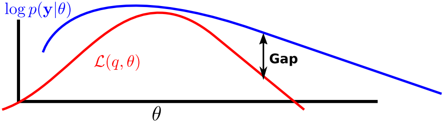


$\mathcal{L}(q)$ can be used to approximate $\log p(\mathbf{y})$ if $\mathbf{KL}(q|p)$ is small!

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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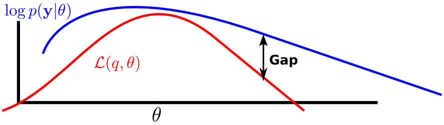

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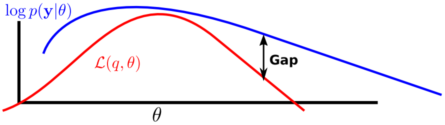

$$= \log \int p(\mathbf{y}, \mathbf{f}, \mathbf{u}|\theta) \frac{q(\mathbf{f}, \mathbf{u})}{q(\mathbf{f}, \mathbf{u})} d\mathbf{f} d\mathbf{u} \geq \int q(\mathbf{f}, \mathbf{u}) \log \frac{p(\mathbf{y}, \mathbf{f}, \mathbf{u}|\theta)}{q(\mathbf{f}, \mathbf{u})} d\mathbf{f} d\mathbf{u} \equiv \mathcal{L}(q, \theta)$$

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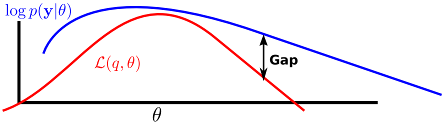

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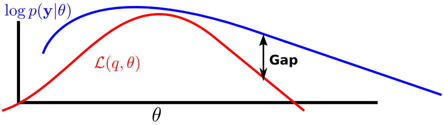

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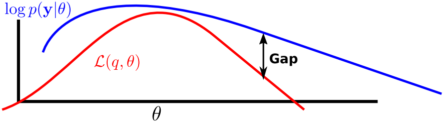

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By maximizing $\mathcal{L}(q, \theta)$ w.r.t q we are enforcing that $q(\mathbf{f}, \mathbf{u})$ looks similar to $p(\mathbf{f}, \mathbf{u}|\mathbf{y})$ in terms of the KL!

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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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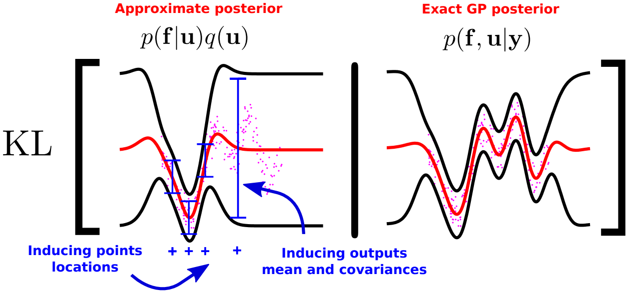

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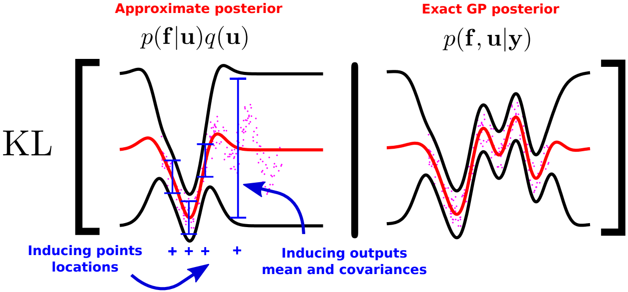

The inducing points are now parameters of the approx. dist. q!

Variational Free Energy (VFE)

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- KL between Gaussians (→ $\mathbf{KL}[q(\mathbf{u})|p(\mathbf{u})]$)

- No change in the model is made and the cost is in $\mathcal{O}(M^2 N)$!
- Predictions are made using $p(\mathbf{f}^\star|\mathbf{u})q(\mathbf{u})$ marginalizing out $\mathbf{u}$.

