Part II: Sparse Gaussian Processes

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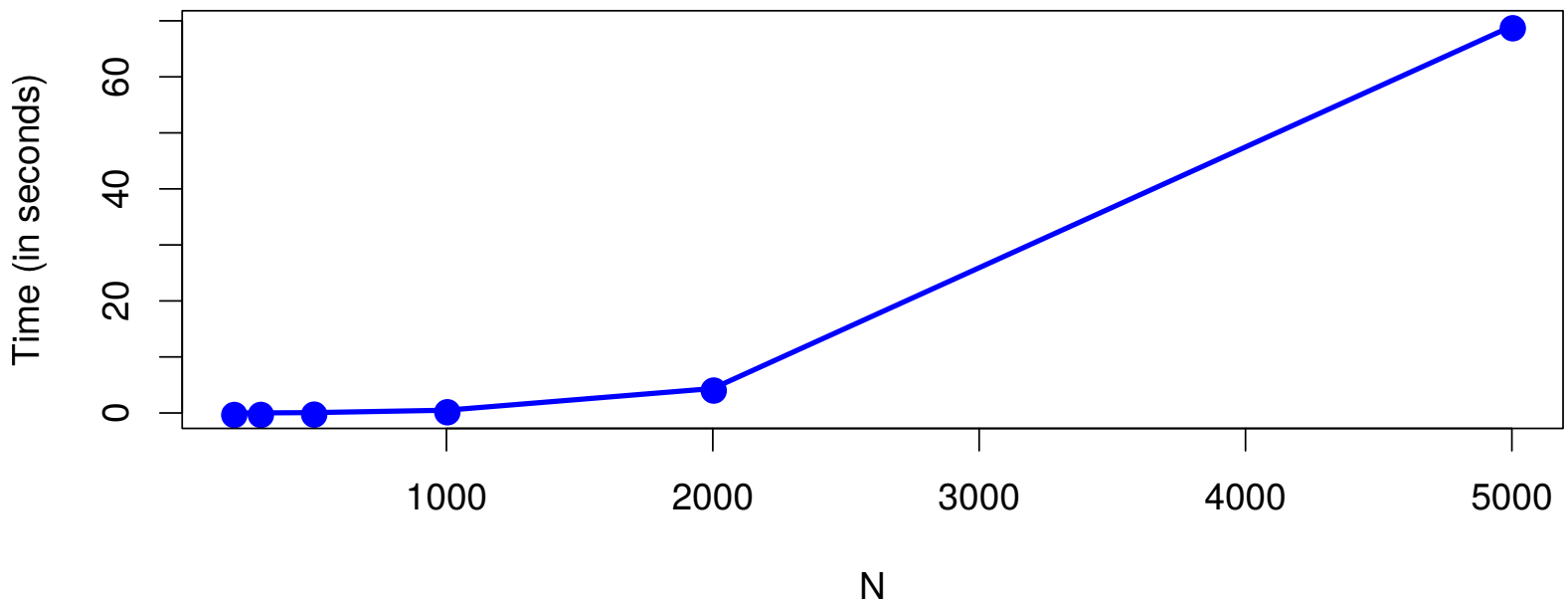

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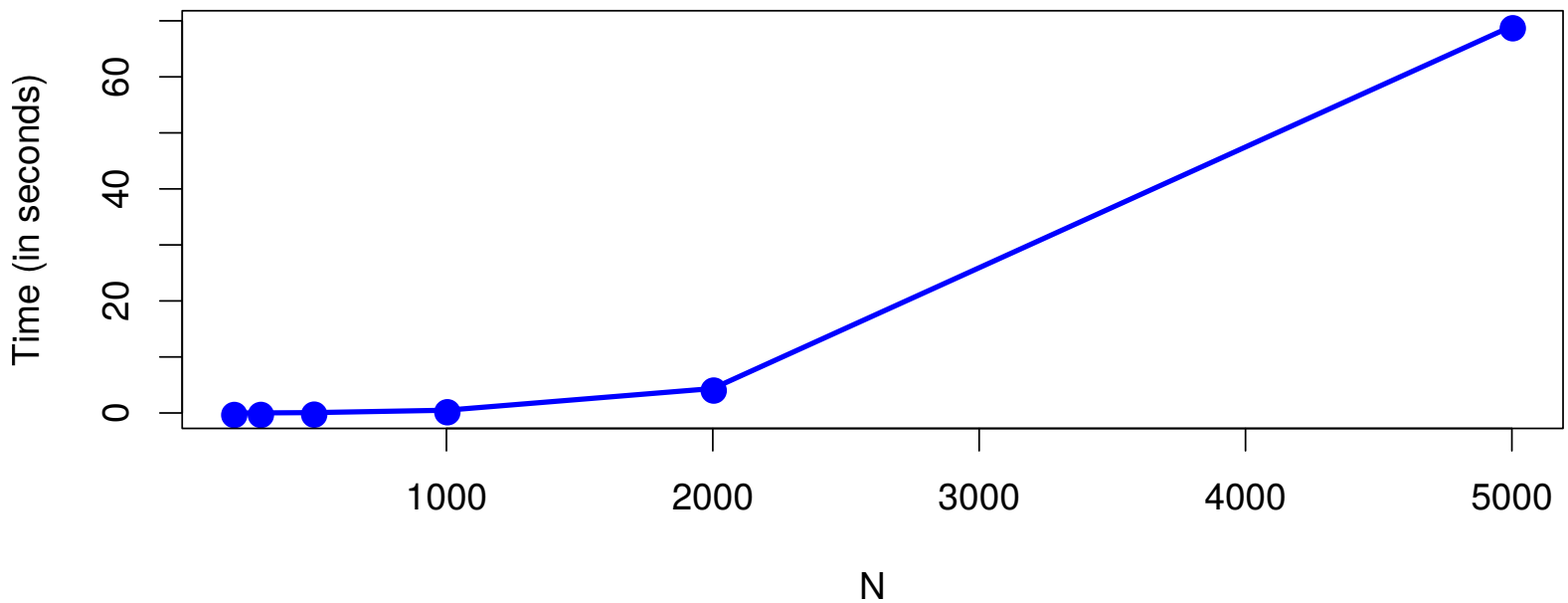

We can handle just a few thousand data instances at most!

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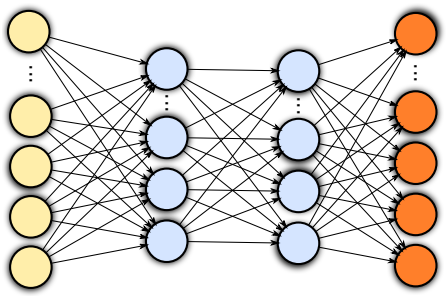

Neural Network
(parametric model)

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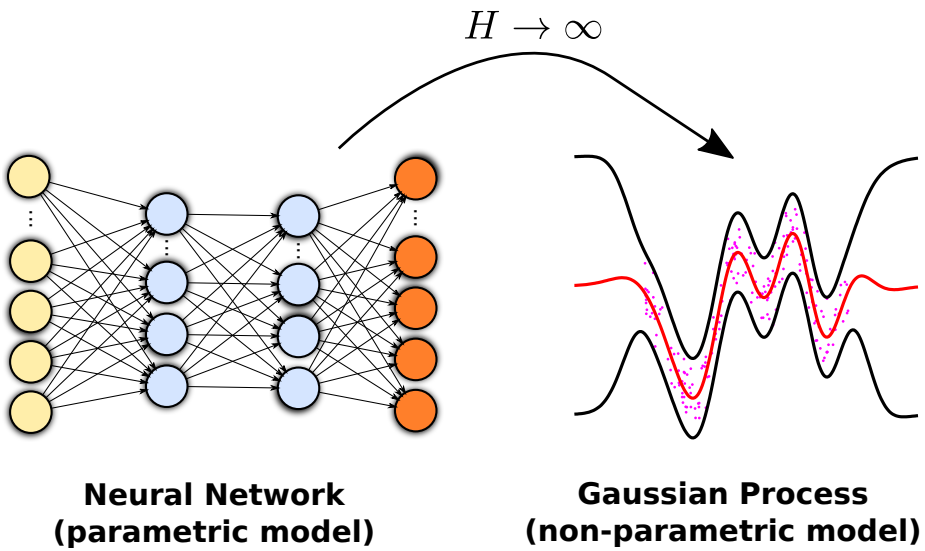

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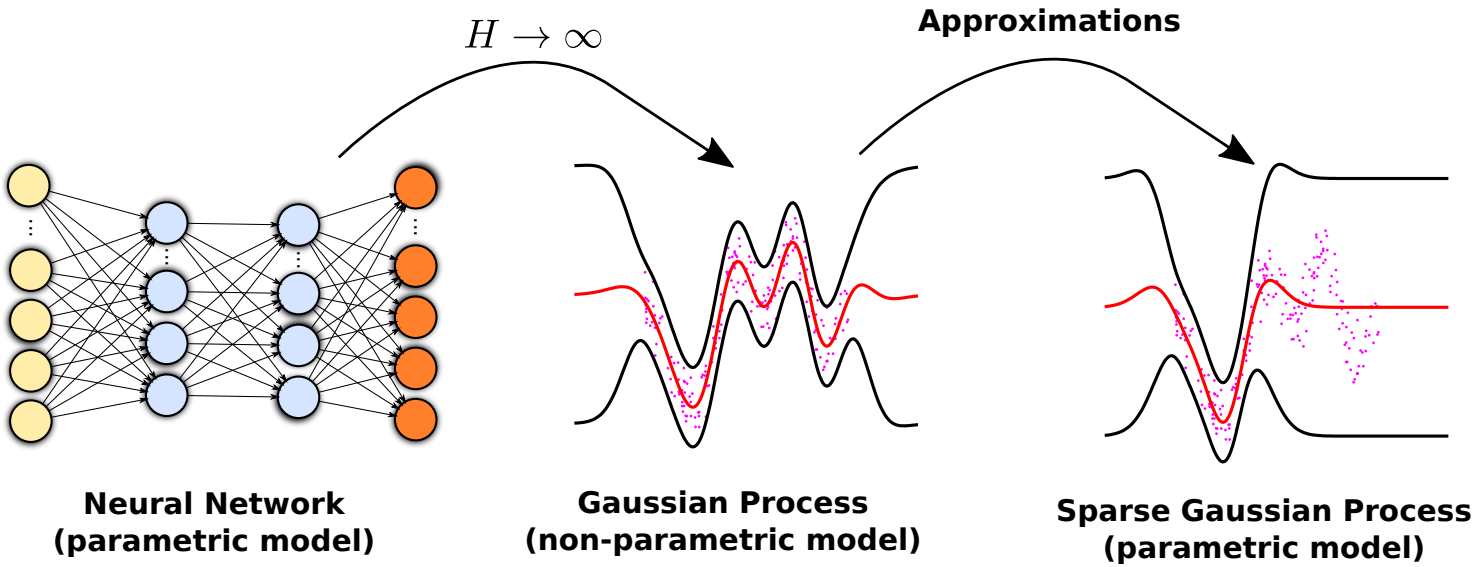

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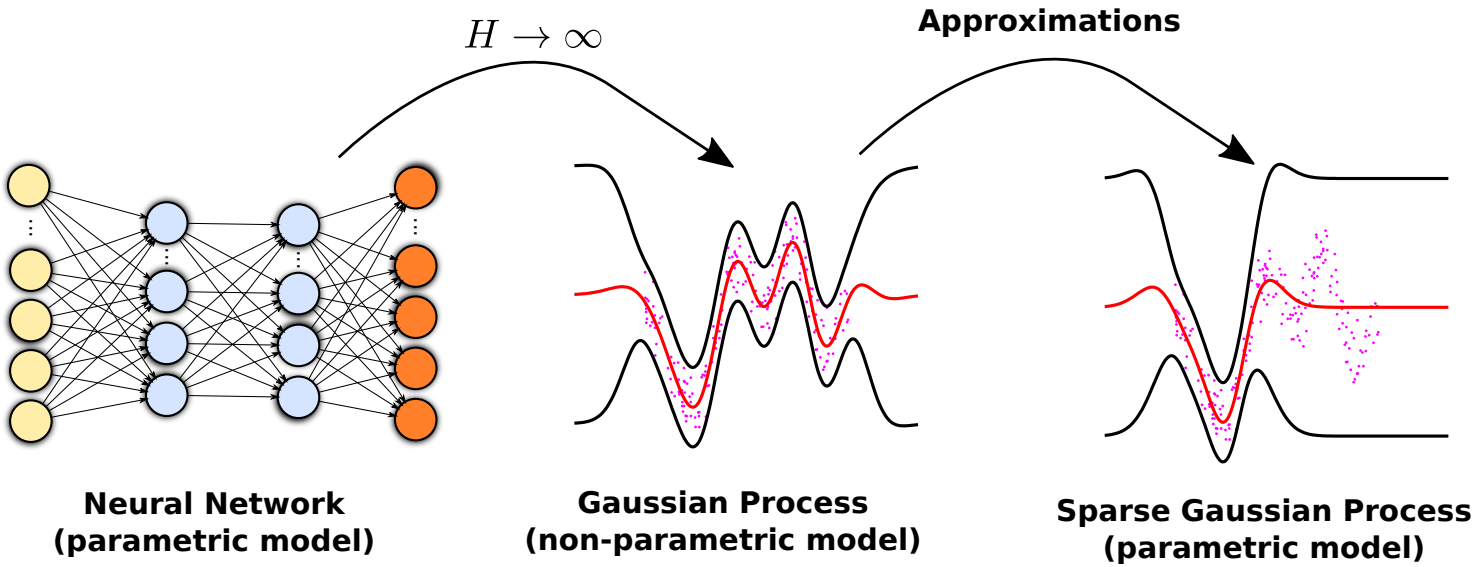

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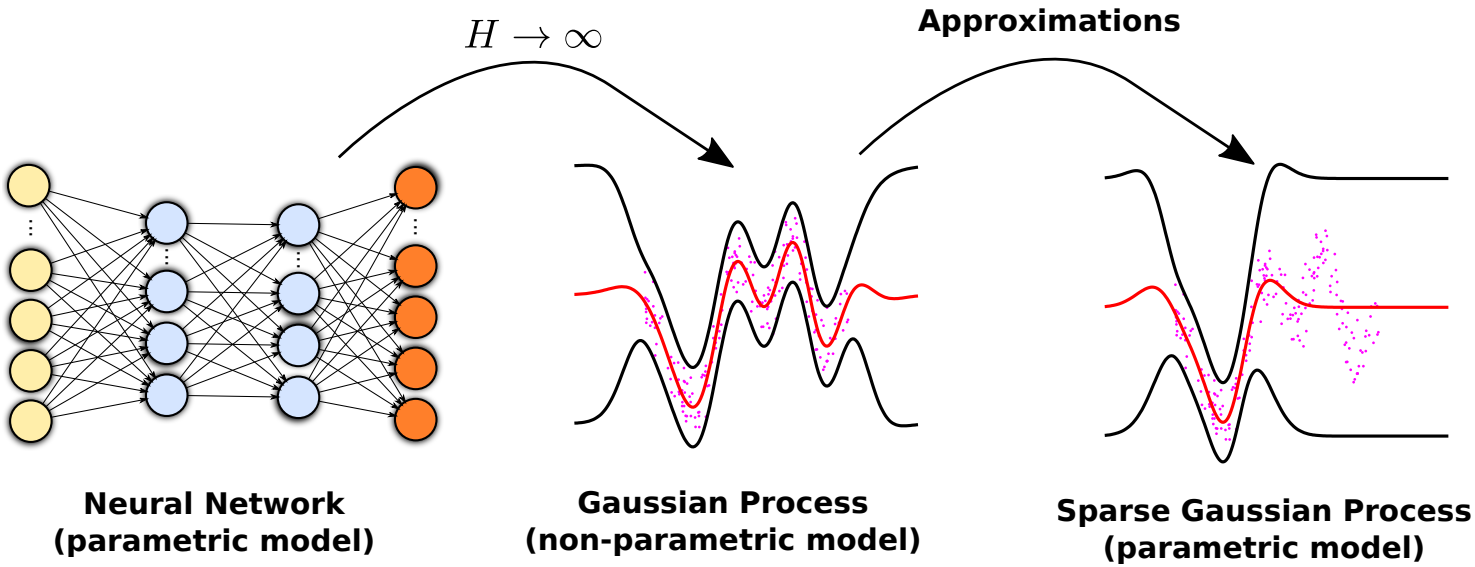

- **Nyström, Random Features and FITC**: approximate GP prior!
- **VFE**: does approximate inference with a simplified distribution q.

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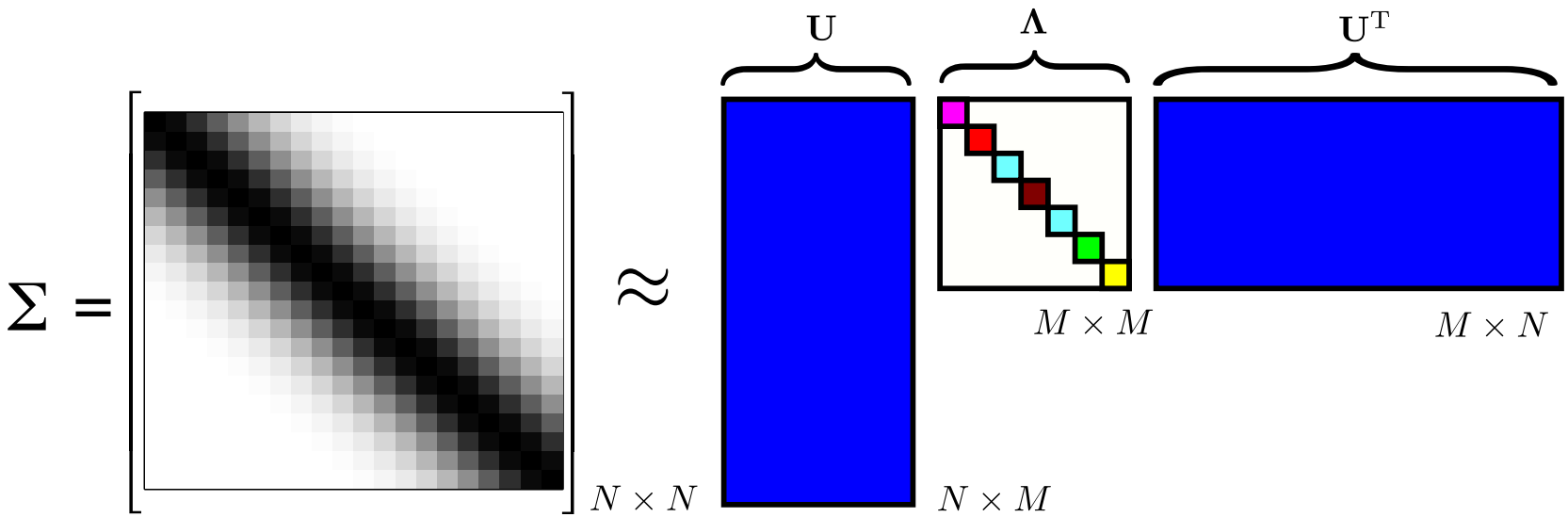

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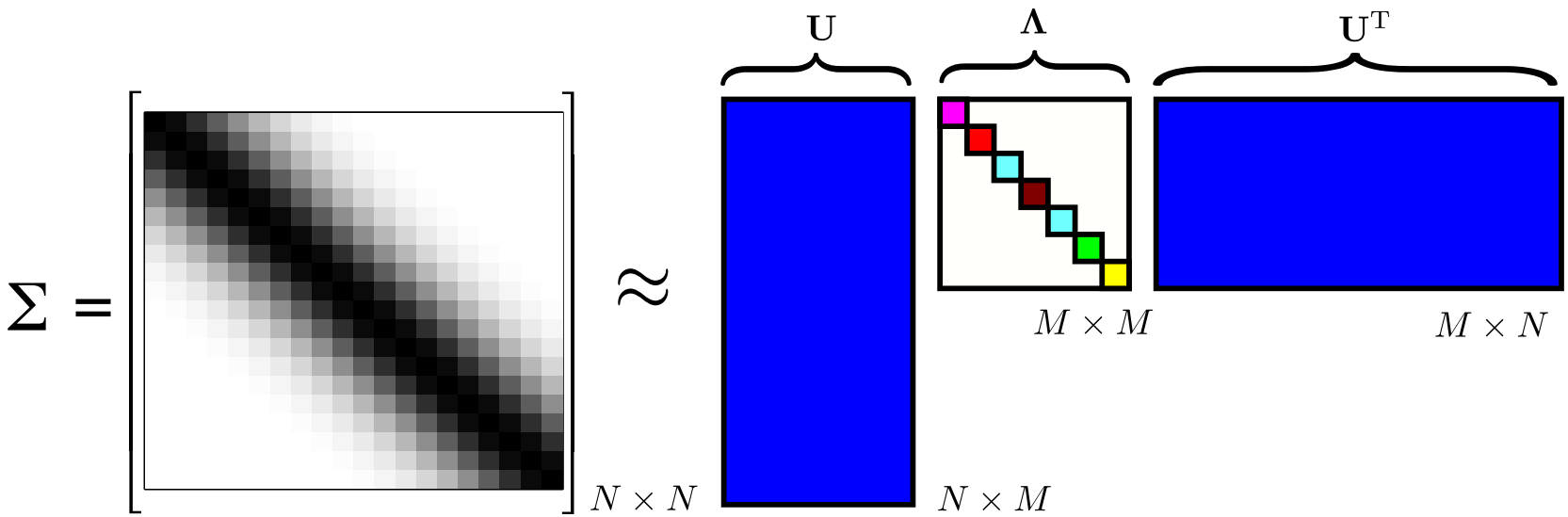

The Woodbury formula gives $(\mathbf{I}\sigma^2 + \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\mathsf{T})^{-1}$ with cost $\mathcal{O}(M^2N)$!

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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$$(\mathbf{I}\sigma^2 + \mathbf{U\Lambda U}^\mathsf{T})^{-1} = \mathbf{I}\sigma^{-2} - \sigma^{-2}\mathbf{U}\left(\mathbf{\Lambda}^{-1} + \mathbf{U}^\mathsf{T}\sigma^{-2}\mathbf{U}\right)^{-1}\mathbf{U}^\mathsf{T}\sigma^{-2}$$

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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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is an eigenfunction of $C(\cdot, \cdot)$ with eigenvalue λ, w.r.t., $p(\mathbf{x})$.