VFE: Predictions for Test Instances

We want to compute the value of $\mathbf{f}^\star$ at a new $\mathbf{x}^\star$:

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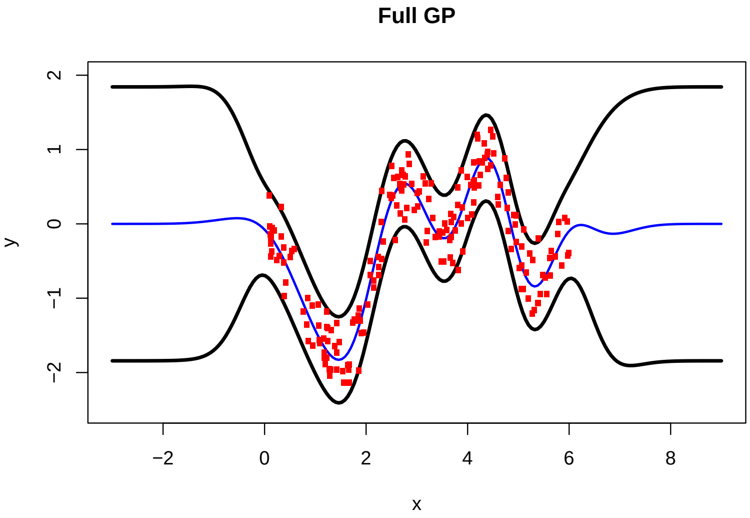
After marginalizing $\mathbf{u}$ w.r.t. $q(\mathbf{u})$, we obtain the predictive distribution:

$$\begin{aligned} p(\mathbf{f}^\star|\mathbf{y}) &= \int p(\mathbf{f}^\star|\mathbf{u})q(\mathbf{u})d\mathbf{u} \\ &= \mathcal{N}\left(\mathbf{f}^\star \middle| \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{u}}\boldsymbol{\Sigma}_{\mathbf{u}\mathbf{u}}^{-1}\mathbf{m}, \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{f}^\star} - \boldsymbol{\Sigma}_{\mathbf{f}^\star\mathbf{u}}\left(\boldsymbol{\Sigma}_{\mathbf{u}\mathbf{u}}^{-1} - \boldsymbol{\Sigma}_{\mathbf{u}\mathbf{u}}^{-1}\mathbf{S}\boldsymbol{\Sigma}_{\mathbf{u}\mathbf{u}}^{-1}\right)\boldsymbol{\Sigma}_{\mathbf{u}\mathbf{f}^\star}\right) \end{aligned}$$

VFE: Illustrative Example



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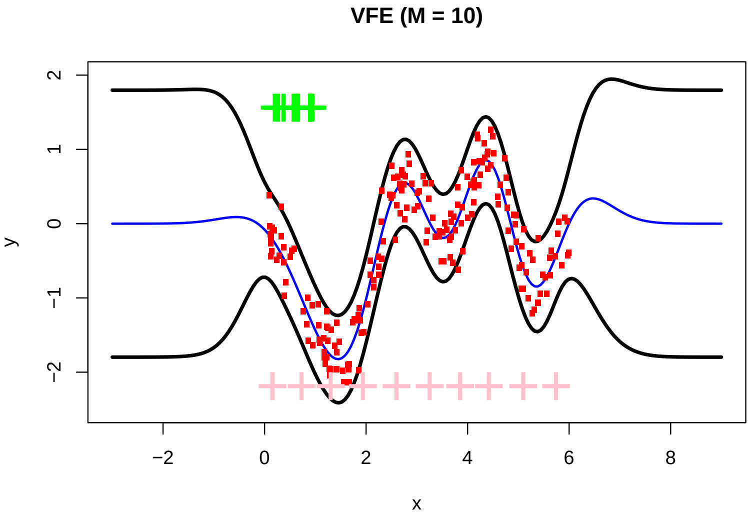

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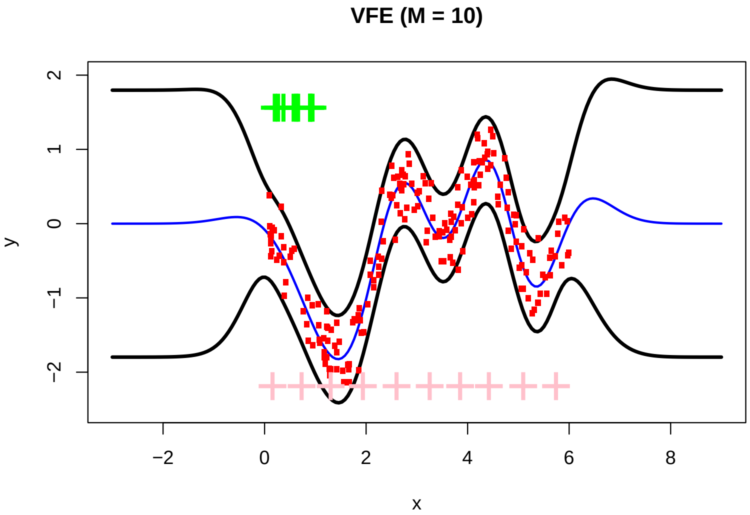
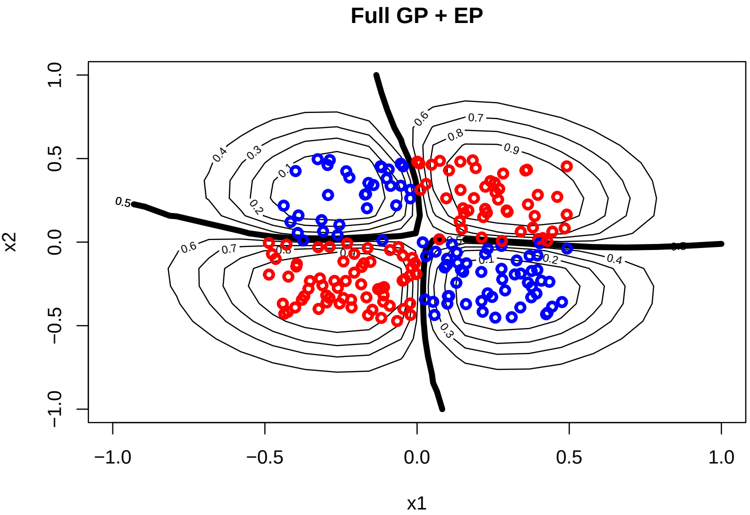


The inducing points cover the regions where the function changes!

VFE: Illustrative Classification Example



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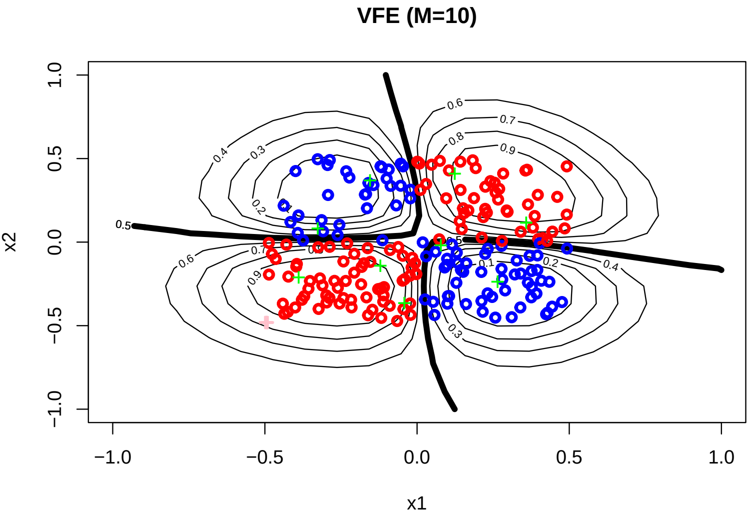