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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,

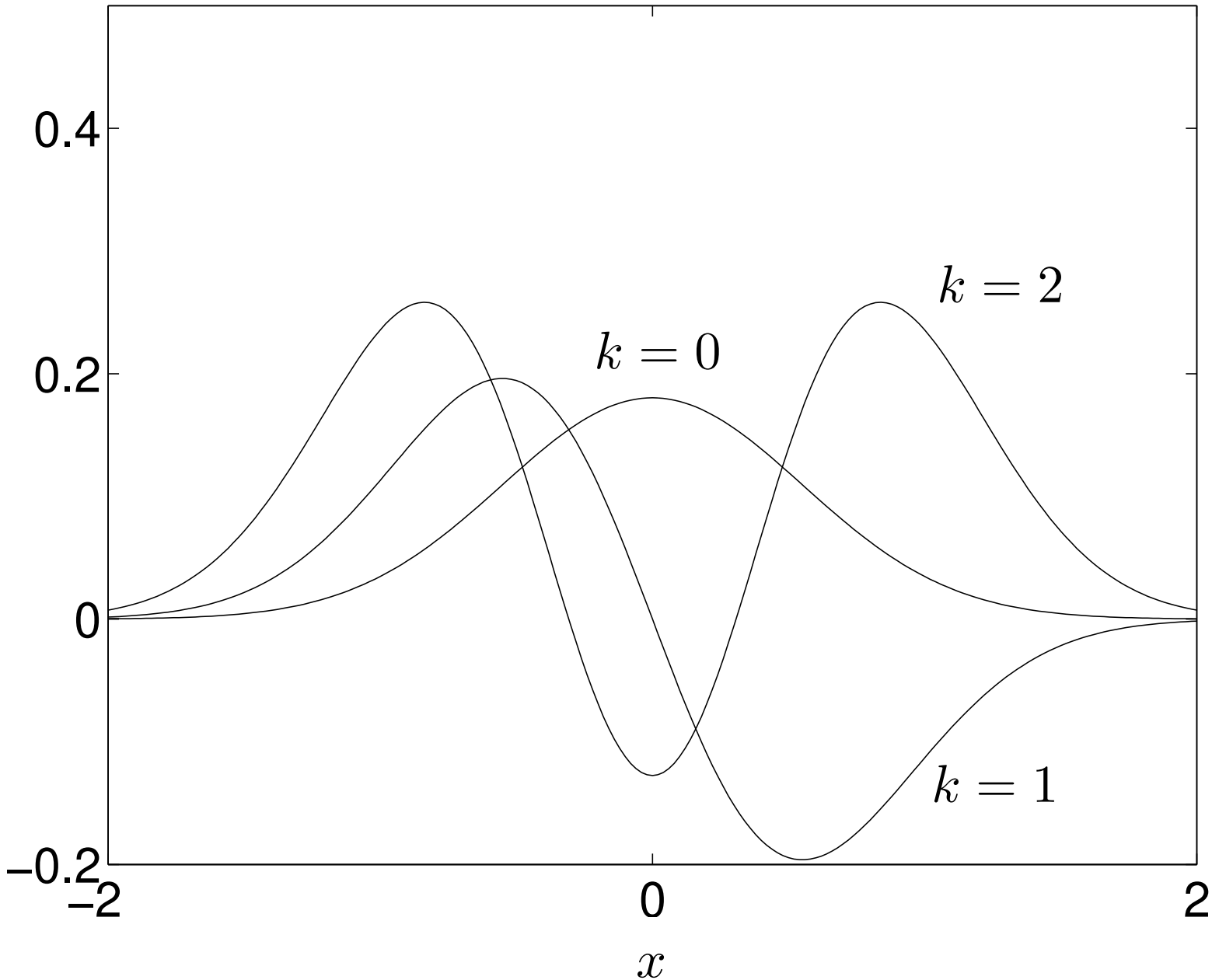
$$\lambda_k = \sqrt{\frac{2a}{A}}B^k\,, \qquad \phi_k(x) = \exp\left\{-(c - a)x^2\right\} H_k(\sqrt{2c}x)\,,$$

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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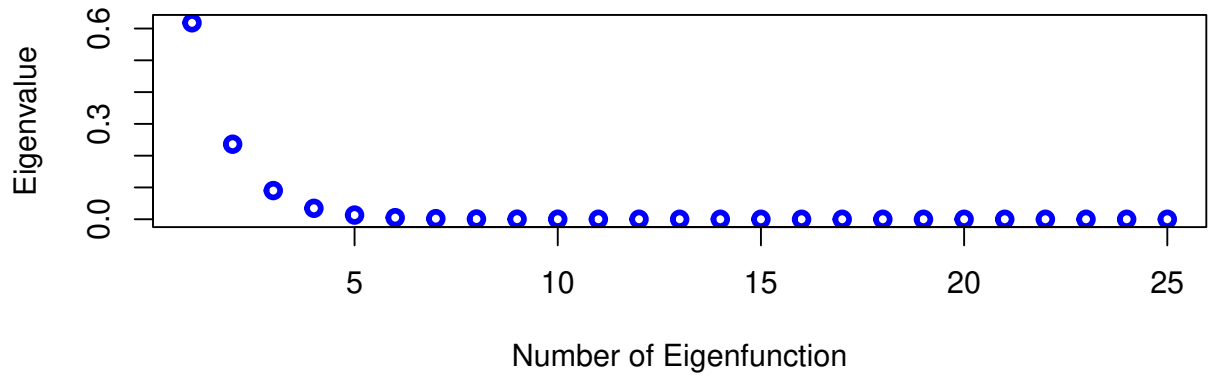

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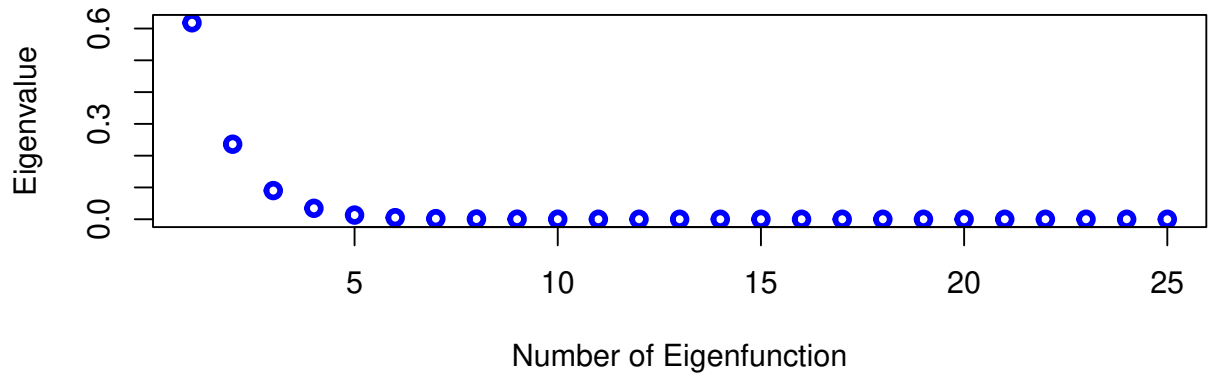
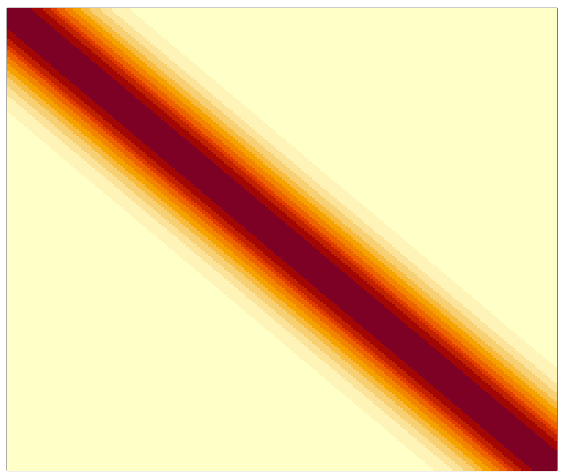
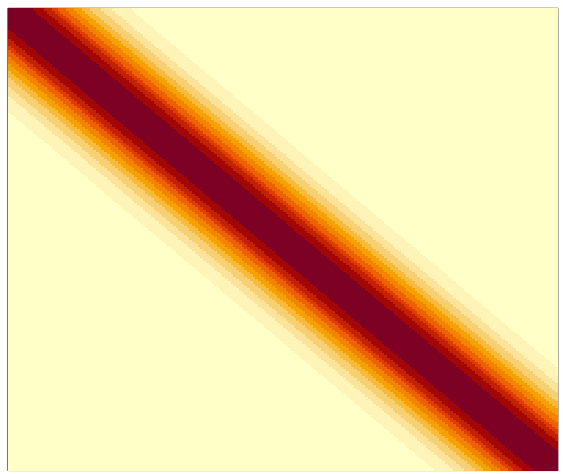


Exact Covariance Matrix



Approx. Covariance Matrix



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

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 $\lambda_i \approx \lambda_i^{\text{mat}}/N = \tilde{\lambda}_i$, which guarantees that $\boldsymbol{\Sigma} = \tilde{\boldsymbol{\Phi}} \tilde{\boldsymbol{\Lambda}} \tilde{\boldsymbol{\Phi}}^{\mathsf{T}}$.

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

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

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Using Mercer's theorem and the previous approximation, we approximate the covariance function as:

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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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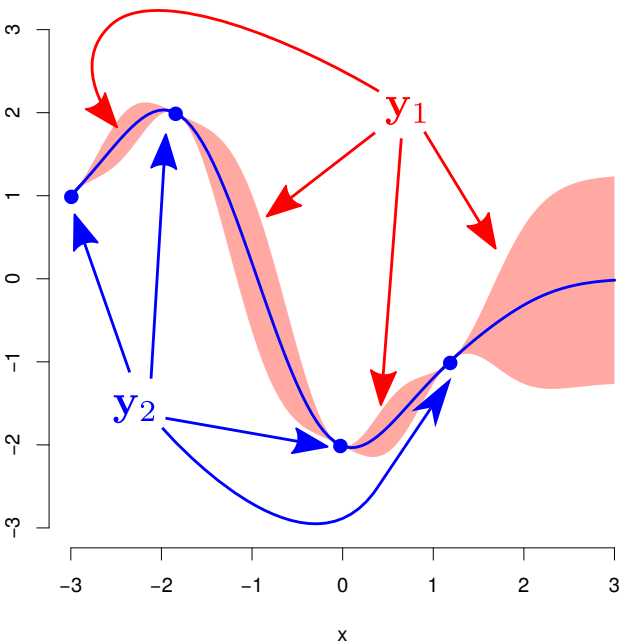

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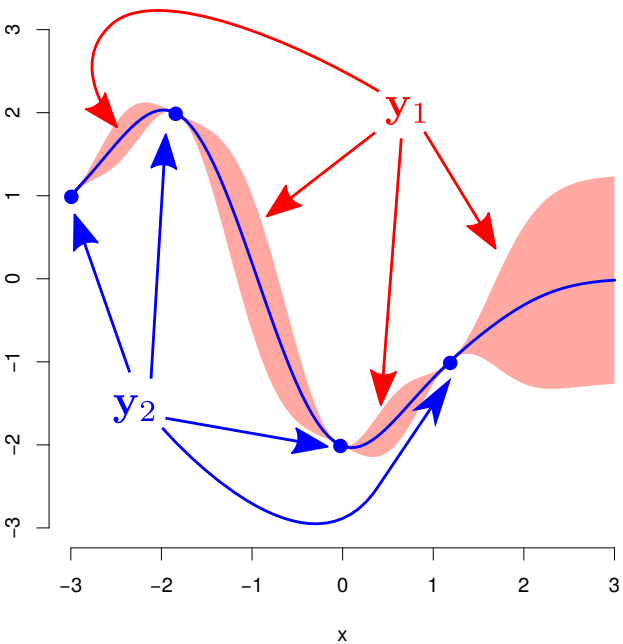

$$p(\mathbf{y}_1, \mathbf{y}_2) = \mathcal{N}\left(\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\mathsf{T} & \mathbf{B} \end{bmatrix}\right),$$

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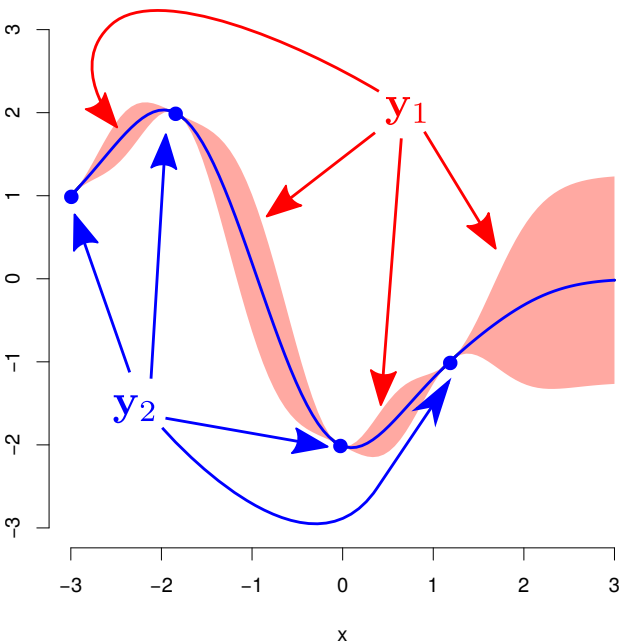

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$$p(\mathbf{y}_1|\mathbf{y}_2) = \mathcal{N}\left(\mathbf{y}_1 \middle| \mathbf{a} + \mathbf{C}\mathbf{B}^{-1}(\mathbf{y}_2 - \mathbf{b}), \mathbf{A} - \mathbf{C}\mathbf{B}^{-1}\mathbf{C}^\mathsf{T}\right)$$

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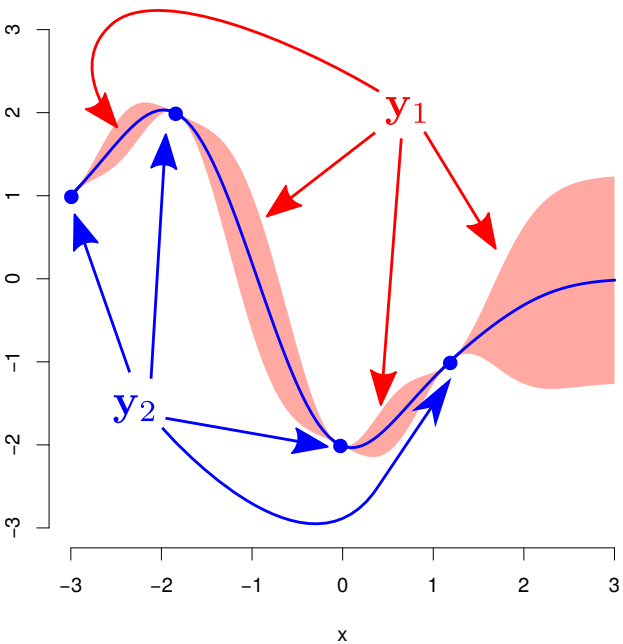

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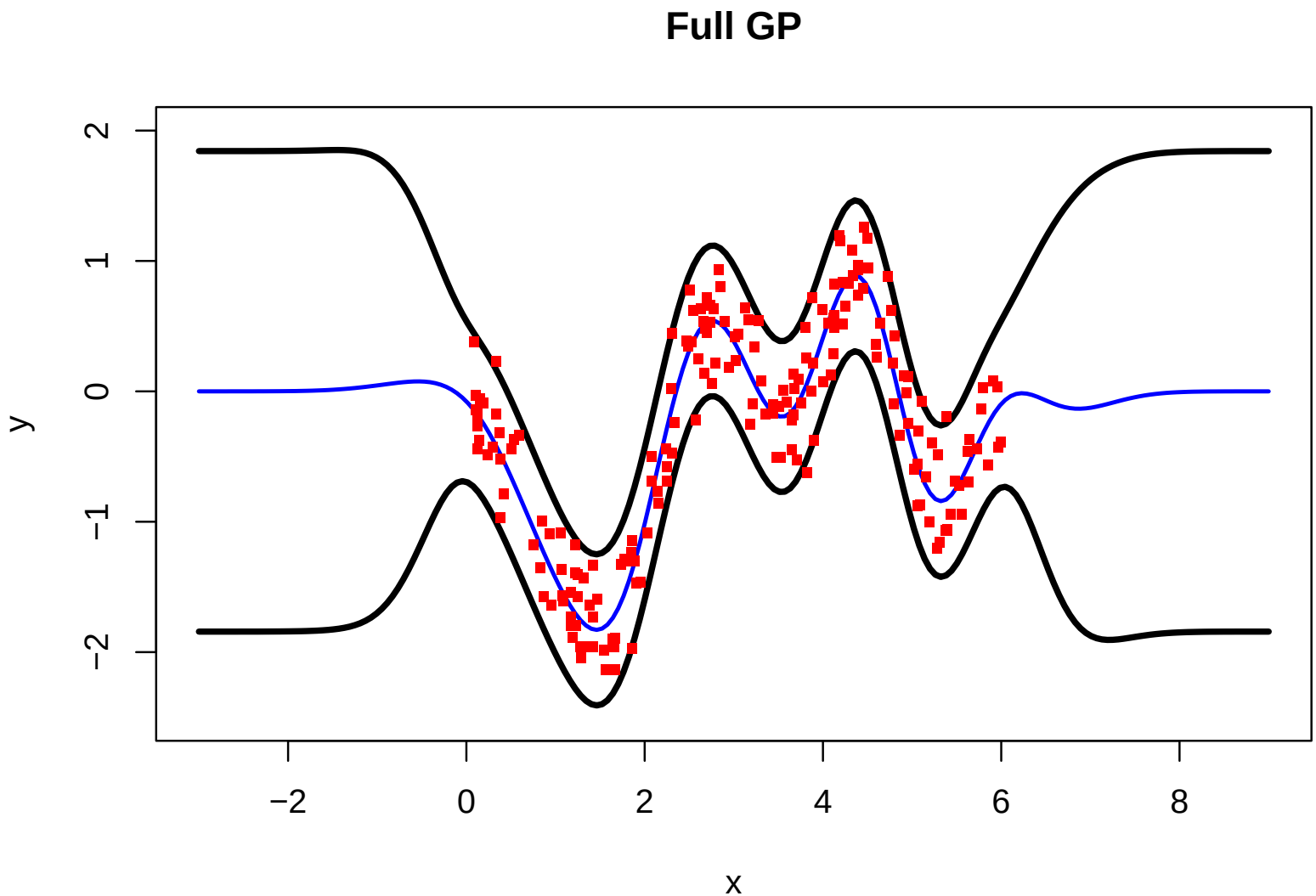
Nyström Approximation: Illustrative Example



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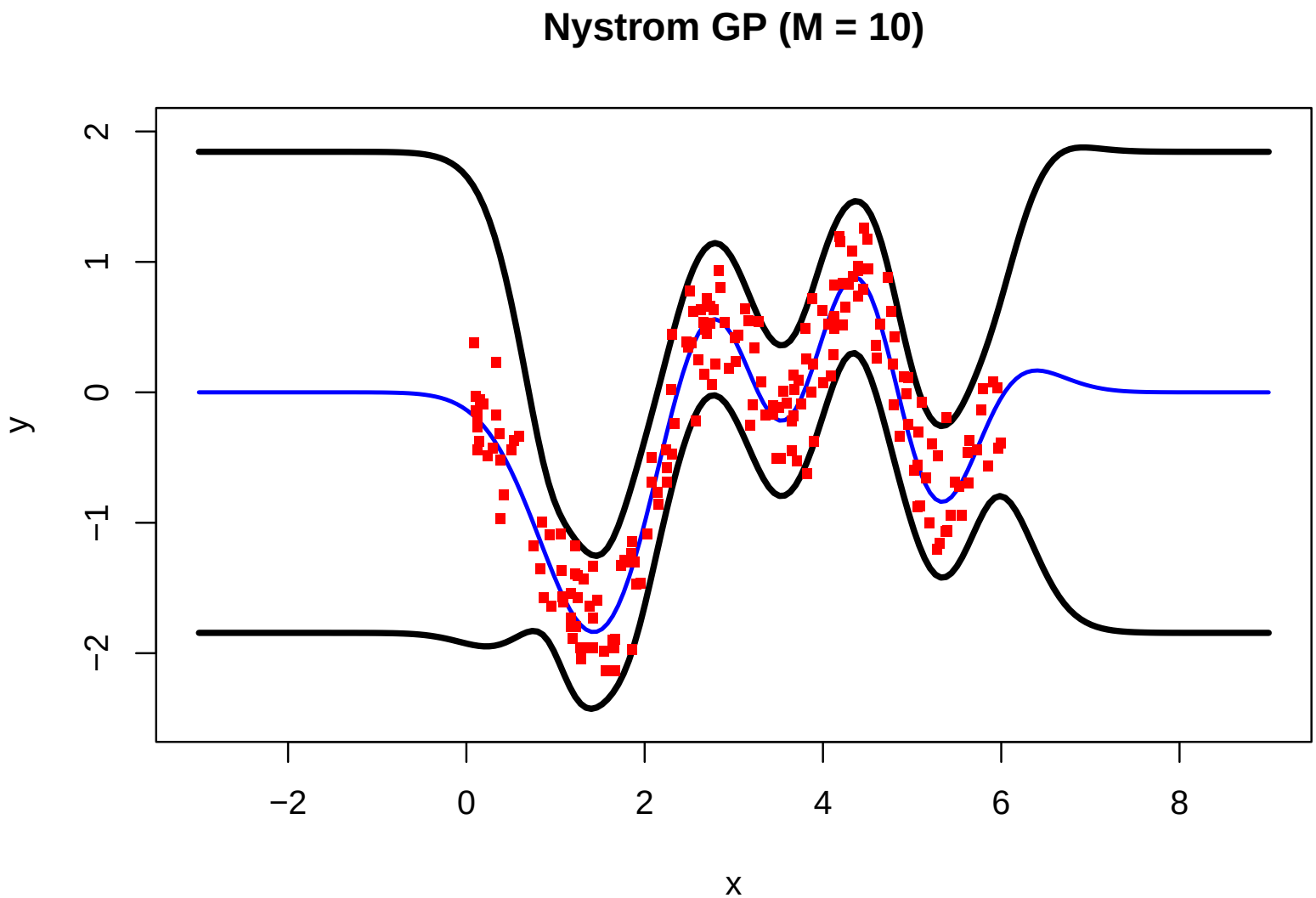

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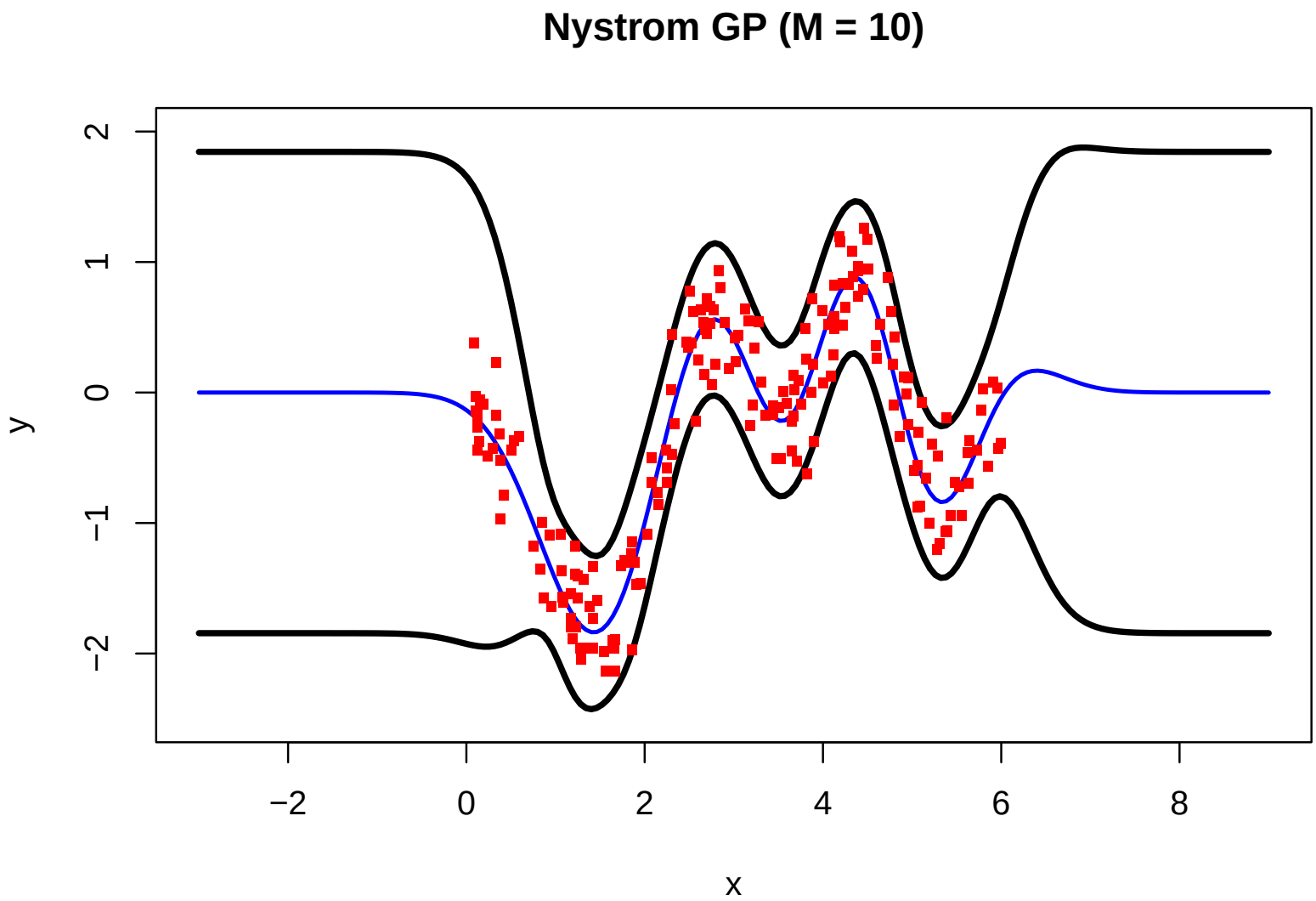

The approximation is similar to the full GP in some regions!

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- 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.