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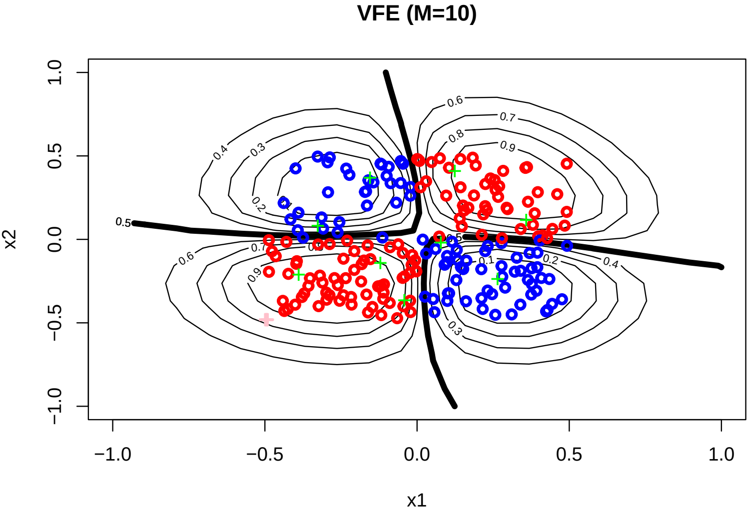

The inducing points spread across the input space!

FITC vs. VFE

Two approaches:

FITC vs. VFE

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- FITC: optimize the marginal likelihood of an approximate GP model.
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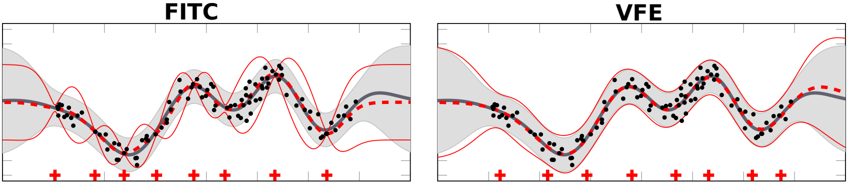

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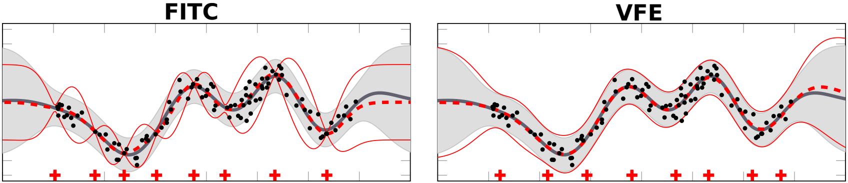

- FITC: less local optima and easier to optimize, also less accurate.
- VFE: more accurate, more local optima, more difficult to optimize.

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

Run the cells of the notebook to fit a sparse GP using the VFE approximation and complete task 6!

Whitened Parameterization for VFE

Alternative VFE objective expected to be easier to optimize!

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Instead of making inference about $\mathbf{u}$, the whitened VFE objective makes inference about:

$$\mathbf{e} \quad \text{such that} \quad \mathbf{u} = \mathbf{L}\mathbf{e}\,, \qquad\qquad \mathbf{e} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})\,,$$

with $\mathbf{u}$ the latent process values at the inducing points and $\mathbf{L}^{\mathsf{T}}\mathbf{L} = \mathbf{\Sigma}_{\mathbf{uu}}$.

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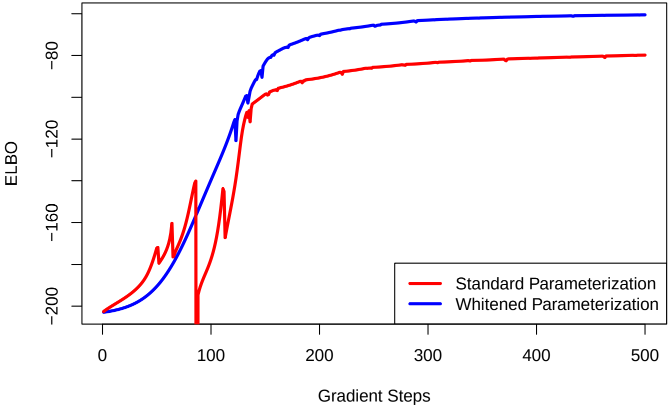
The VFE objective becomes:

$$\sum_{i=1}^{N} \mathbb{E}_{q(\mathbf{e})p(f(\mathbf{x}_i)|\mathbf{e})} [\log p(y_i|f(\mathbf{x}_i))] - \text{KL}(q(\mathbf{e})|\mathcal{N}(\mathbf{0}, \mathbf{I}))\,,$$

with $p(f(\mathbf{x}_i)|\mathbf{e})$ using the covariances between $f(\mathbf{x}_i)$ and $\mathbf{e}$.

Whitened Parameterization: Illustrative Example



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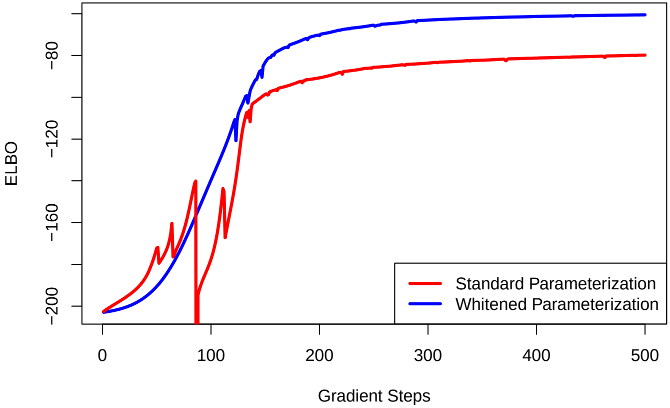

Whitening significantly improves convergence!

Run the cells of the notebook to fit a sparse GP using the VFE approximation with whitening!

Natural Gradient Ascent

Gradient ascent moves in the direction of the gradient $\nabla_{\xi}\mathcal{L}(\xi)$.

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Formally:

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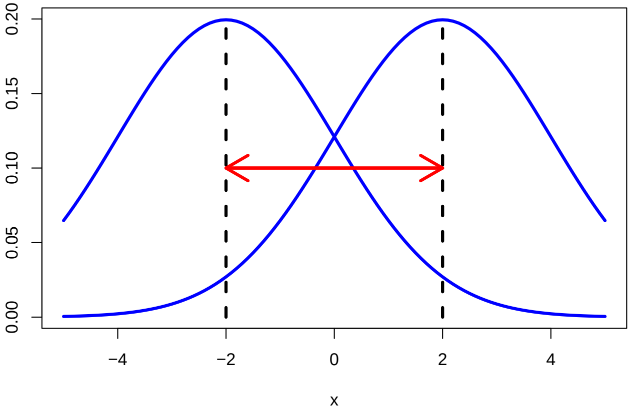
If $\boldsymbol{\xi}$ represents the parameters of probability distributions, the Euclidean norm may be problematic!

Illustration with Two Gaussians



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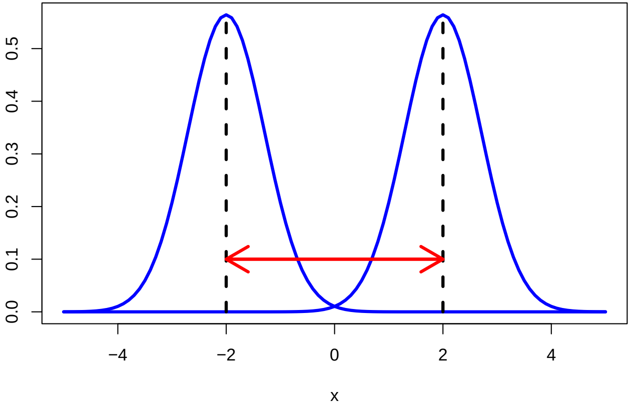