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

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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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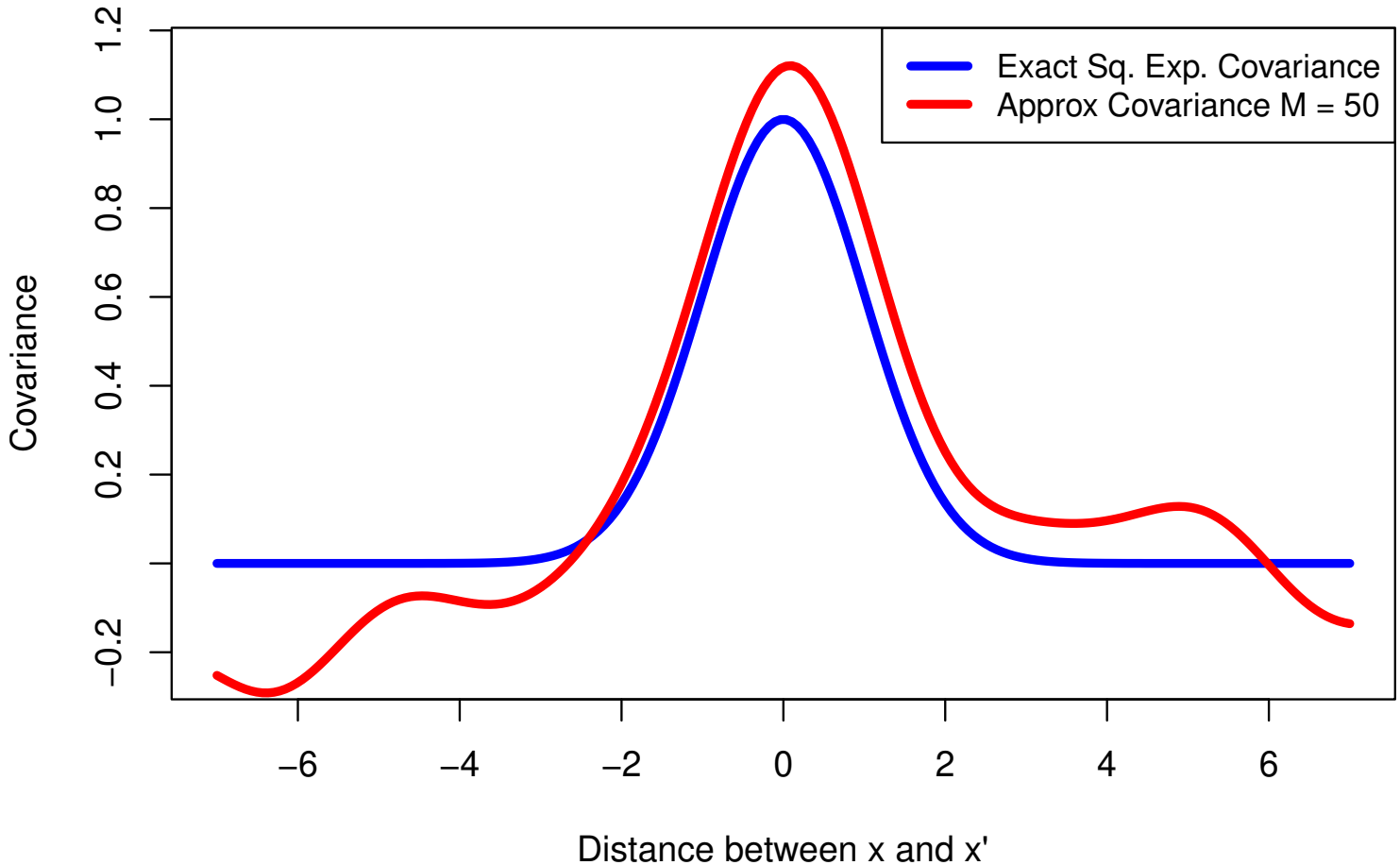

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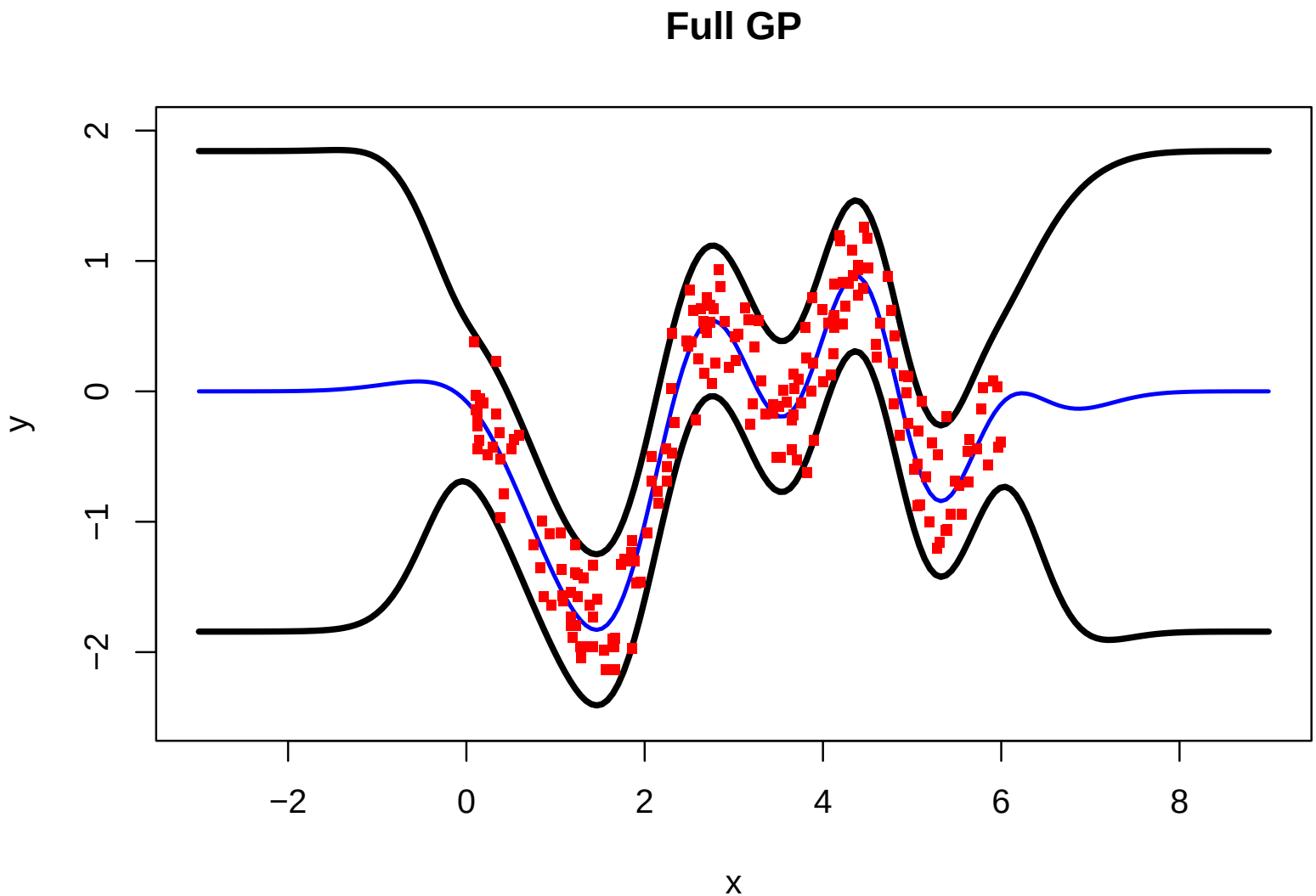
The computational cost is $\mathcal{O}(NM^2)$!

Random Features: Illustrative Example



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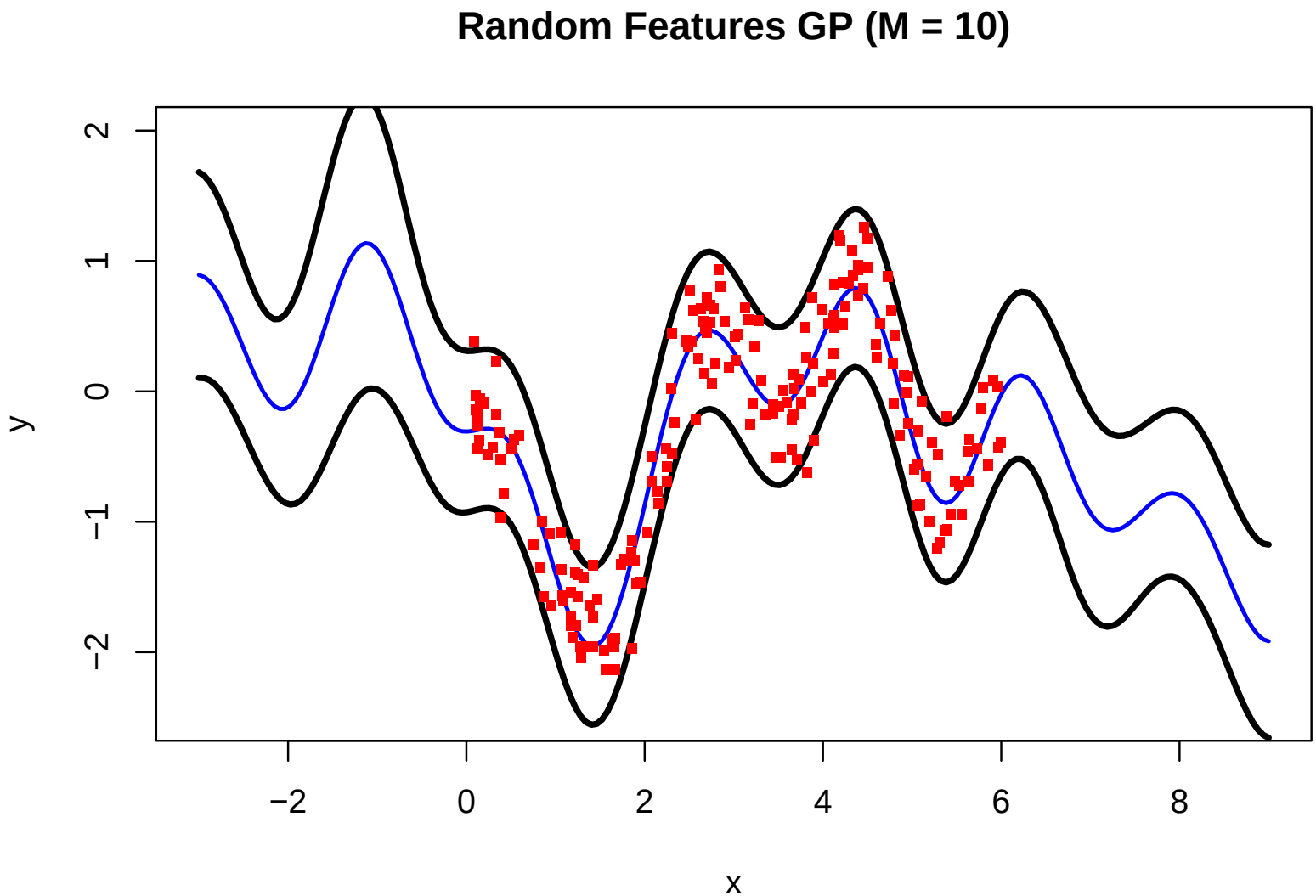

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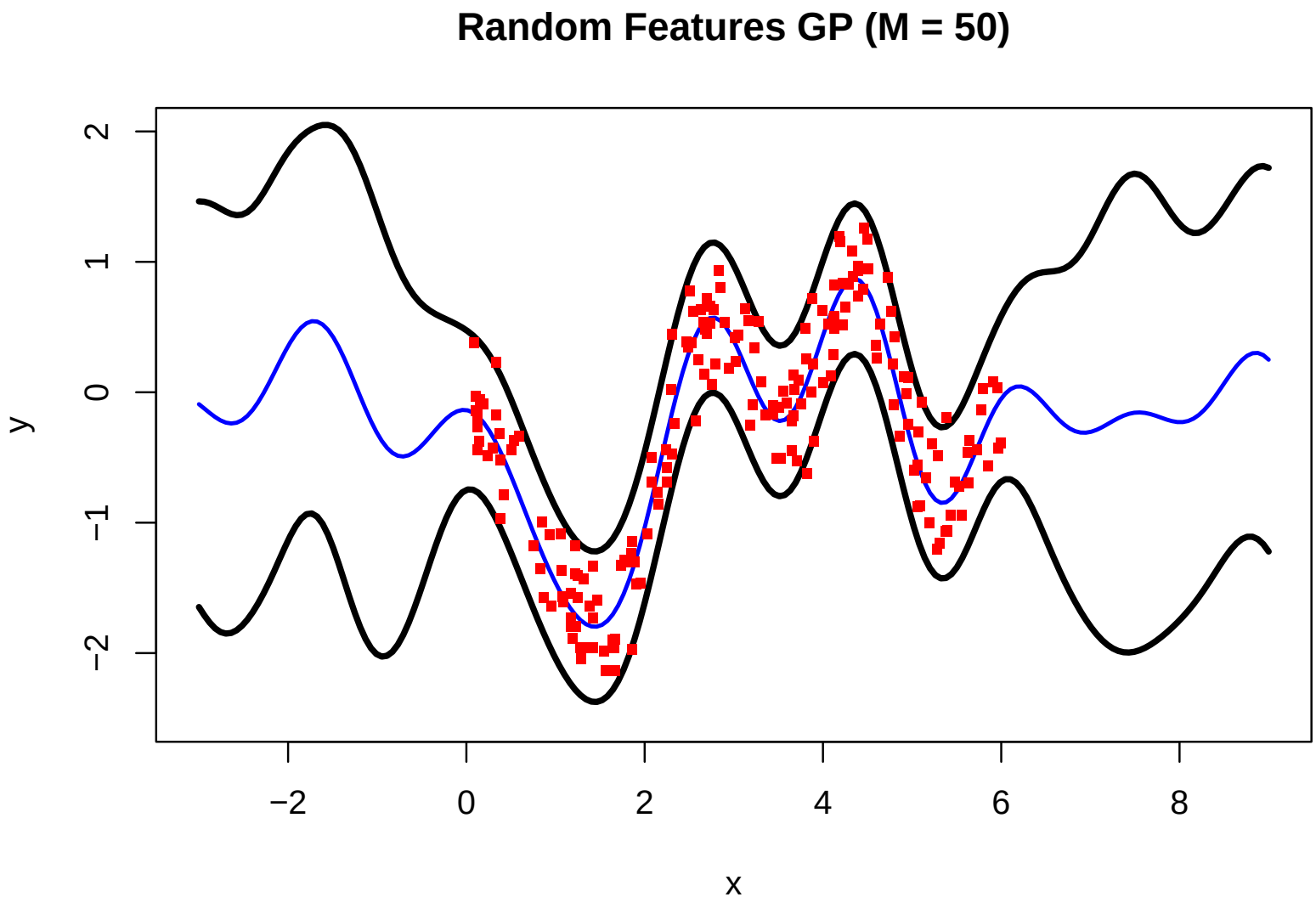

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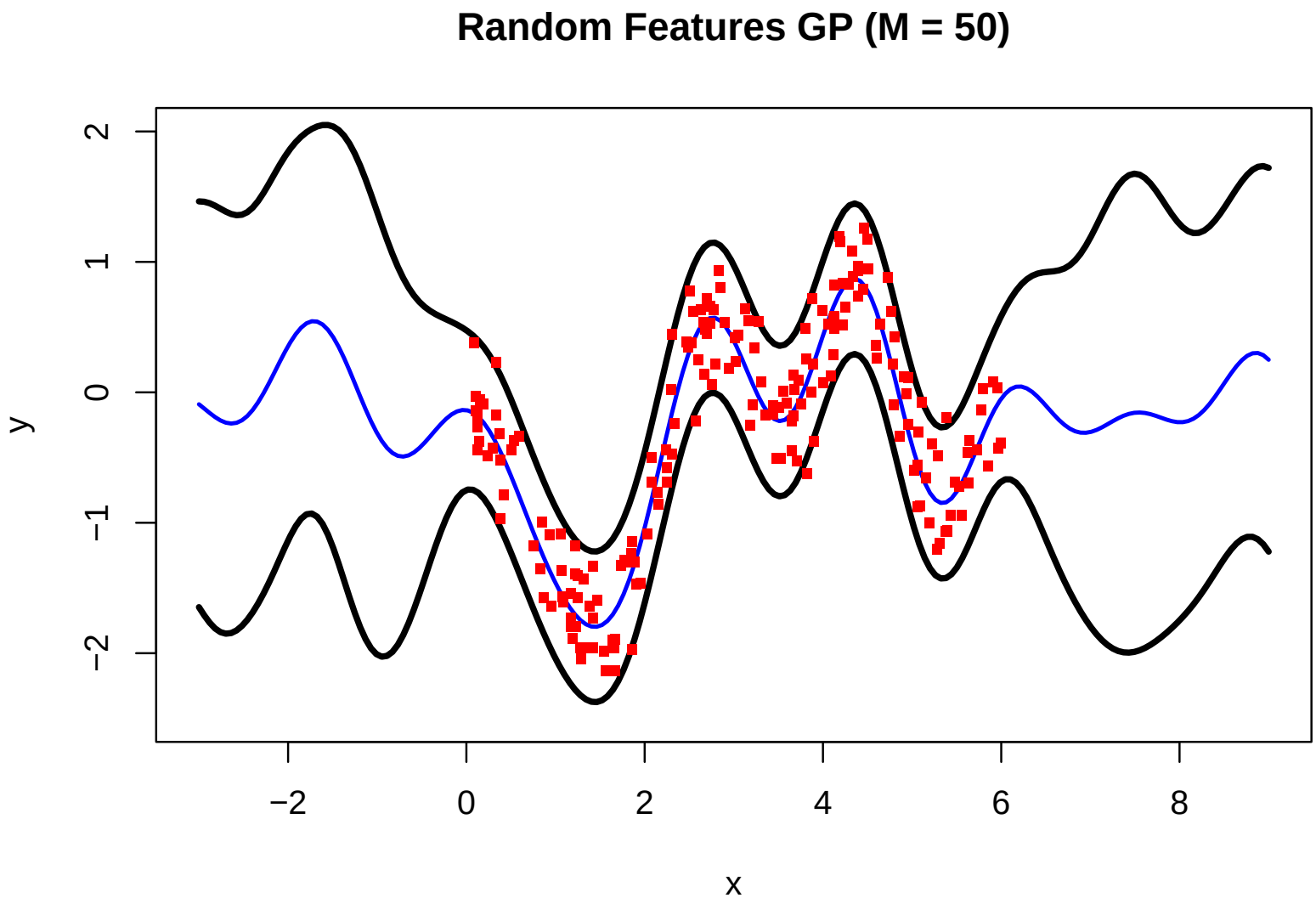

In regions with no data the approximation may be wiggling a lot!

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

Full Independent Training Conditional (FITC)

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

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

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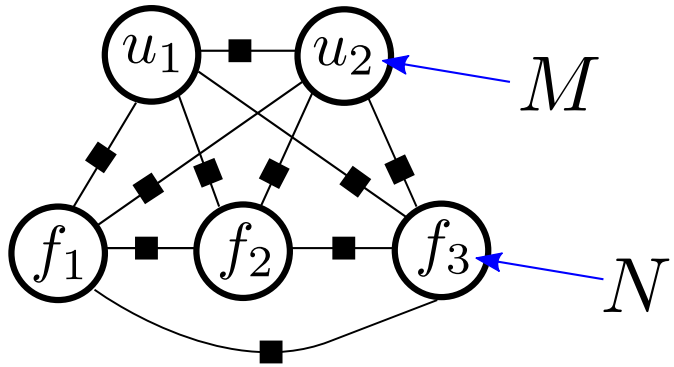

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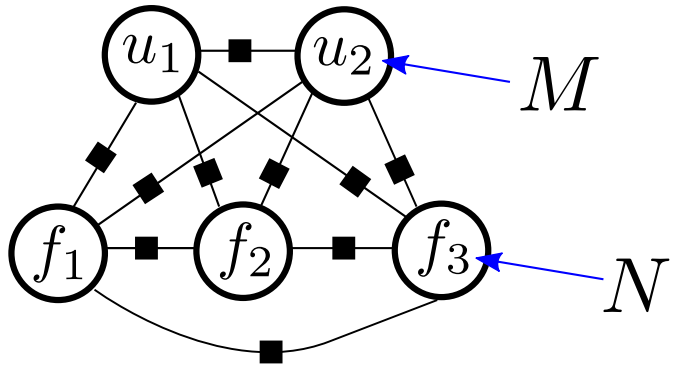

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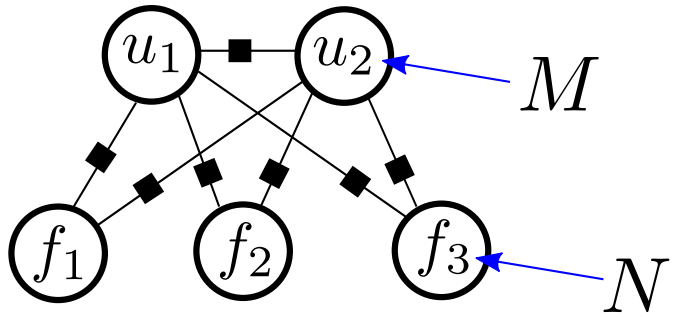

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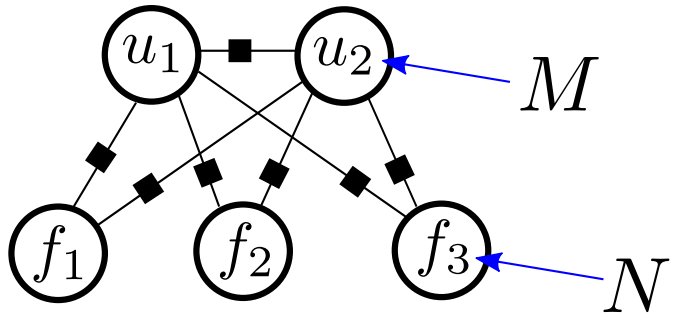

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where $\tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}} = \mathbf{D} + \mathbf{Q}_{\mathbf{ff}}$ with $\mathbf{D}$ diagonal and $\mathbf{Q}_{\mathbf{ff}} = \boldsymbol{\Sigma}_{\mathbf{fu}}\boldsymbol{\Sigma}_{\mathbf{uu}}^{-1}\boldsymbol{\Sigma}_{\mathbf{uf}}$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

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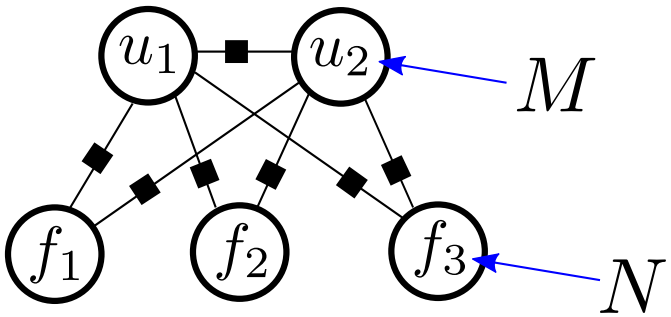

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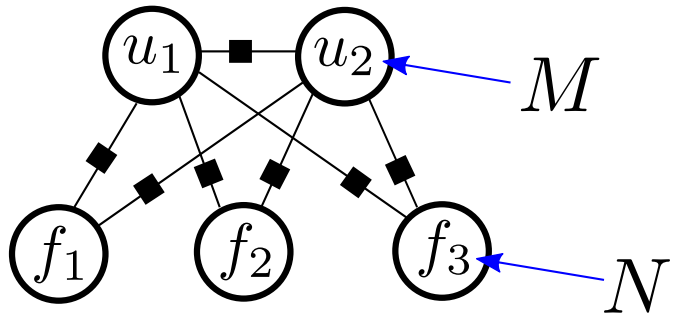

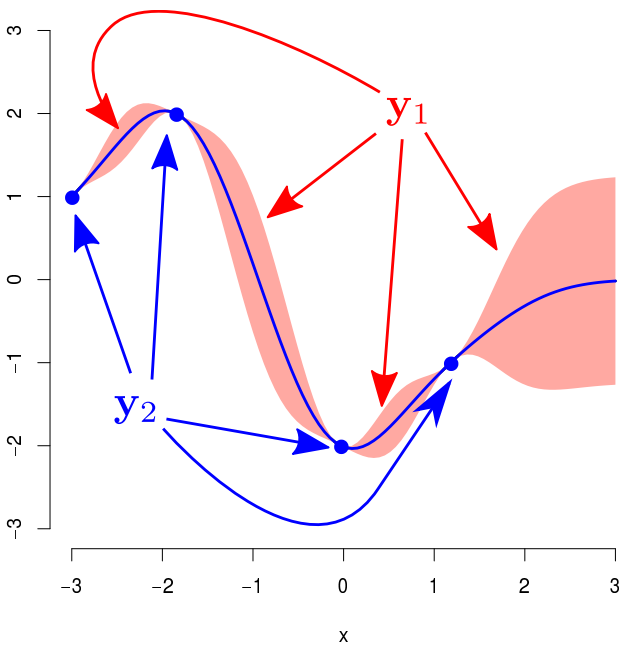

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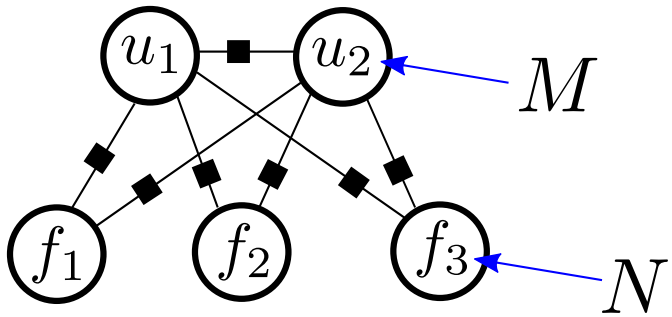

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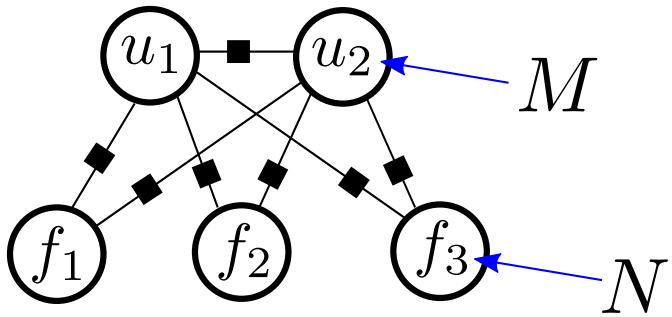

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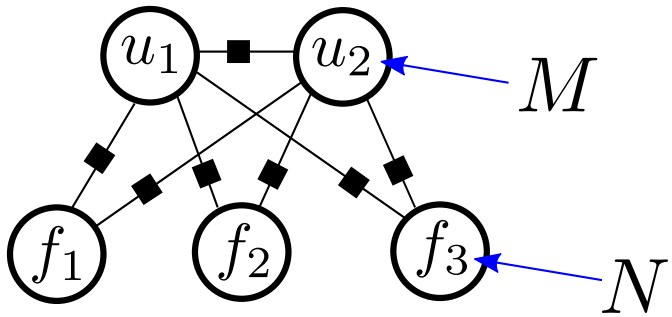

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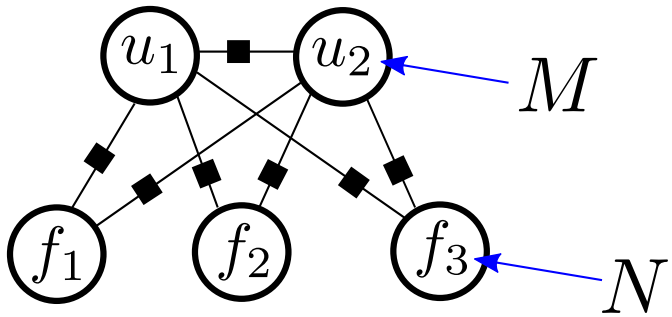

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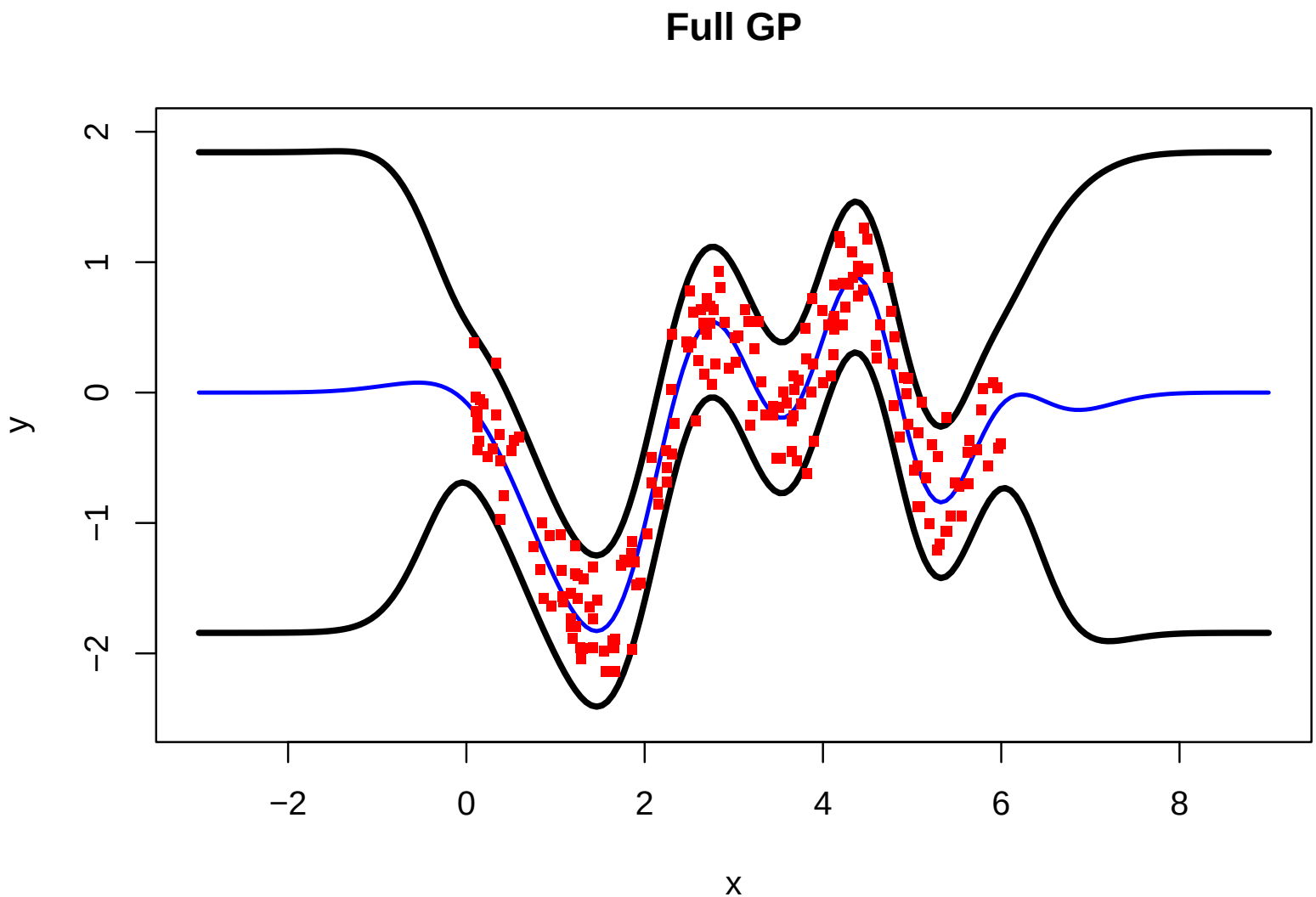
Simply treat them as prior parameters and maximize the approximate marginal likelihood $p(\mathbf{f}|\mathbf{0}, \tilde{\boldsymbol{\Sigma}}_{\mathbf{ff}})$!

FITC: Illustrative Example



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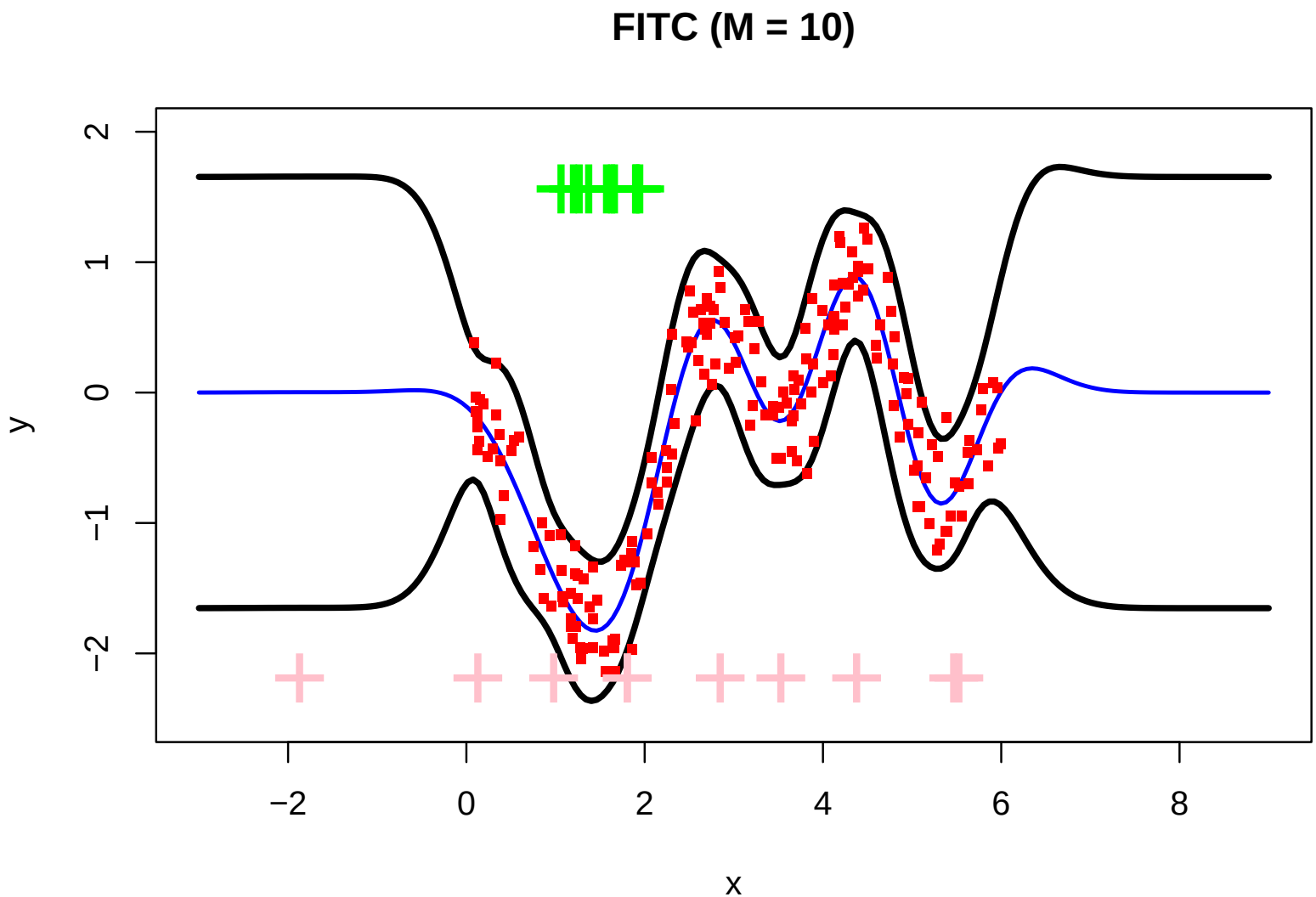

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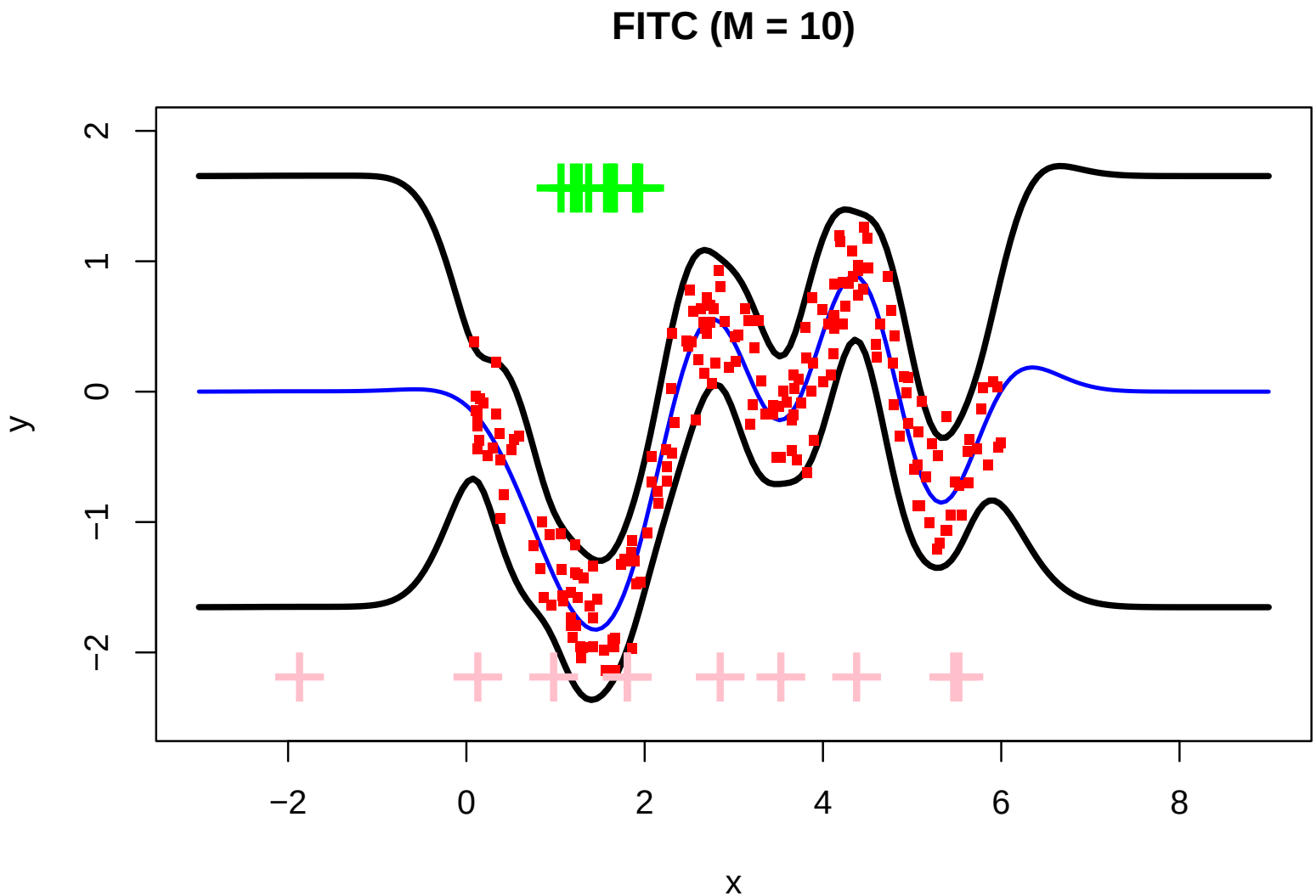

The inducing points cover the regions where the function changes!

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- It can be understood as considering heteroscedastic (input dependent) noise!

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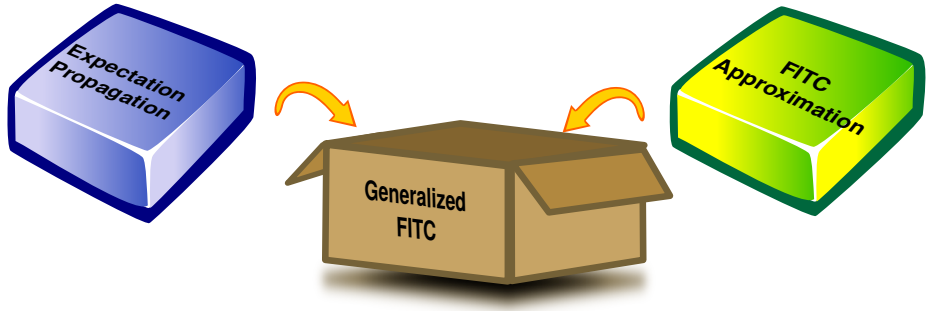

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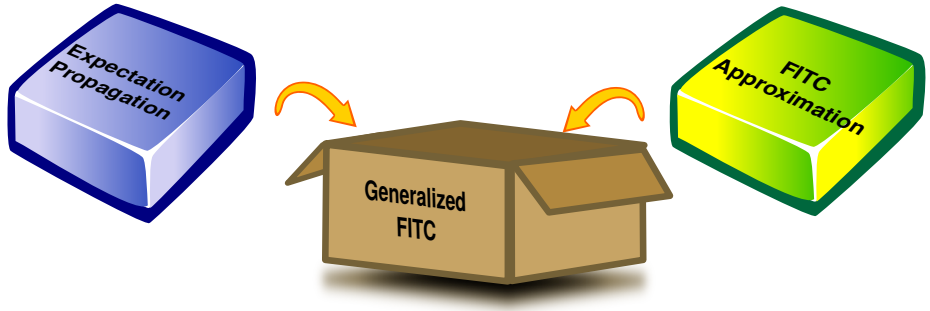

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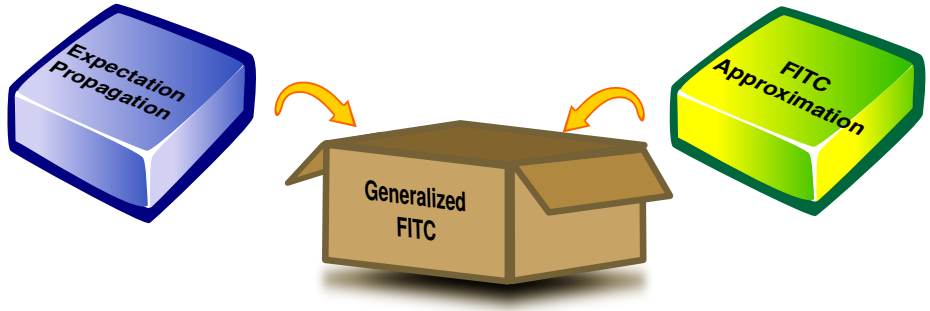

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where $\tilde{\mathbf{\Sigma}}$ is the **approximate FITC covariance matrix**.

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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!

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Consider these two Gaussian distributions:

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

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

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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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}:

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

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

which ensures that $\tilde{t}_j(\mathbf{f})q^{\setminus j}(\mathbf{f})$ and $t_j(\mathbf{f})q^{\setminus j}(\mathbf{f})$ **integrate the same**.

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

Graphical Illustration

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

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

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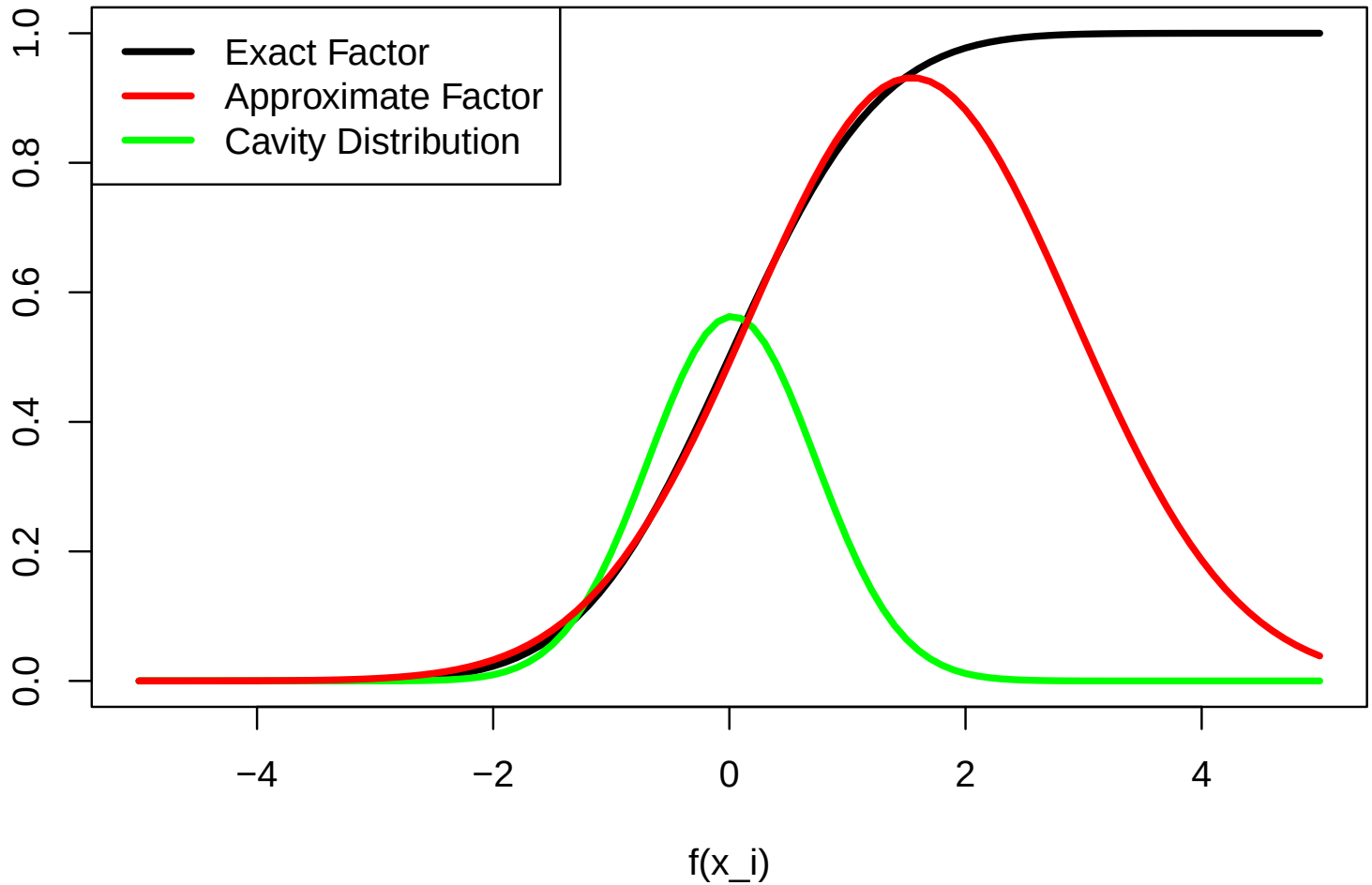
If the exact factor already belongs to the exponential family it needs not be approximated!

GFITC: Factor Approximation



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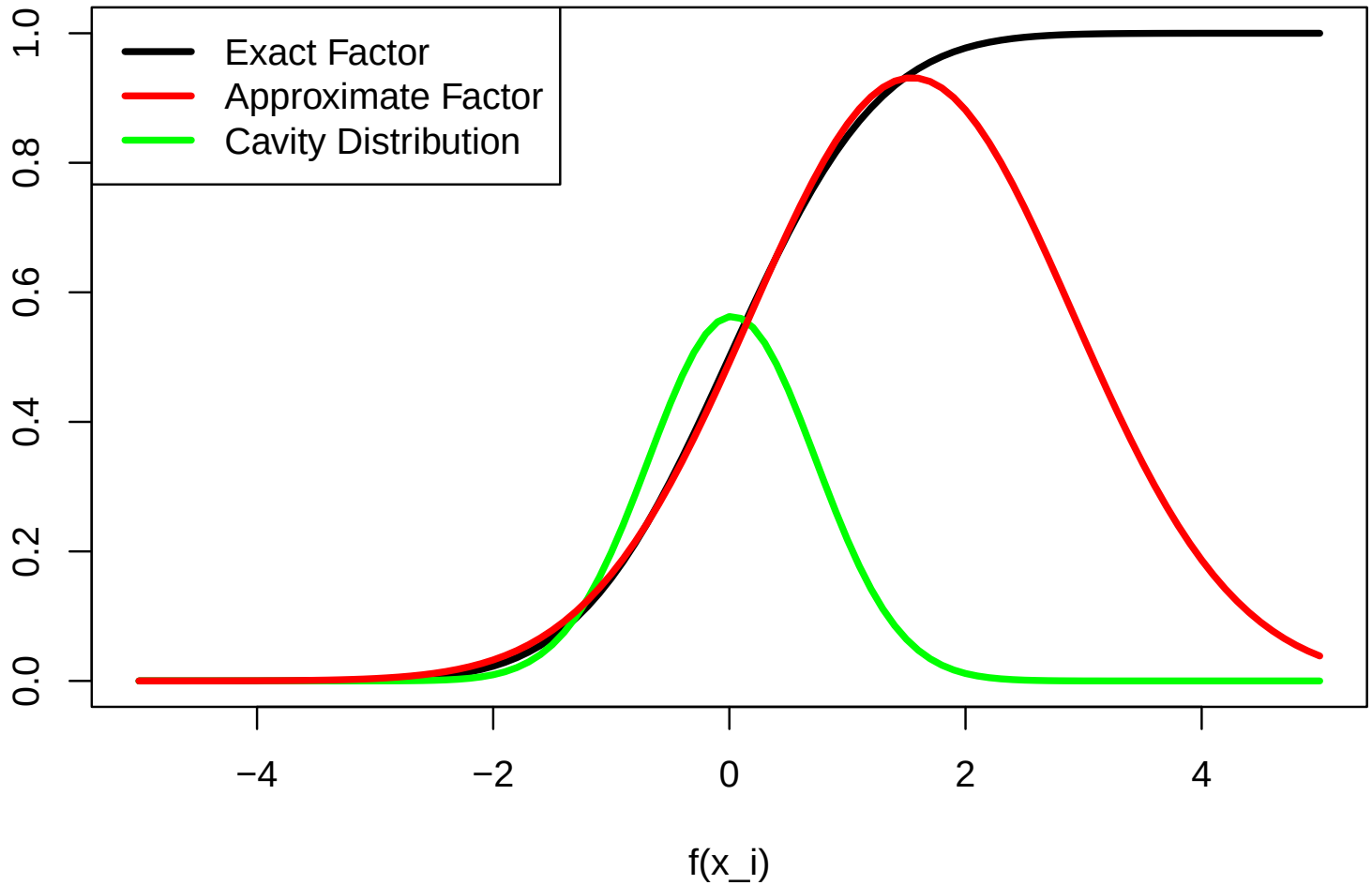

The approximate factor is accurate in regions of high posterior probability as indicated by the cavity distribution!