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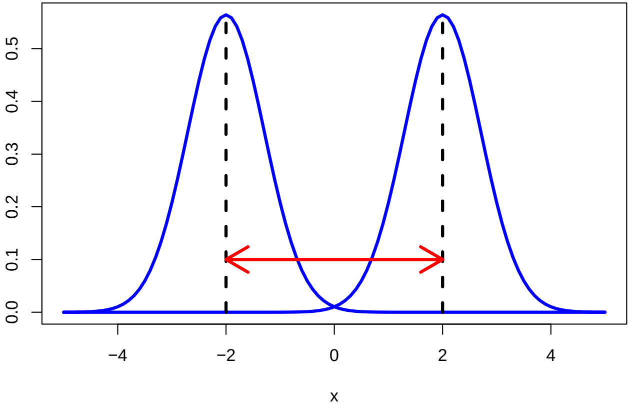
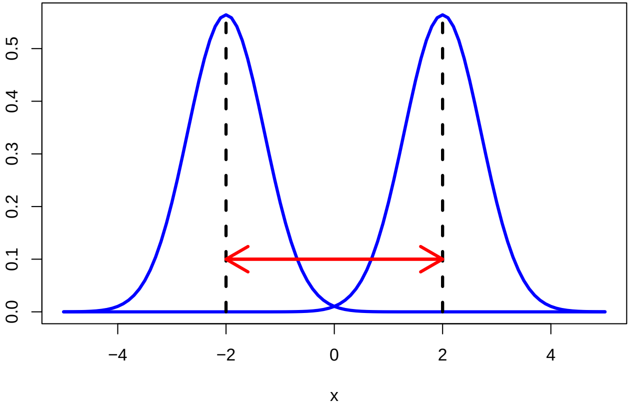


The Euclidean distance between parameters is 4 in both cases!

Illustration with Two Gaussians



A better alternative is the KL-divergence between distributions!

Natural Gradient Ascent

Considers the KL-divergence as a norm:

$$\nabla_{\boldsymbol{\xi}} \mathcal{L}(\boldsymbol{\xi}) \mathbf{F}_{\boldsymbol{\xi}}^{-1} \propto \lim_{\epsilon \to 0} \frac{1}{\epsilon} \underset{\mathbf{d} \, s.t. \mathrm{KL}[q(\mathbf{u}|\boldsymbol{\xi}) | q(\mathbf{u}|\boldsymbol{\xi}+\mathbf{d})] \leq \epsilon}{\arg\max} \mathcal{L}(\boldsymbol{\xi} + \mathbf{d})$$

with $\mathbf{F}_{\boldsymbol{\xi}}$ the Fisher information of q:

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Let $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$ be the natural and expectation parameters of q, respectively:

$$\mathbf{F}_{\boldsymbol{\eta}} = \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\eta}}, \qquad \mathbf{F}_{\boldsymbol{\xi}} = \left(\frac{\partial \boldsymbol{\eta}}{\partial \boldsymbol{\xi}}\right)^{\mathsf{T}} \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\eta}} \frac{\partial \boldsymbol{\eta}}{\partial \boldsymbol{\xi}} = \left(\frac{\partial \boldsymbol{\eta}}{\partial \boldsymbol{\xi}}\right)^{\mathsf{T}} \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\xi}}.$$

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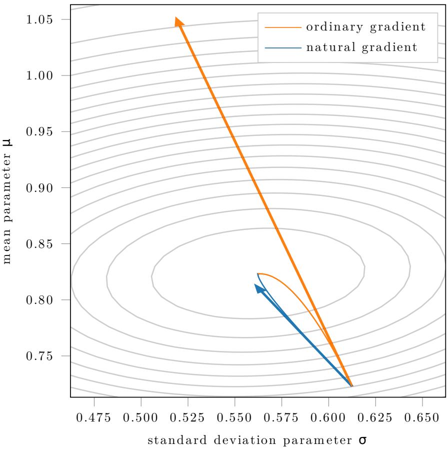
Thus,