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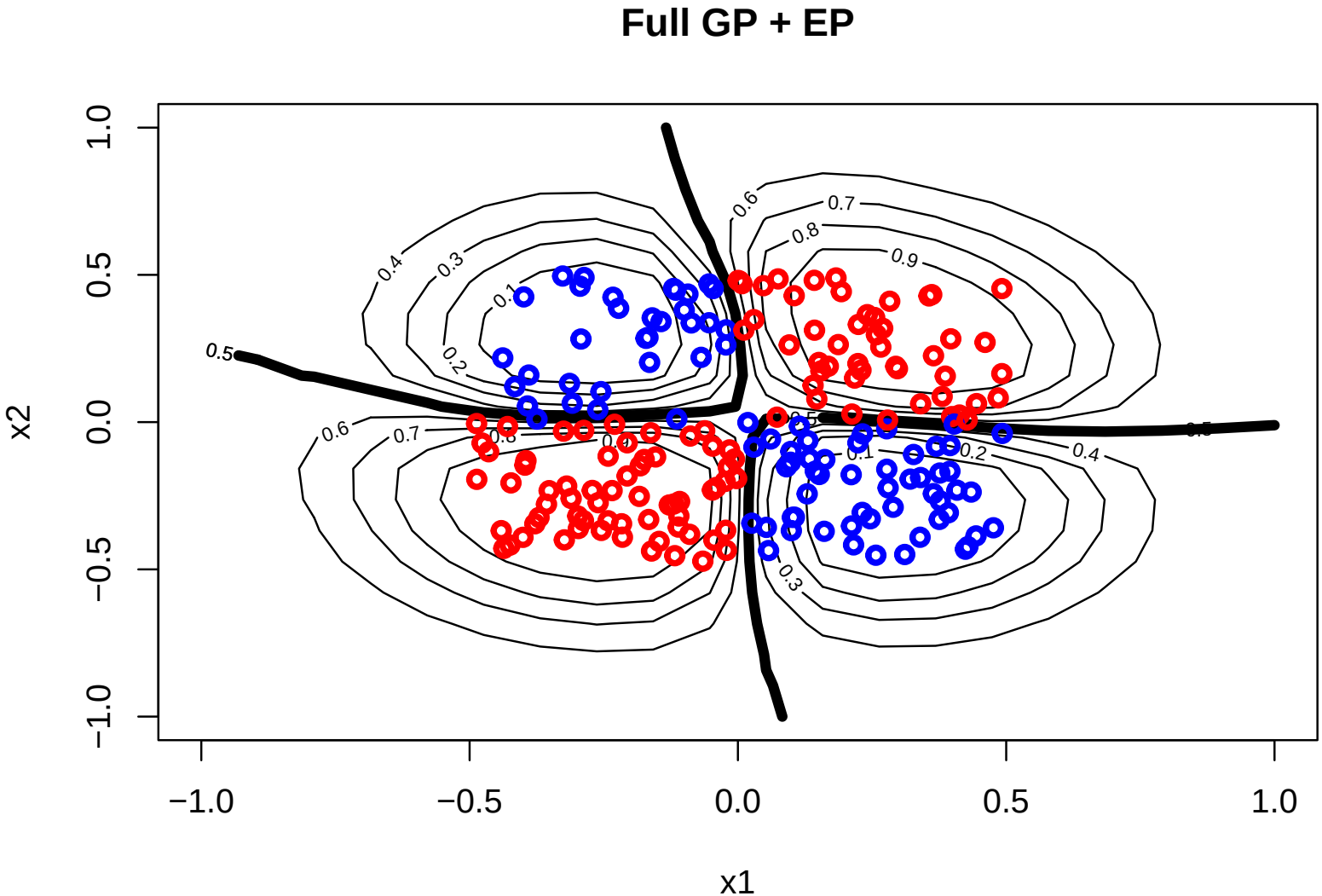
After marginalizing $\mathbf{f}$ w.r.t. $q(\mathbf{f})$, we obtain the predictive distribution:

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

GFITC: Illustrative Example



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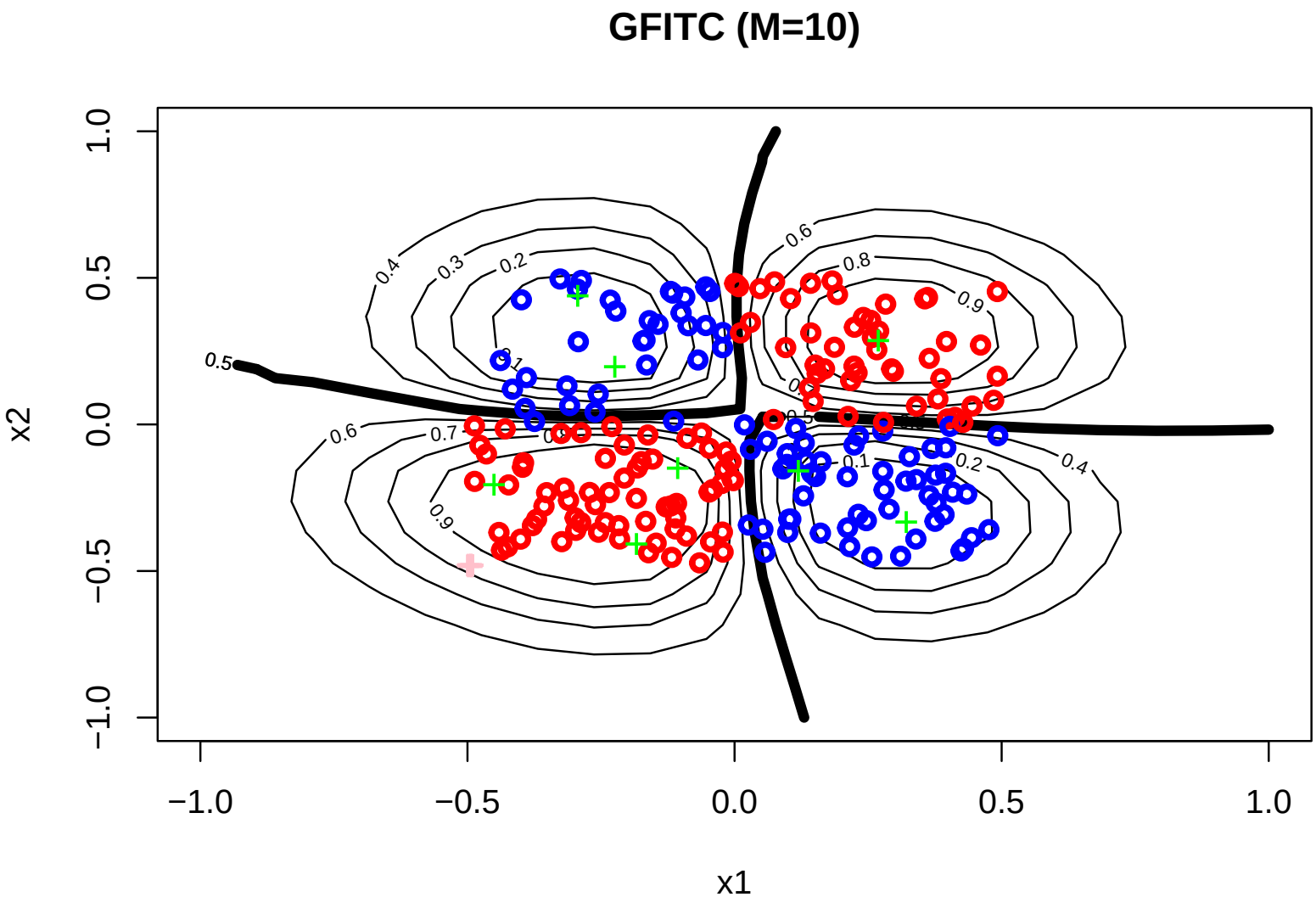

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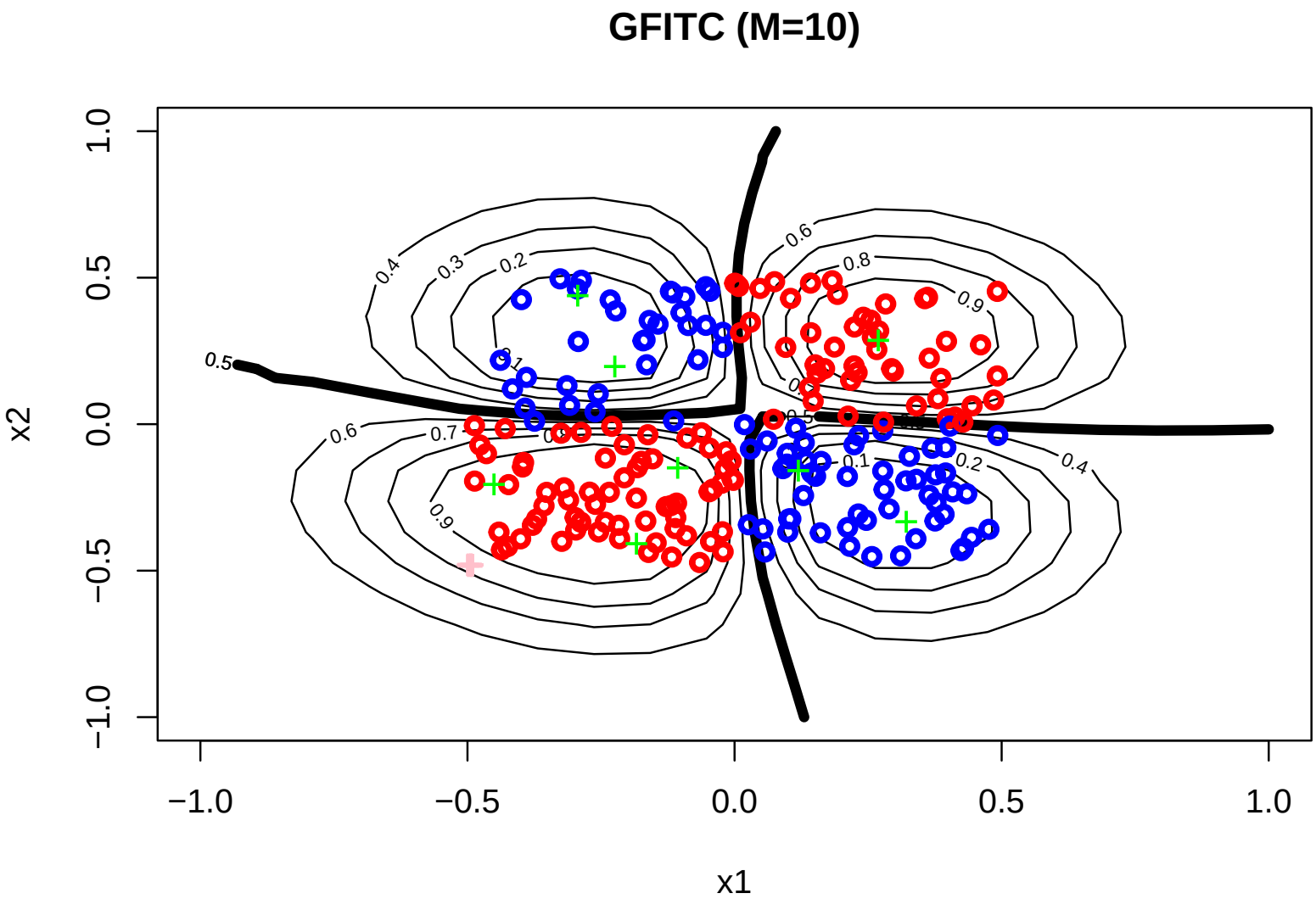

The inducing points spread across the input space!

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

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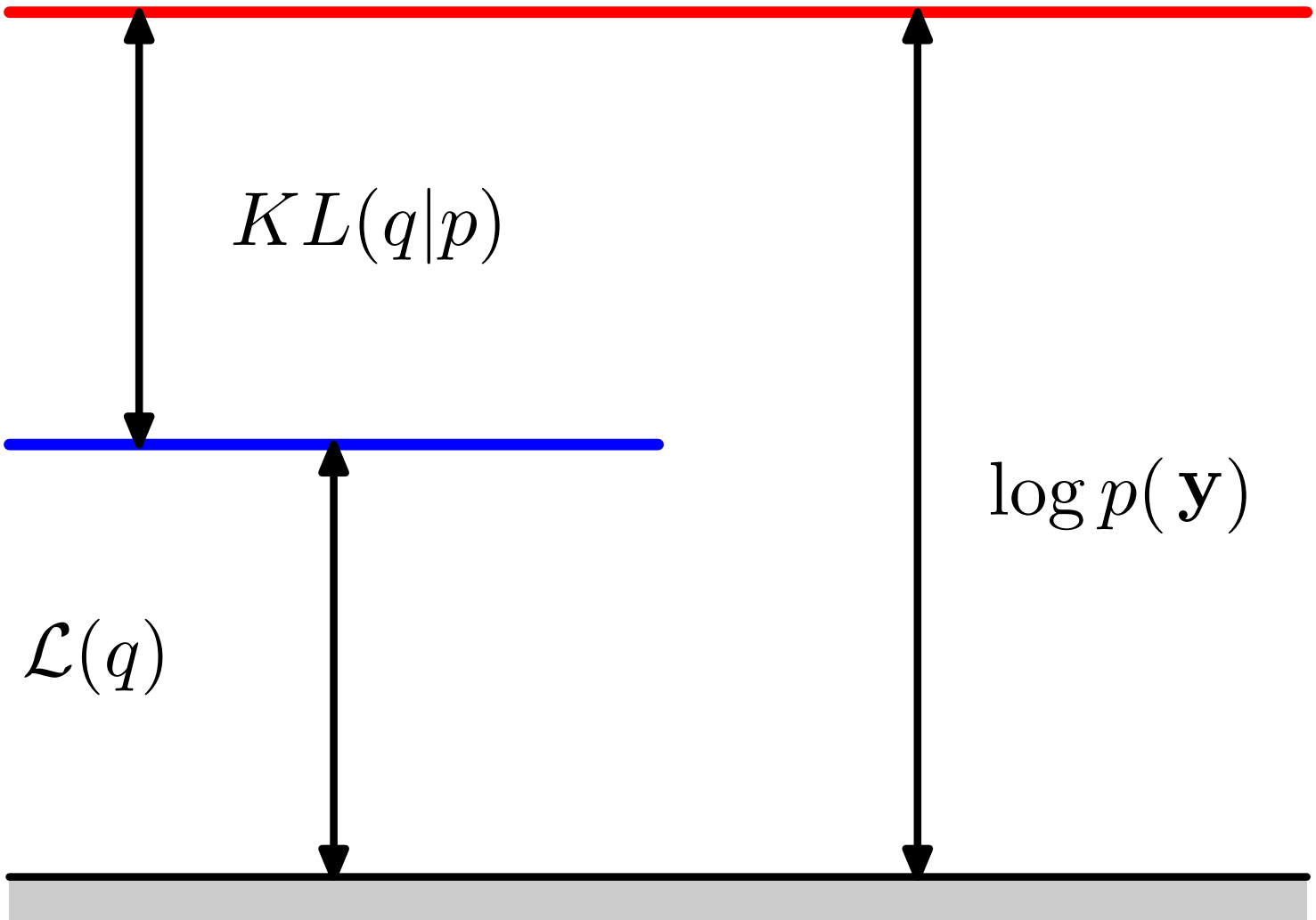
Let the target be $p(\mathbf{f}|\mathbf{y})$. Consider the decomposition of $p(\mathbf{y})$:

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

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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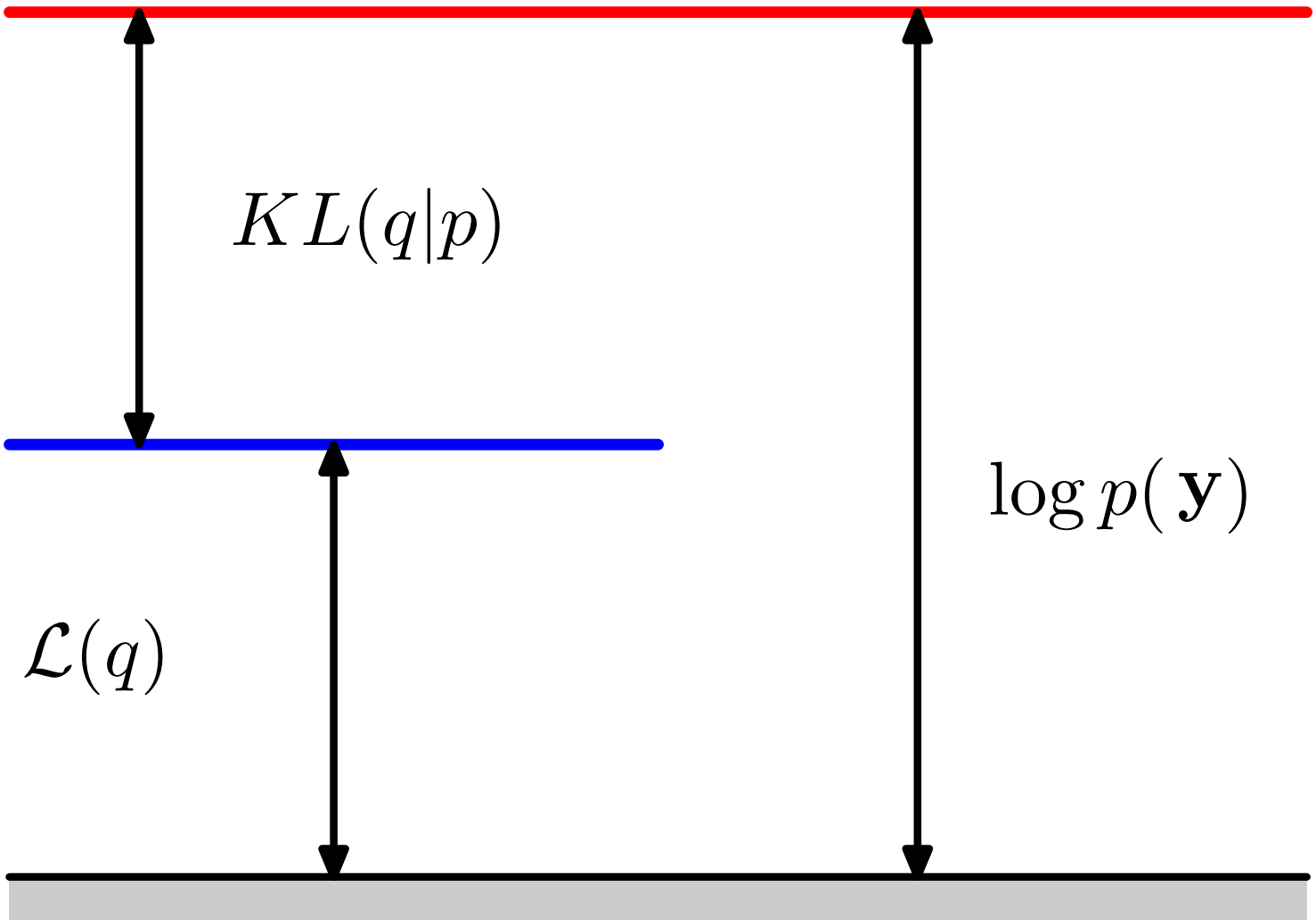
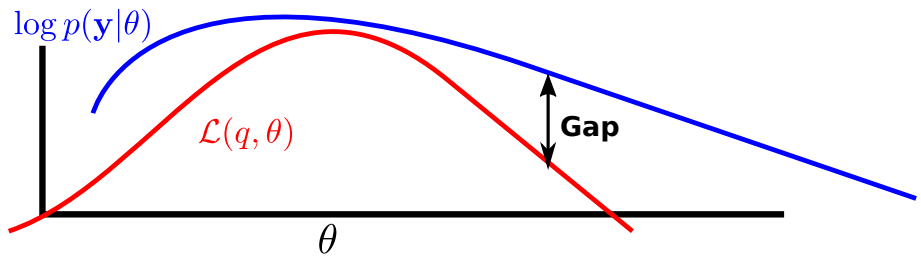


$\mathcal{L}(q)$ **can be used to approximate** $\log p(\mathbf{y})$ **if KL**$(q|p)$ **is small!**

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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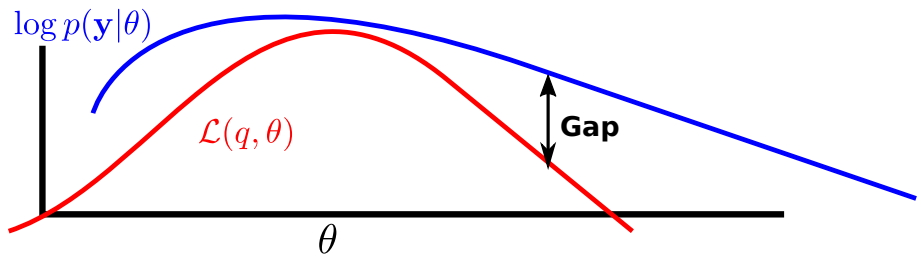

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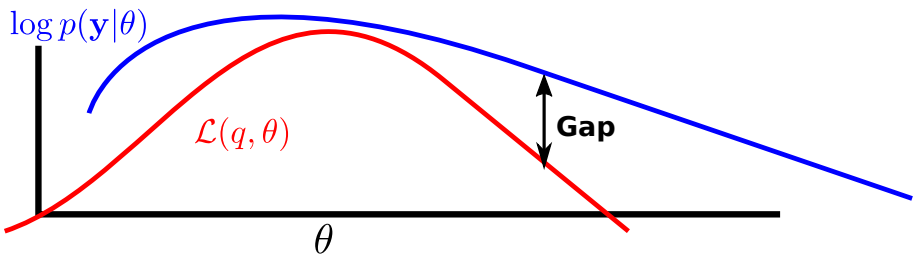

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$$= \log \int p(\mathbf{y},\mathbf{f},\mathbf{u}|\theta)\frac{q(\mathbf{f},\mathbf{u})}{q(\mathbf{f},\mathbf{u})}d\mathbf{f}d\mathbf{u} \geq \int q(\mathbf{f},\mathbf{u}) \log \frac{p(\mathbf{y},\mathbf{f},\mathbf{u}|\theta)}{q(\mathbf{f},\mathbf{u})}d\mathbf{f}d\mathbf{u}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

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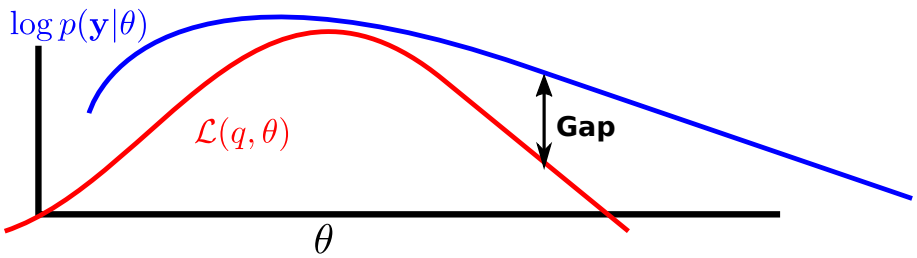

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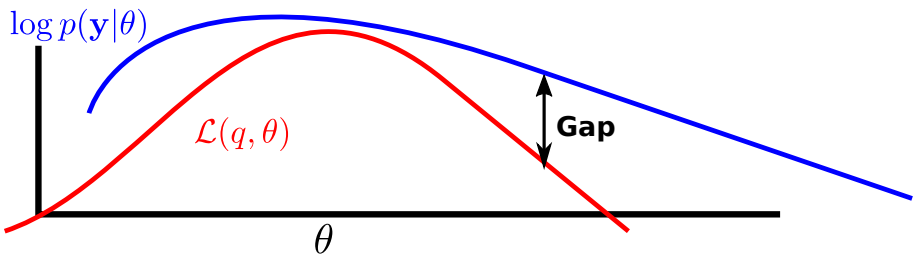
Variational Free Energy (VFE)

Lower bound the log-likelihood:



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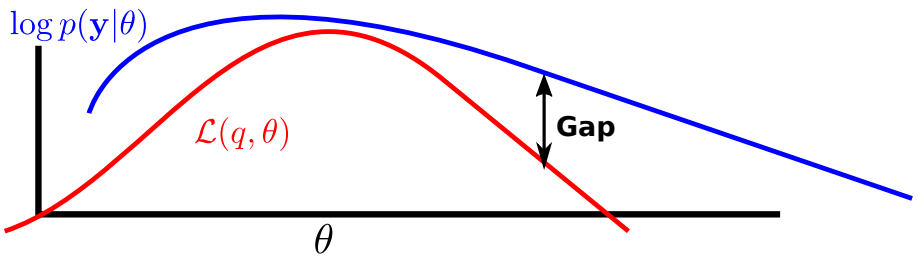

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By maximizing $\mathcal{L}(q,\theta)$ w.r.t q we are enforcing that $q(\mathbf{f},\mathbf{u})$ looks similar to $p(\mathbf{f},\mathbf{u}|\mathbf{y})$ in terms of the KL!

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

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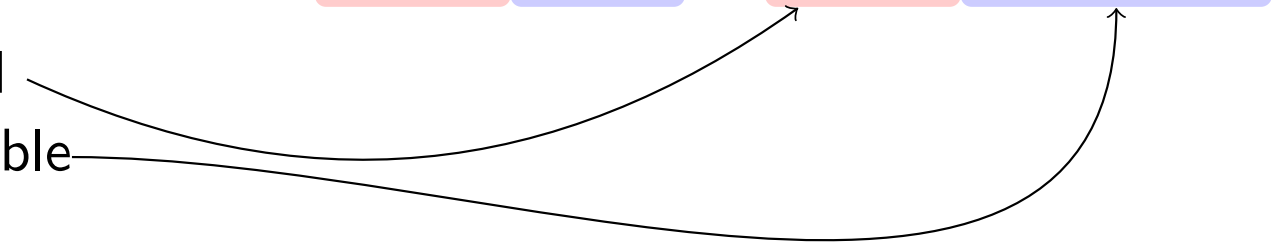

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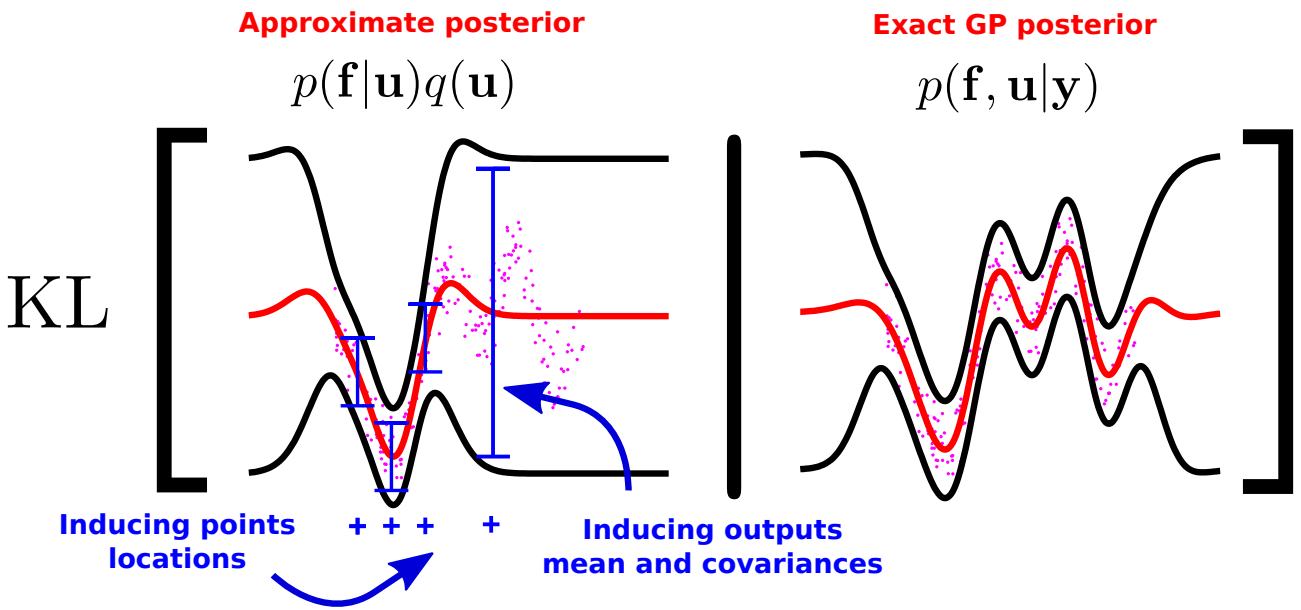

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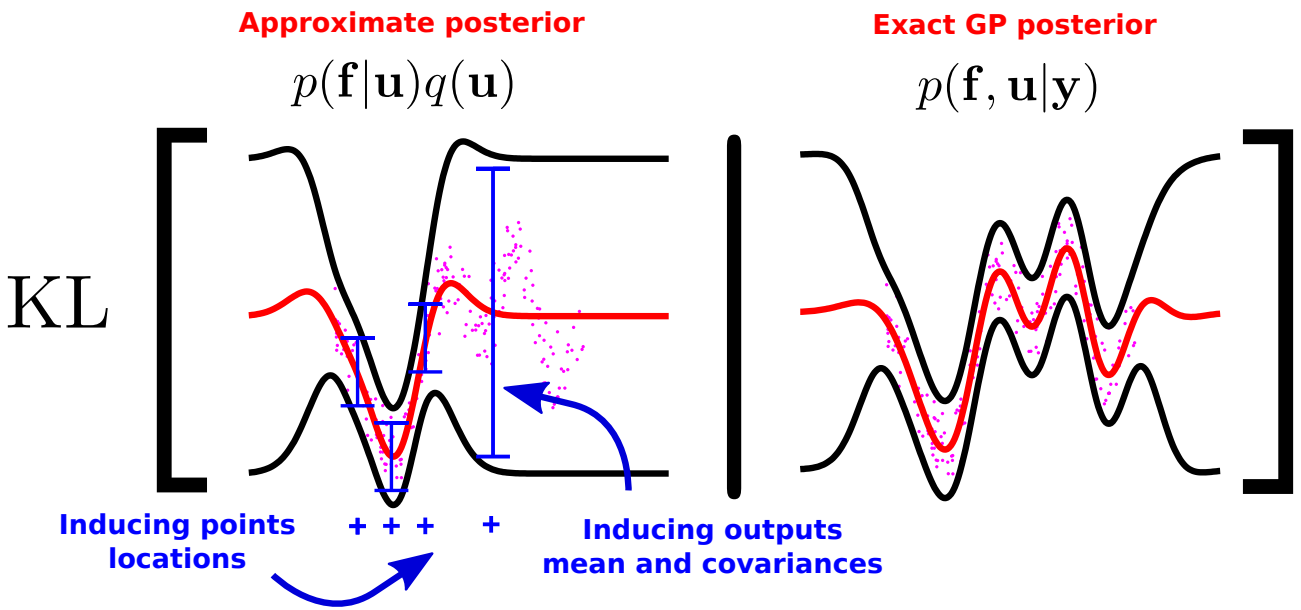

The inducing points are now parameters of the approx. dist. q!

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- Mean squared prediction error
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- 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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The conditional $p(\mathbf{f}^\star|\mathbf{u})$ is:

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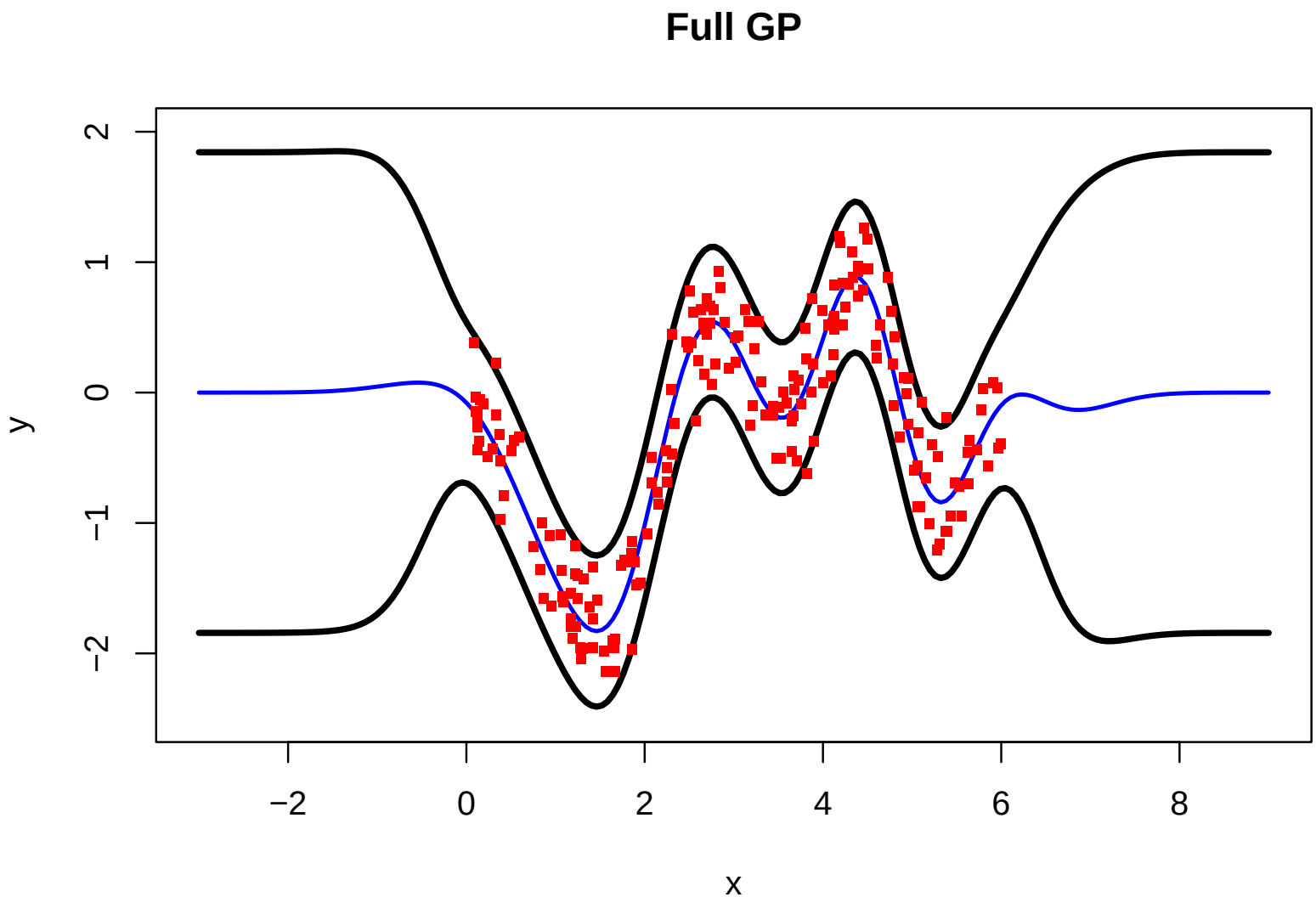
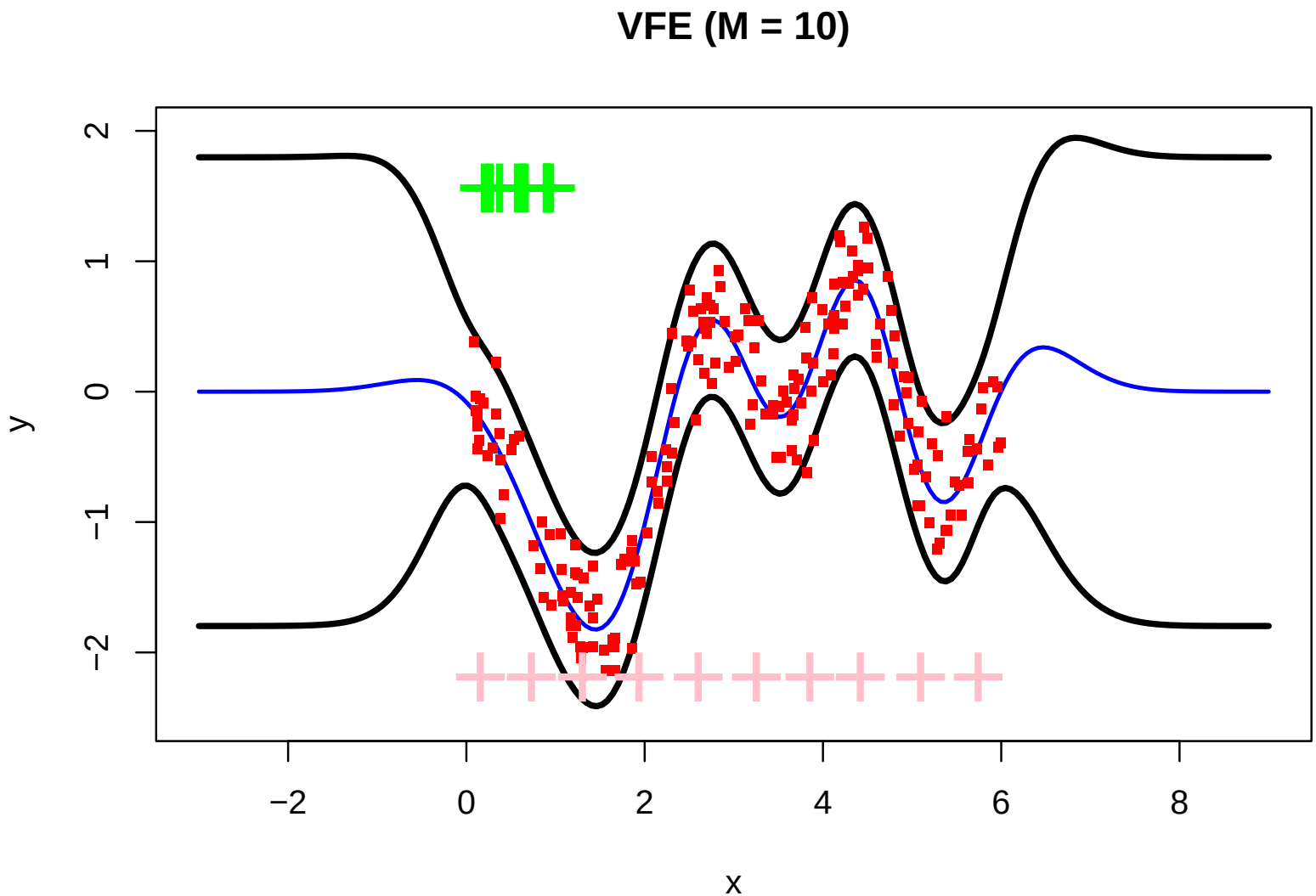
After marginalizing $\mathbf{u}$ w.r.t. $q(\mathbf{u})$, we obtain the predictive distribution:

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

VFE: Illustrative Example



VFE: Illustrative Example



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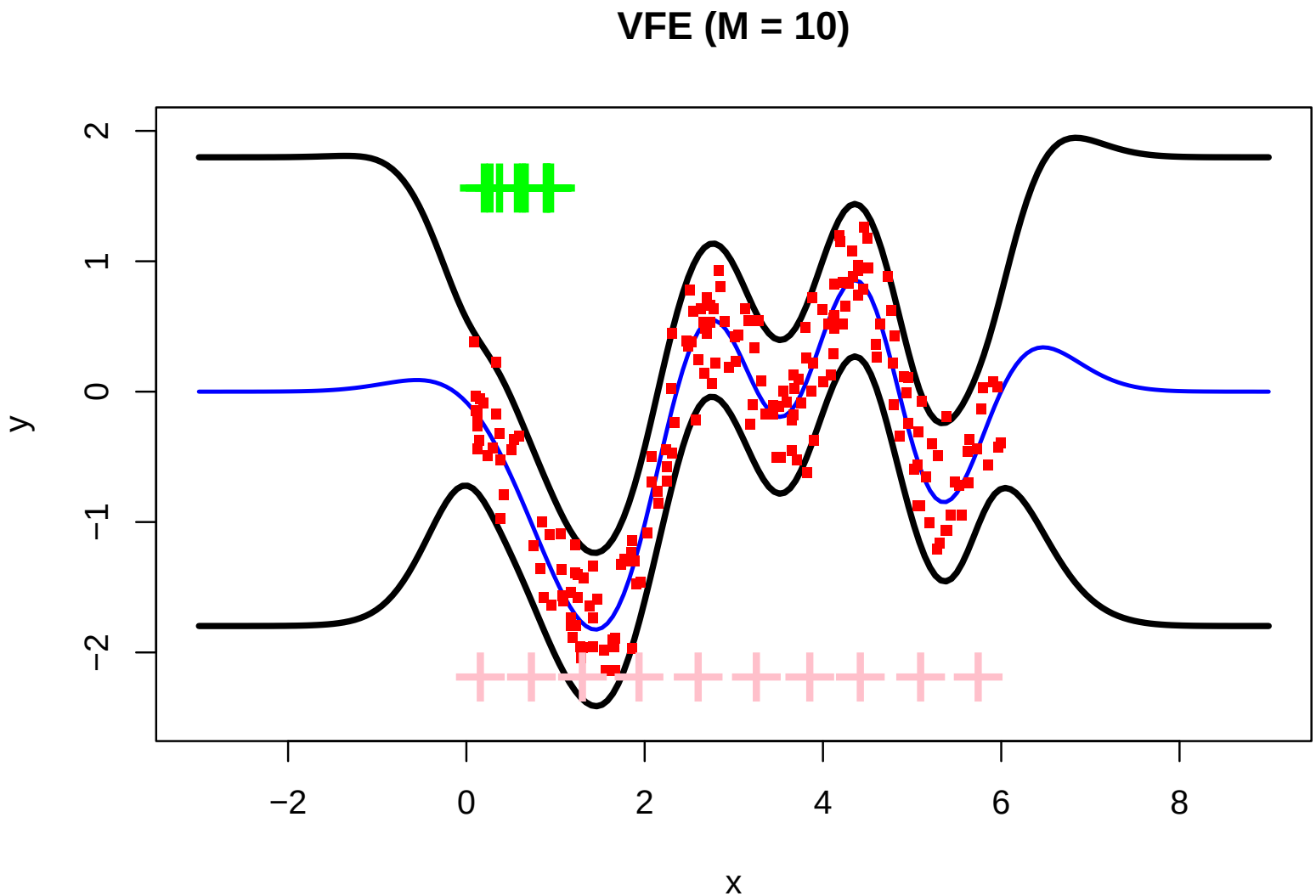
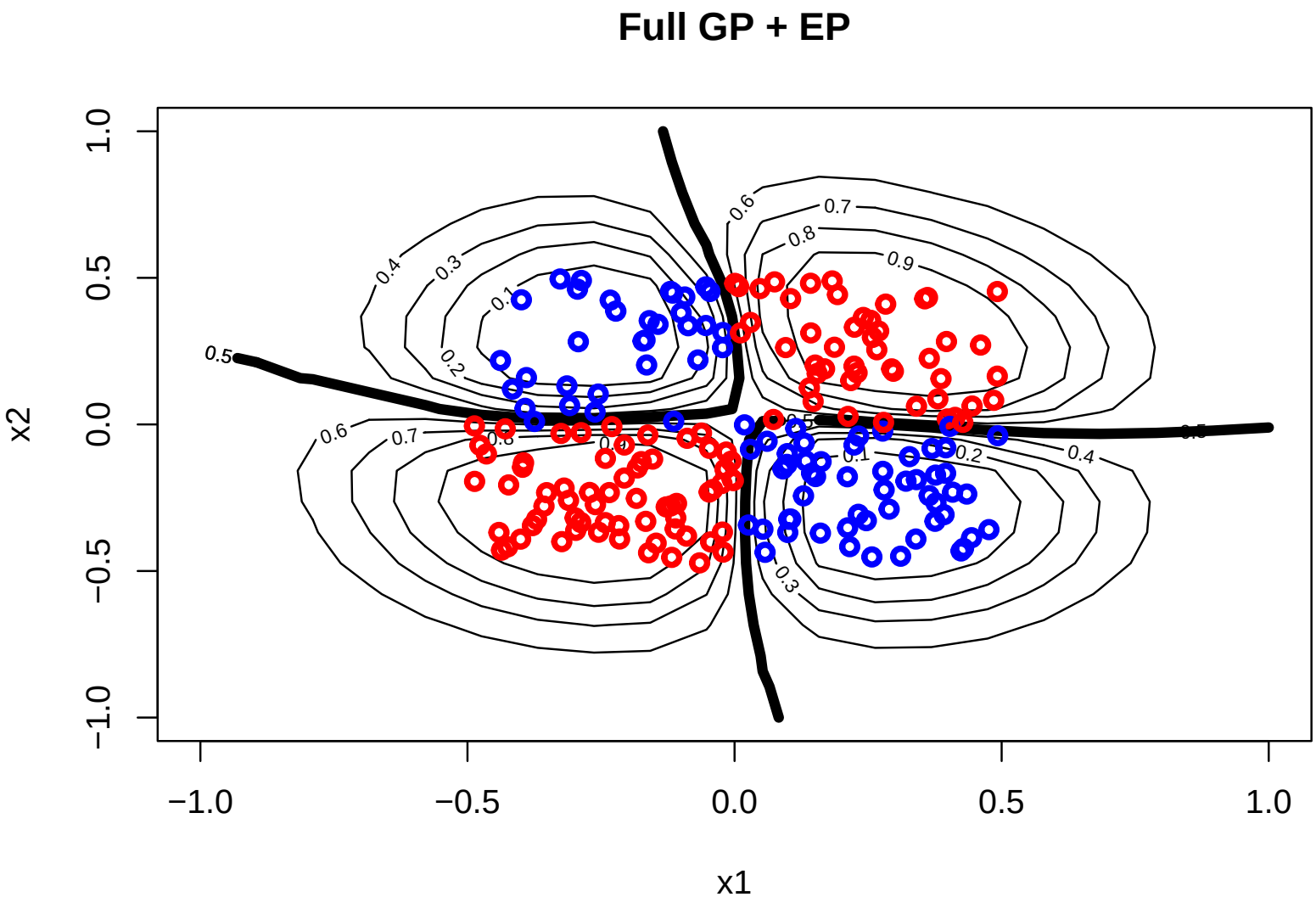


The inducing points cover the regions where the function changes!

VFE: Illustrative Classification Example



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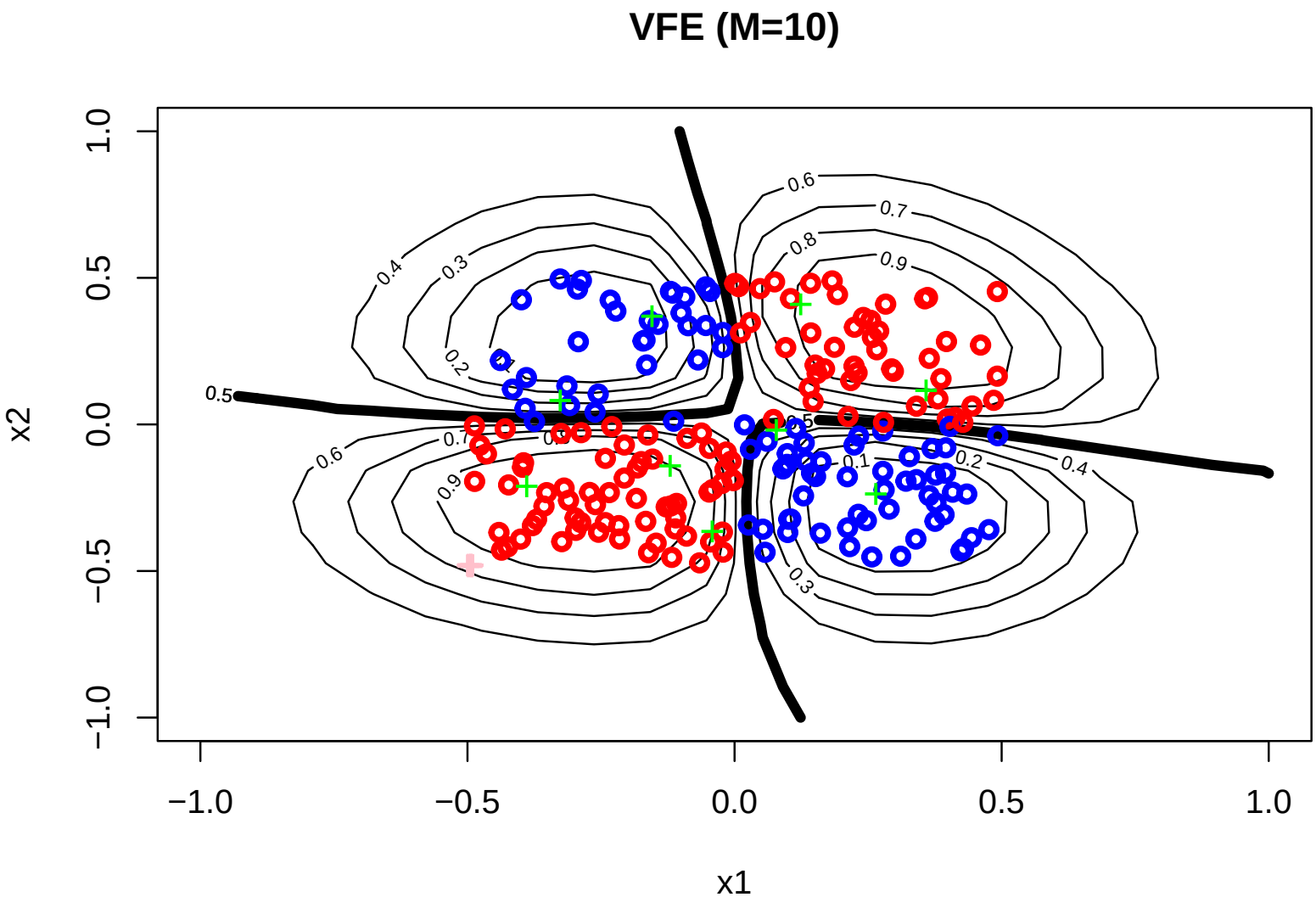

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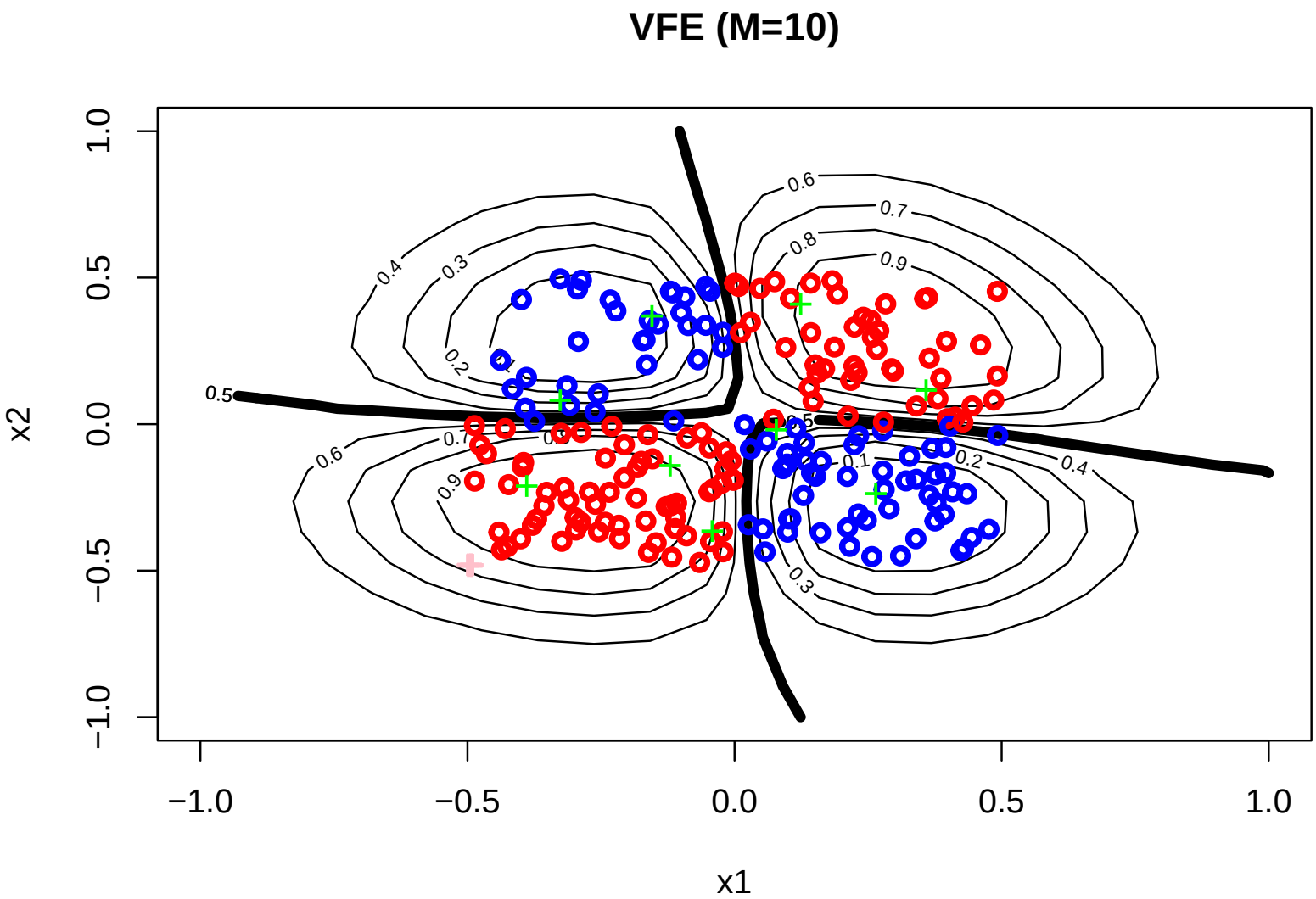

The inducing points spread across the input space!