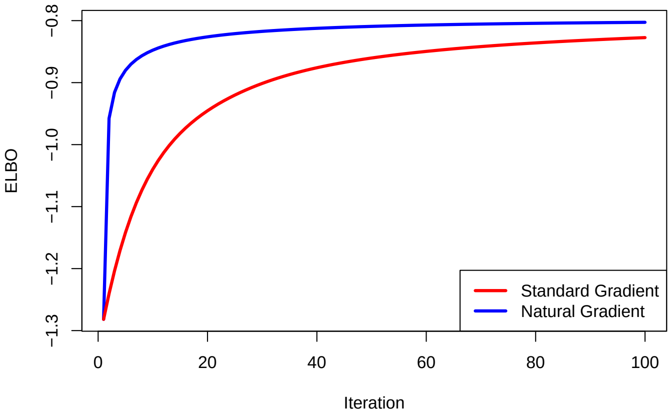
$$\nabla_{\boldsymbol{\xi}} \mathcal{L}(\boldsymbol{\xi}) \mathbf{F}_{\boldsymbol{\xi}}^{-1} = \nabla_{\boldsymbol{\xi}} \mathcal{L}(\boldsymbol{\xi}) \frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{\theta}} \left(\frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{\eta}}\right)^{\mathsf{T}} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} \left(\frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{\eta}}\right)^{\mathsf{T}}.$$

Natural Gradient Ascent



(Salimbeni et al., 2018)

Natural Gradient: Illustrative Example



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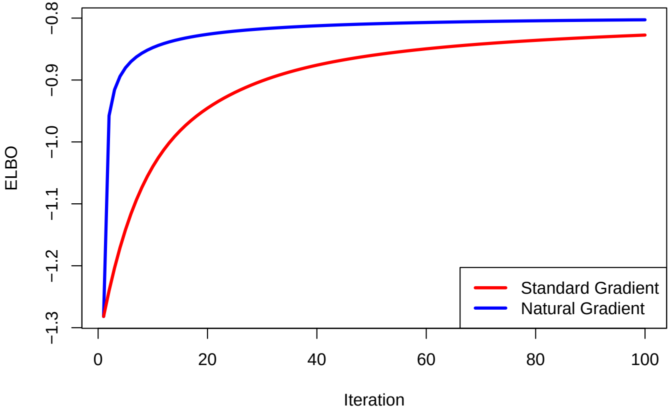

The natural gradient achieves a faster convergence!

Run the cells of the notebook to fit a sparse GP using the VFE approximation with natural gradients!

GPs for Big Data

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

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Straight forward to do that in the VFE approach:

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&\approx \frac{N}{B} \sum_{i\in\mathcal{B}} \mathbb{E}_{q(f_i)}[\log p(y_i|f_i,\theta)] - \mathbf{KL}[q(\mathbf{u})|p(\mathbf{u})]
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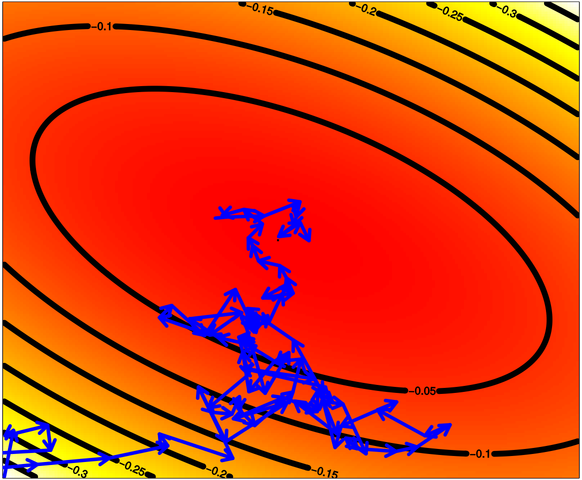
\end{aligned}
$$