FITC vs. VFE

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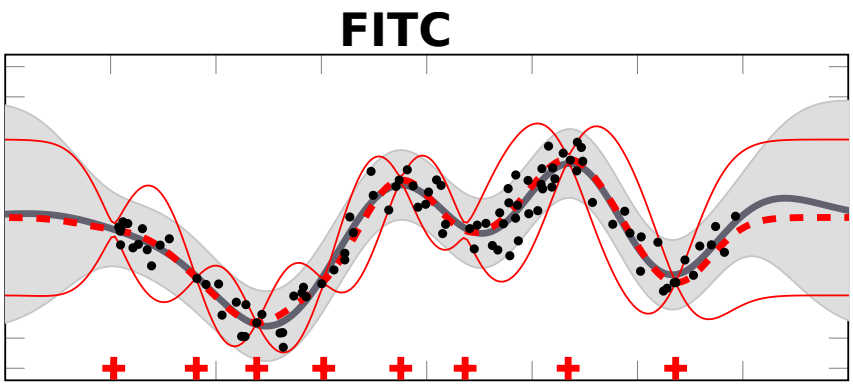

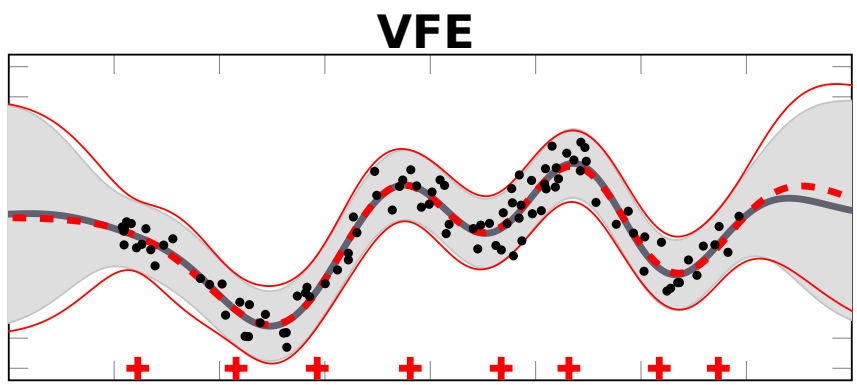

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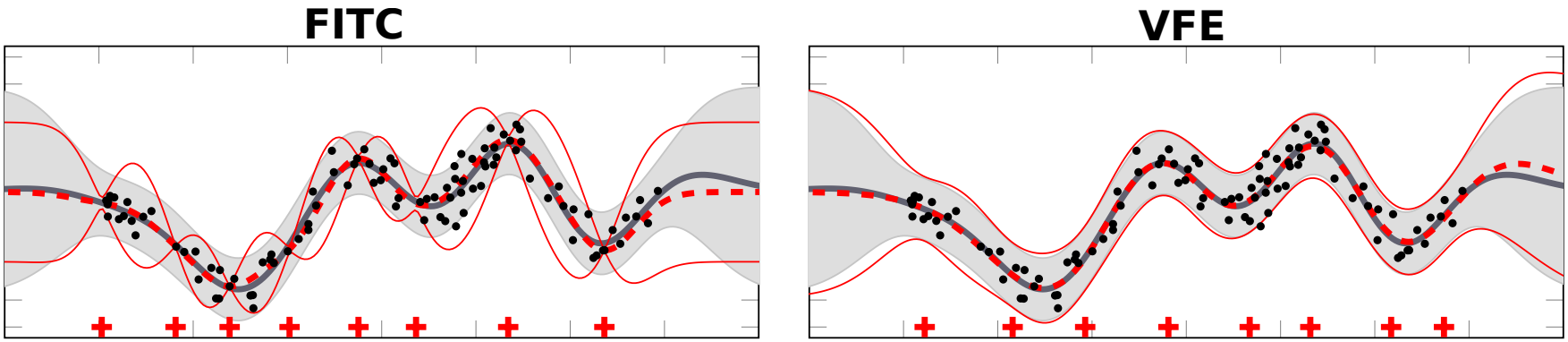

- FITC: less local optima and easier to optimize, also less accurate.
- VFE: more accurate, more local optima, more difficult to optimize.

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

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:

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The VFE objective becomes:

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

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

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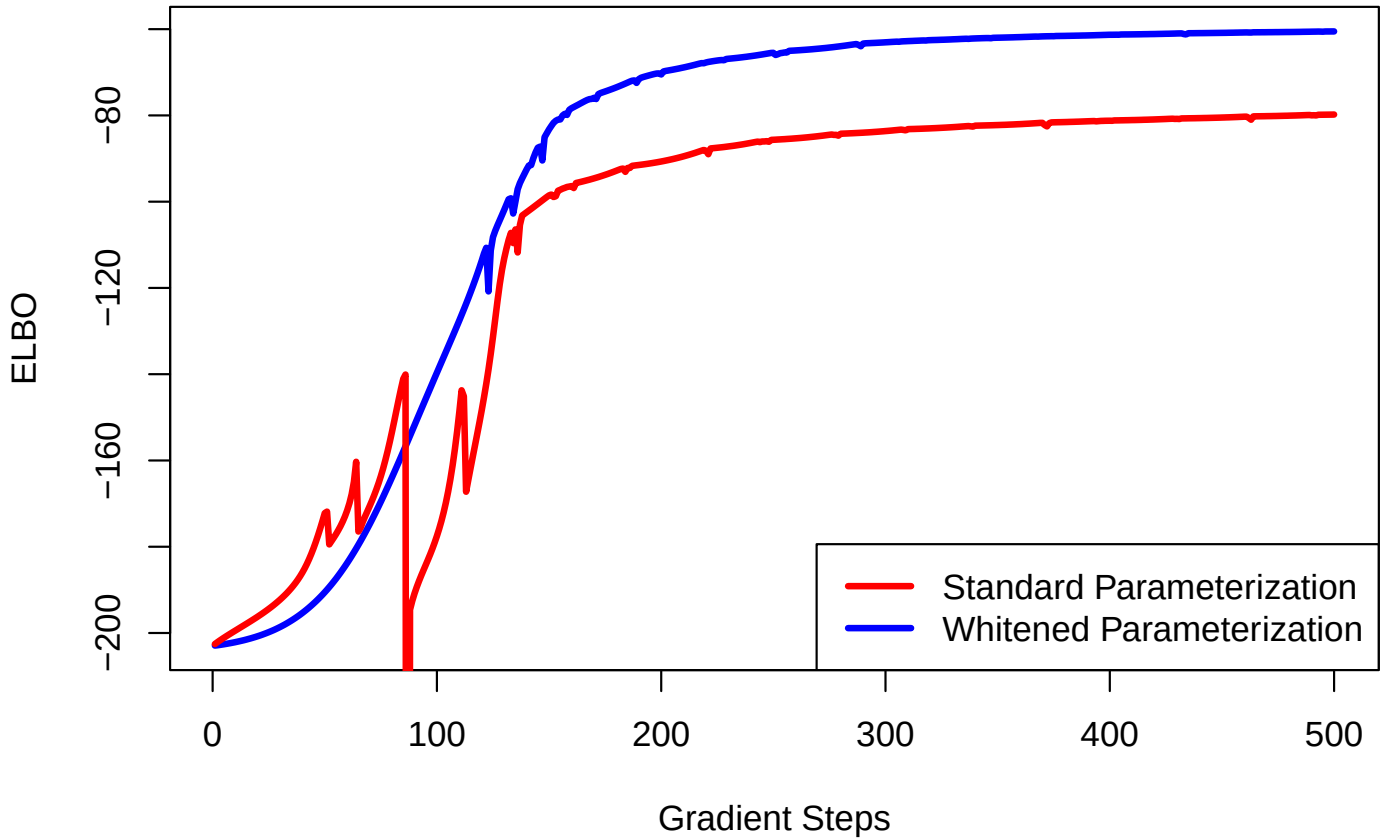

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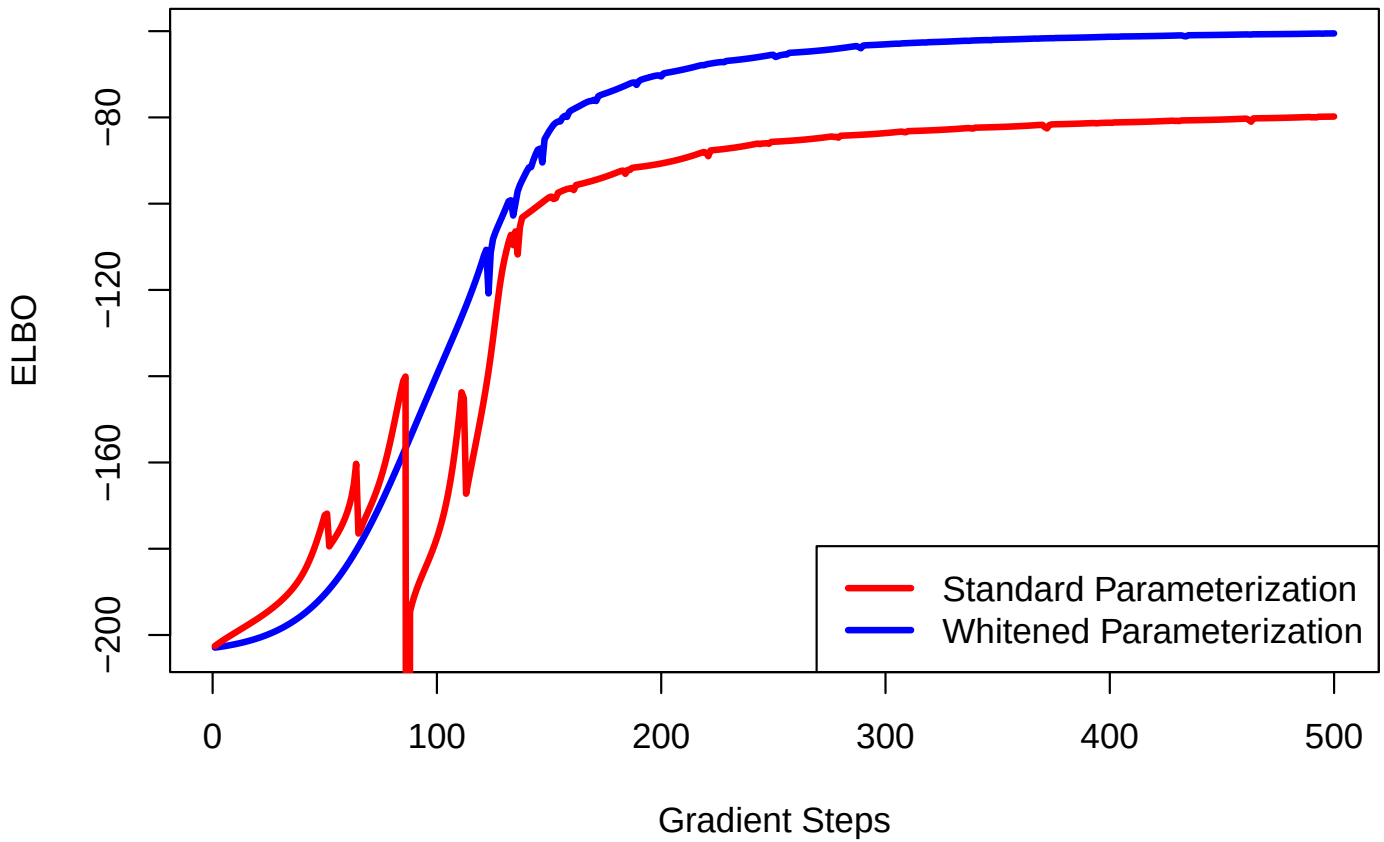

Whitening significantly improves convergence!

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

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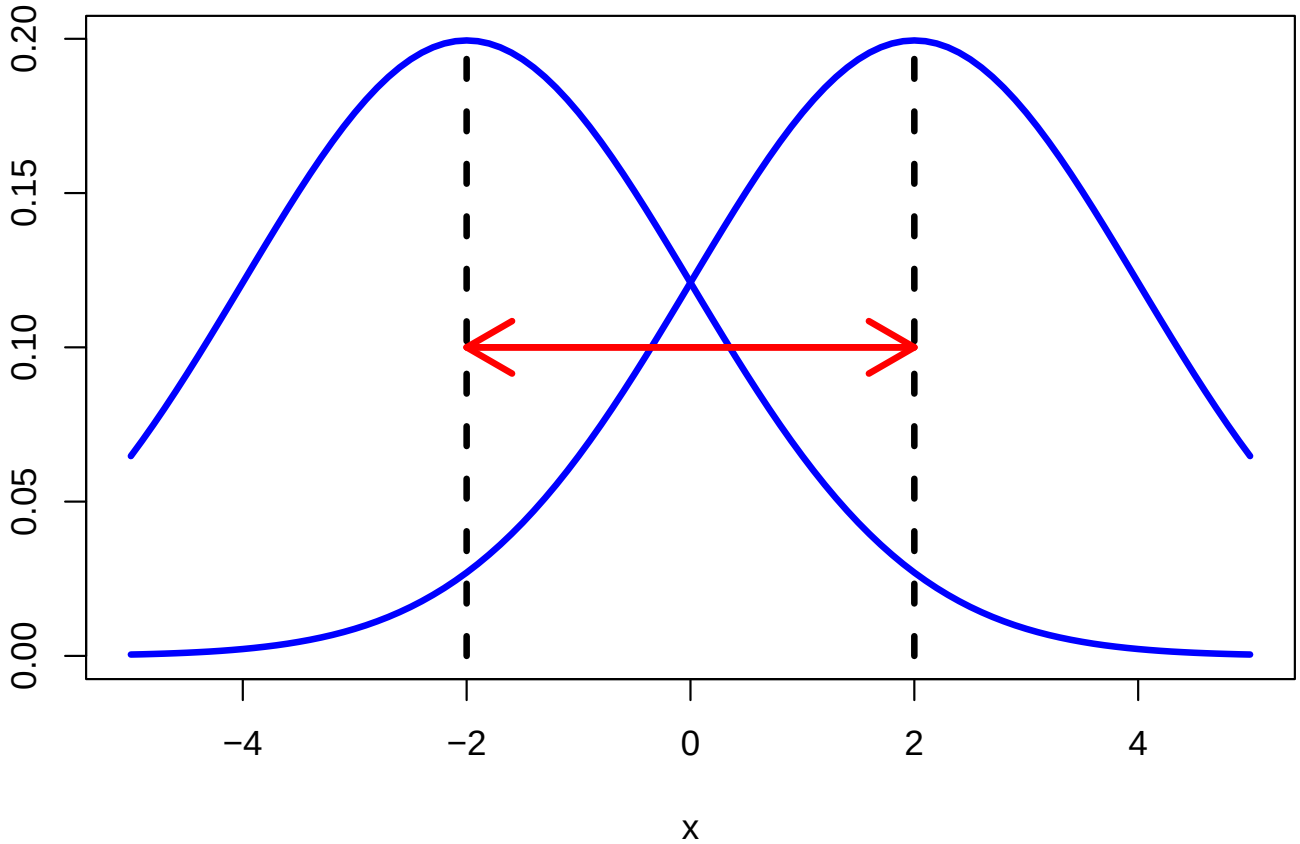
If $\boldsymbol{\xi}$ represents the parameters of probability distributions, the Euclidean norm may be problematic!

Illustration with Two Gaussians



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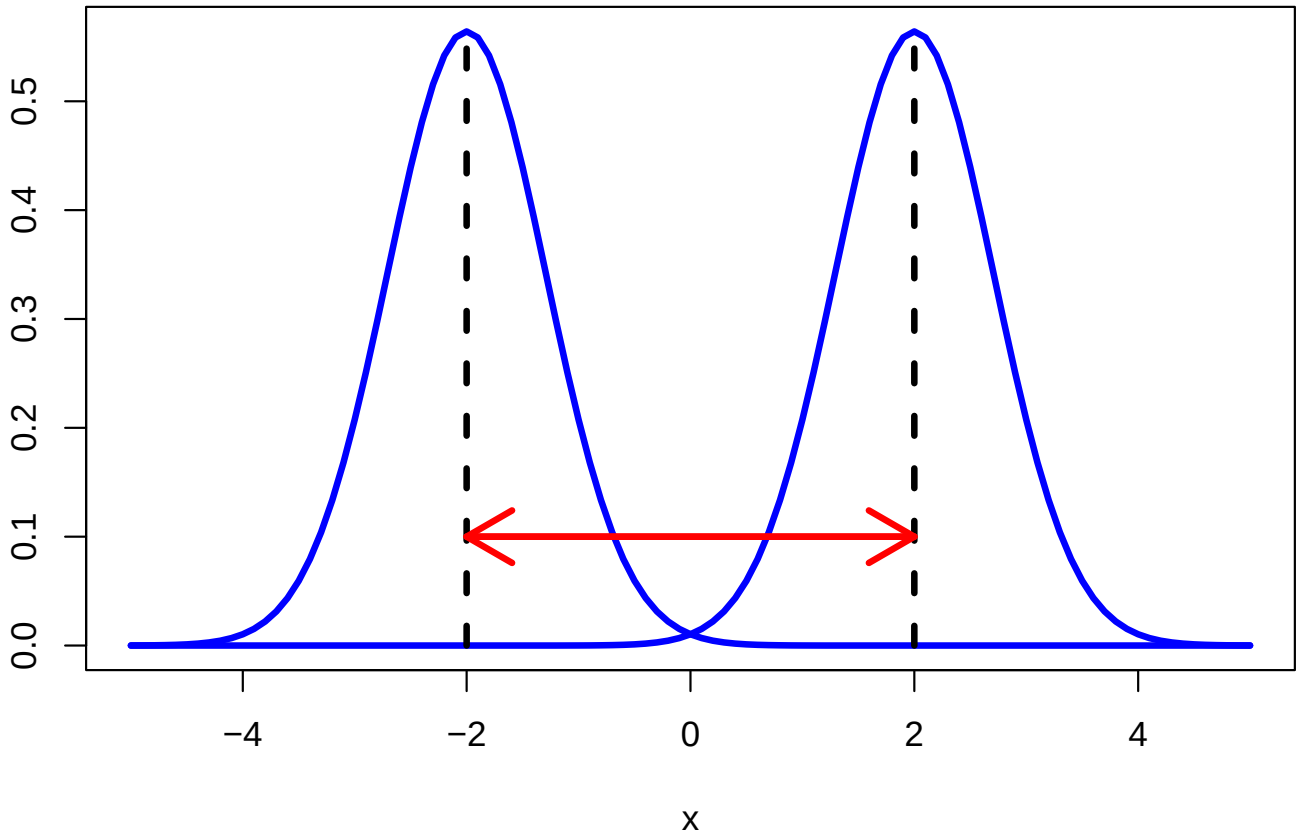

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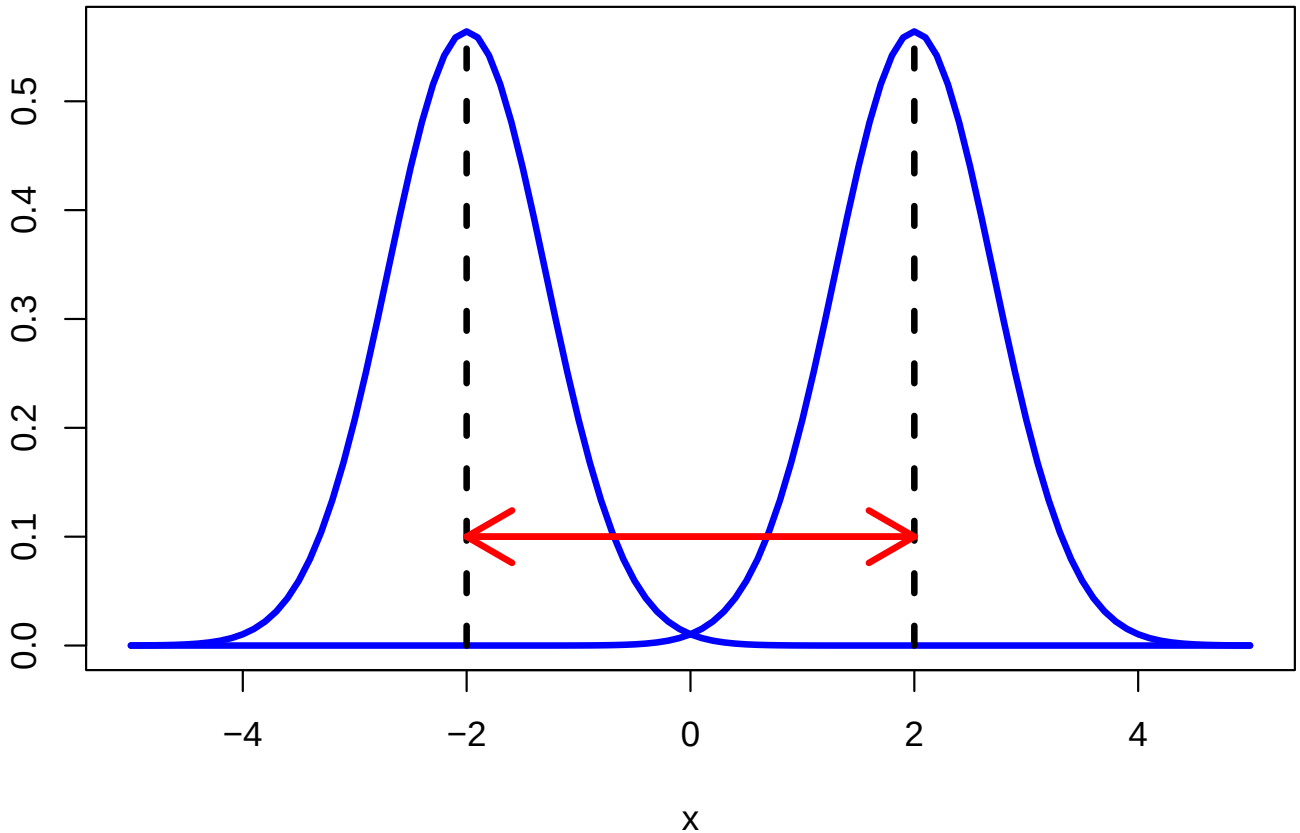
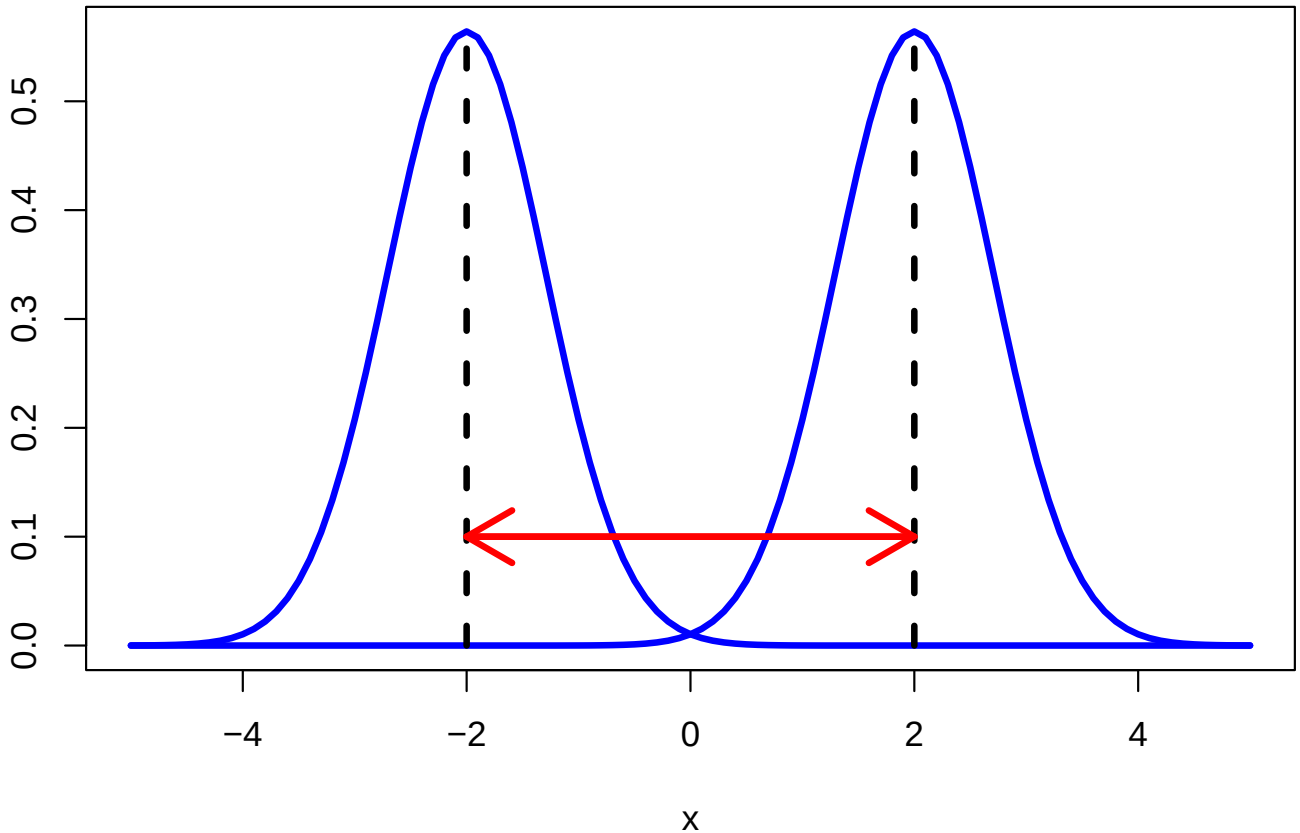


The Euclidean distance between parameters is 4 in both cases!

Illustration with Two Gaussians



A better alternative is the KL-divergence between distributions!

Natural Gradient Ascent

Considers the KL-divergence as a norm:

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

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:

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

Natural Gradient Ascent

Considers the KL-divergence as a norm:

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

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

$$\mathbf{F}_{\boldsymbol{\xi}} = -\mathbb{E}_{q(\mathbf{u}|\boldsymbol{\xi})}[\nabla^2_{\boldsymbol{\xi}}\log q(\mathbf{u}|\boldsymbol{\xi})]$$

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

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

Thus,

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

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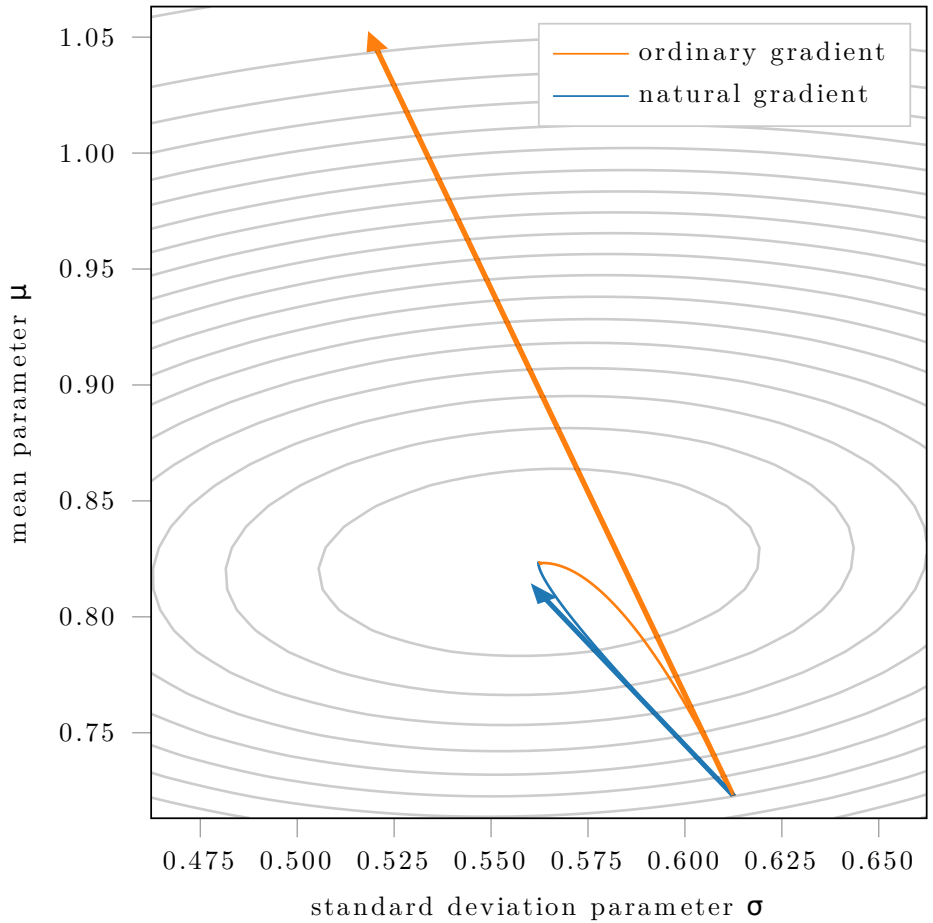
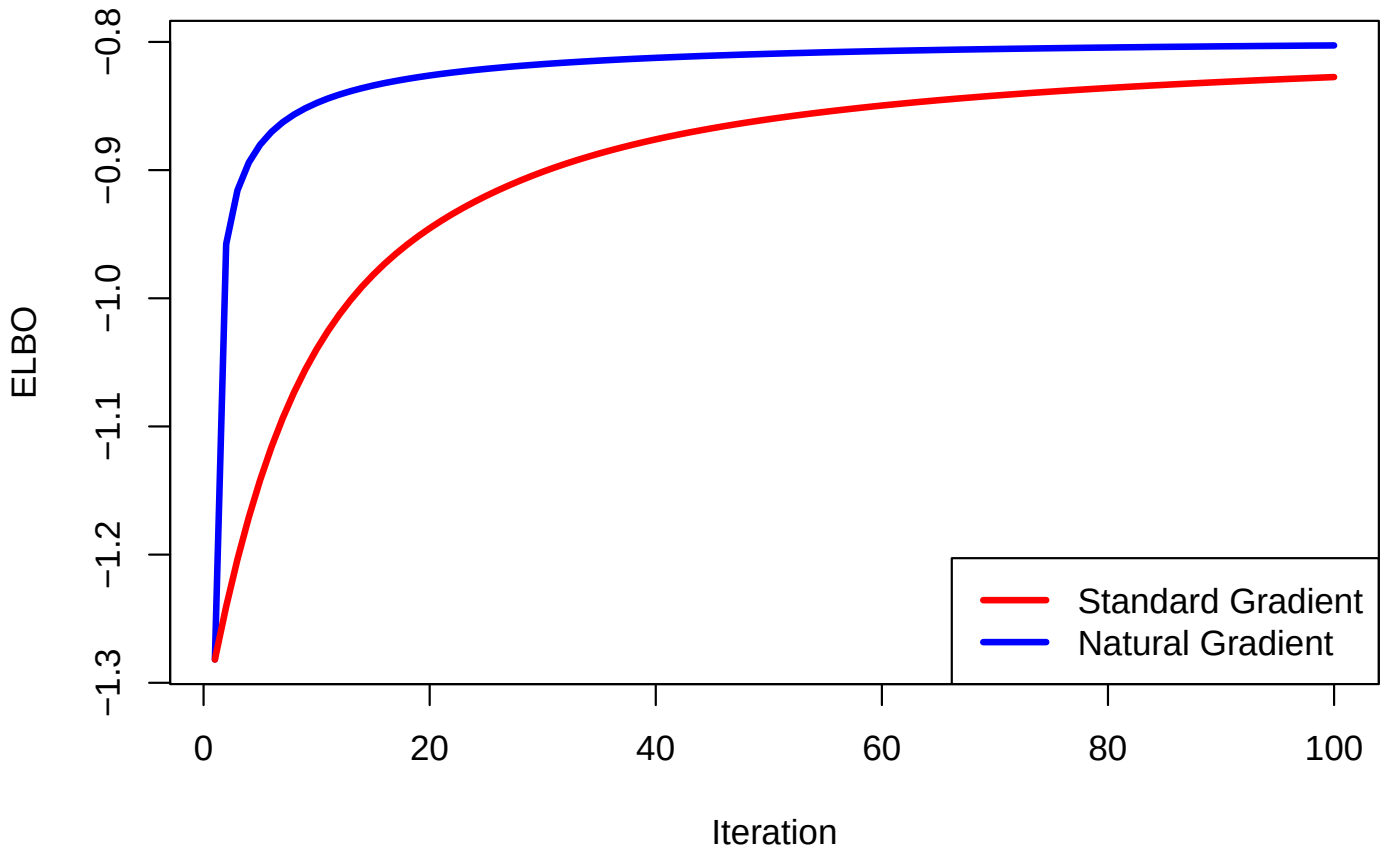


(Salimbeni et al., 2018)

Natural Gradient: Illustrative Example



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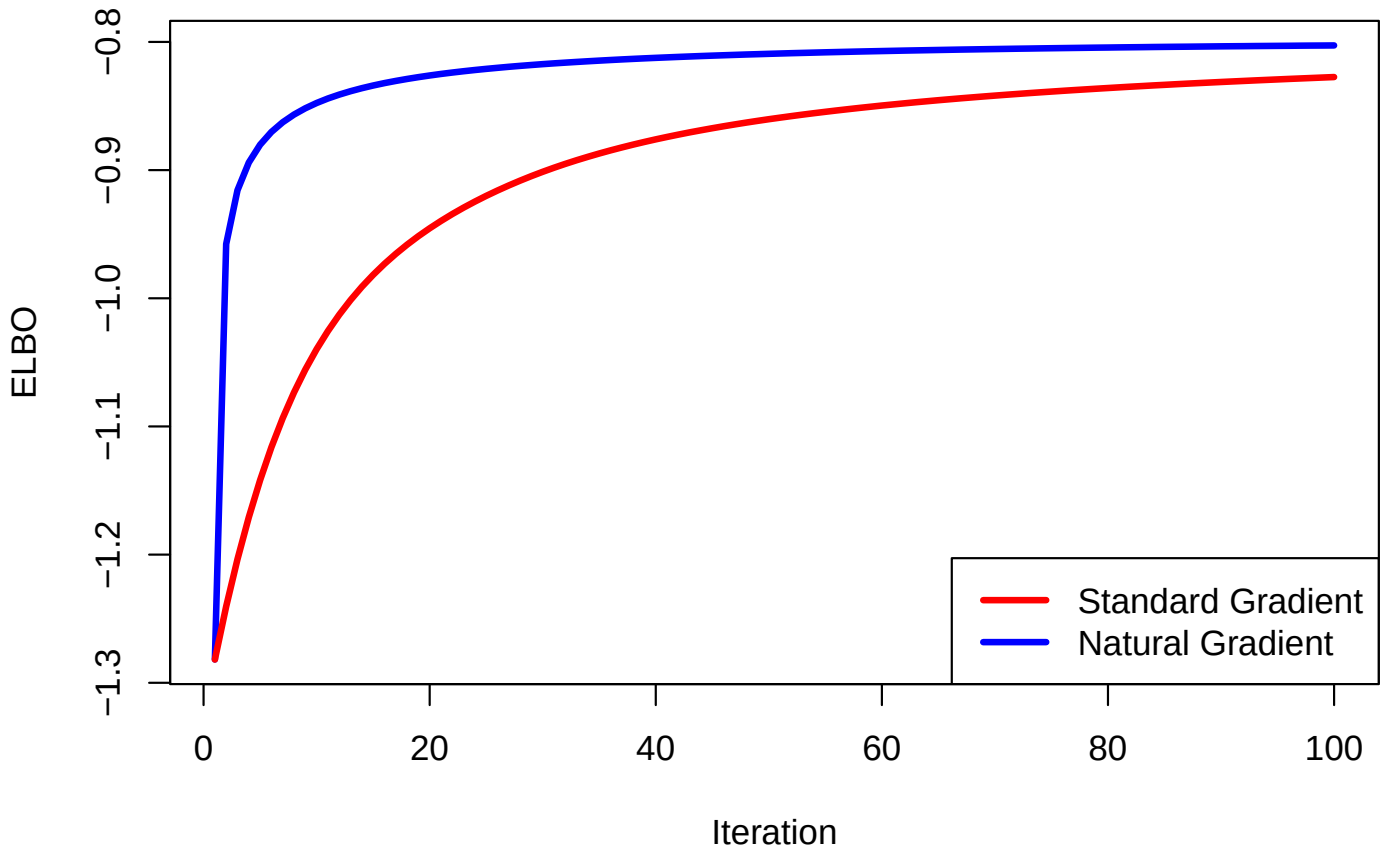

The natural gradient achieves a faster convergence!

GPs for Big Data

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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)

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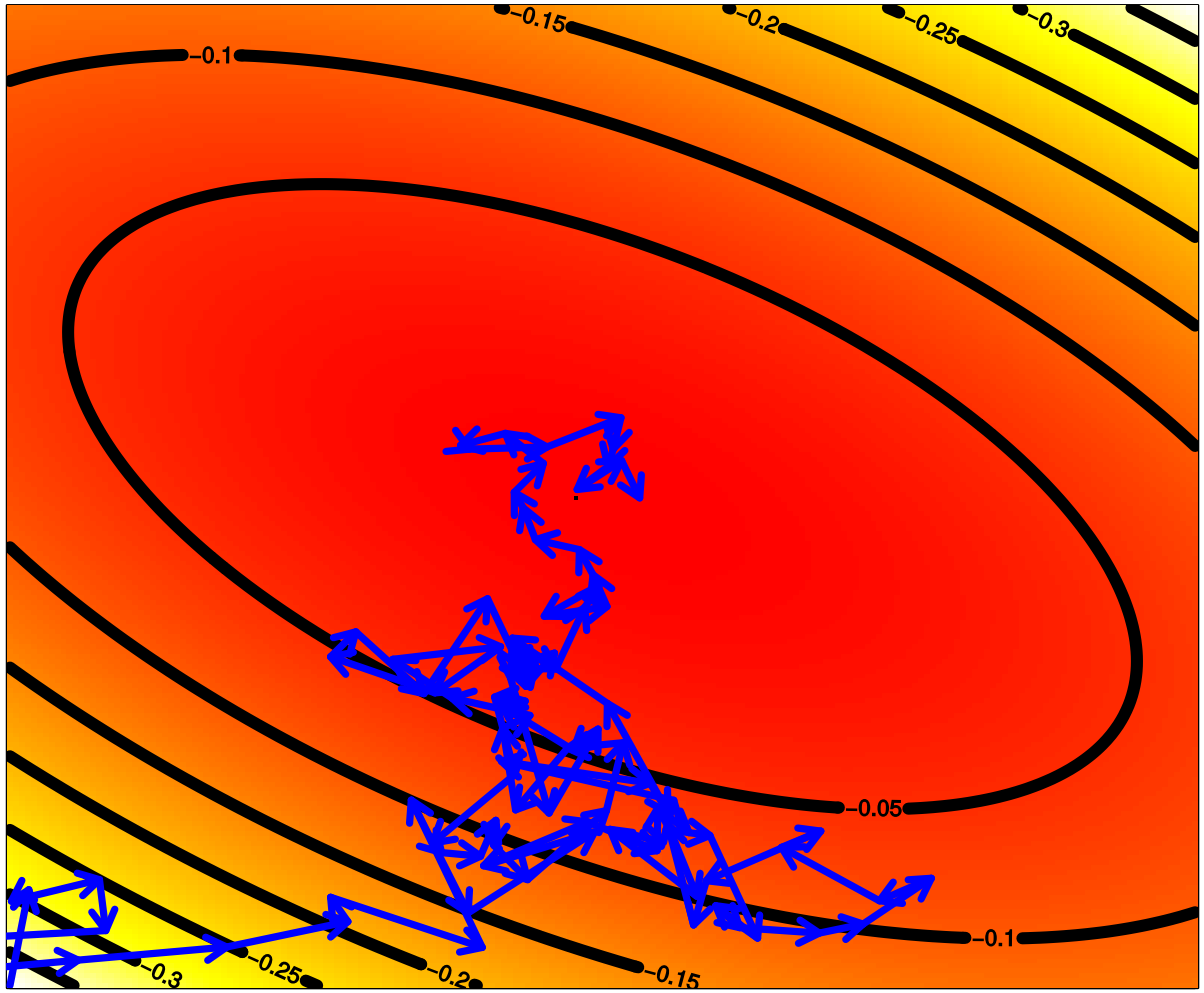

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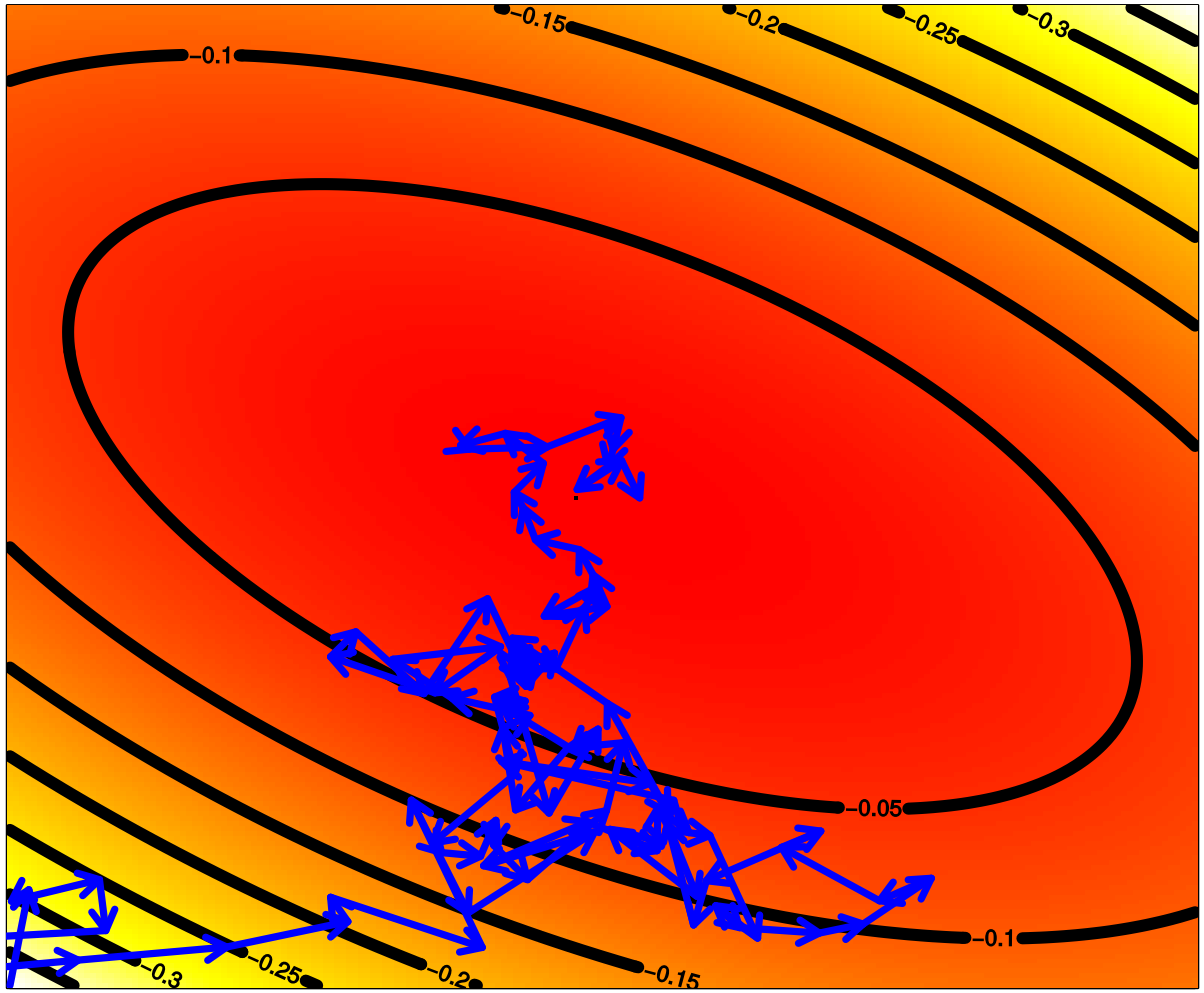
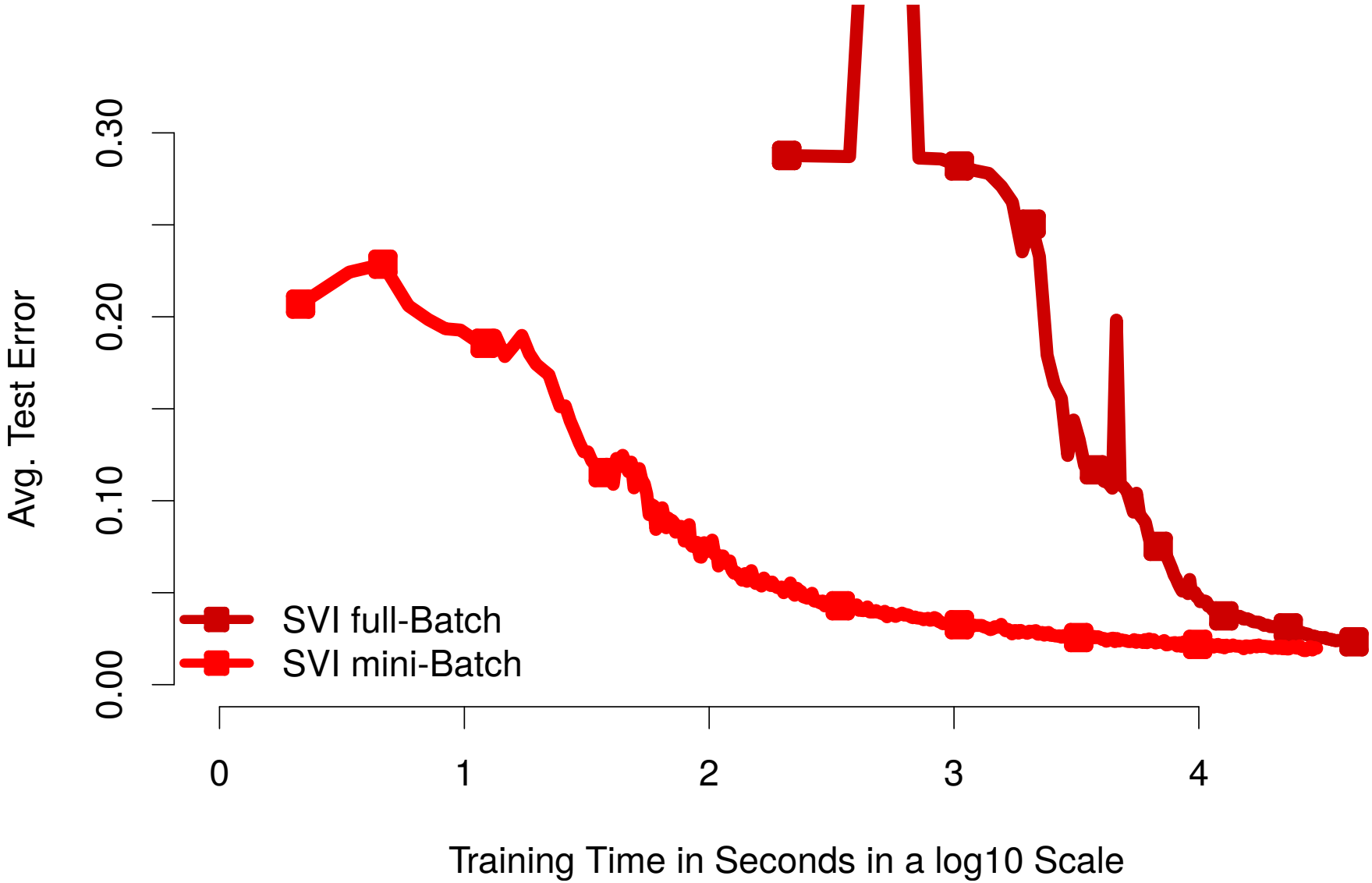


To converge to a local neighborhood of the optimum stochastic methods require an estimate of the gradient which can be very cheap!

GPs for Big Data



(Hernández-Lobato, 2015)

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- The objective is prone to local optima and difficult to optimize.

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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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