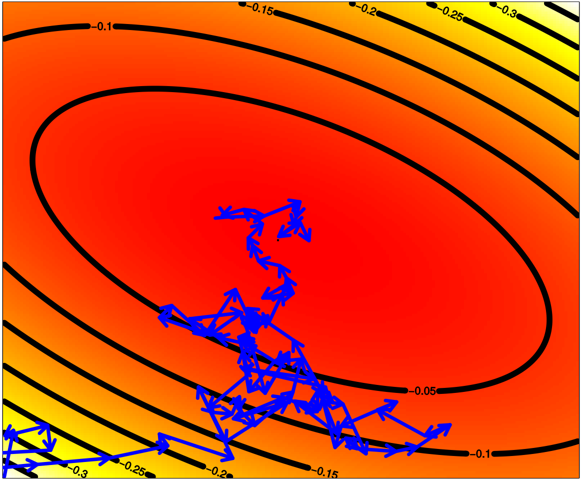
The training cost goes down to $\mathcal{O}(M^3)$ which allows to address datasets with millions of instances!

(Hensman et al., 2013)

GPs for Big Data

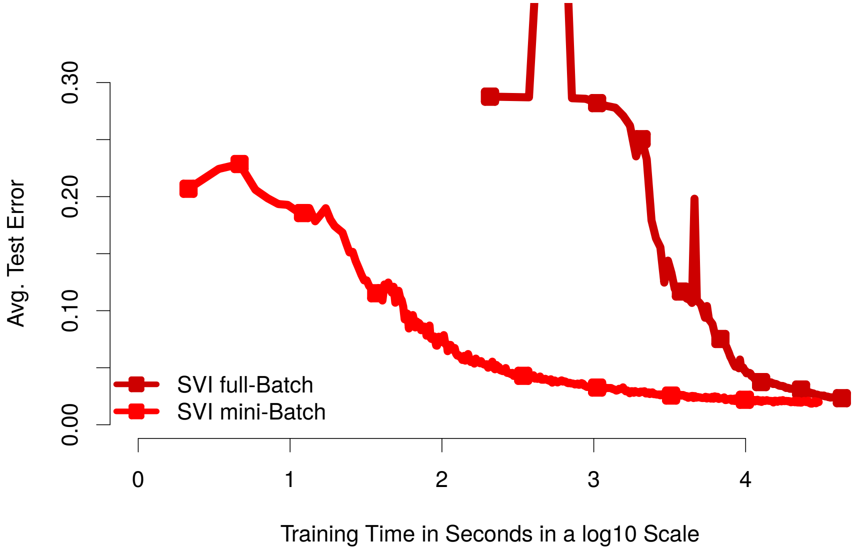


GPs for Big Data



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)

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- It allows for minibatch training which reduces the cost to $\mathcal{O}(M^3)$.

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- Reduces the cost to $\mathcal{O}(M^2 N)$ with $M \ll N$.
- The optimized inducing points spread over the input space where the latent function changes.
- Guaranteed to be exact if $M = N$ and the inducing points are not optimized and located at the training points.
- It does not change the model. It relies on a particular posterior approximation that speeds-up the computations.
- It allows for minibatch training which reduces the cost to $\mathcal{O}(M^3)$.
- The objective is prone to local optima and difficult to optimize.

Run the cells of the notebook to fit a sparse GP using the VFE approximation with mini-batches!

Run the cells of the notebook to fit a sparse GP using the VFE approximation for classification and carry out task 7!

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- The best performing method seems to be the VFE method since it does not modify the prior.
- Some methods allow for stochastic optimization and mini-batch training that further reduce the cost to $\mathcal{O}(M^3)$.

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