Part III: Deep Gaussian Processes

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Summary so Far about GPs

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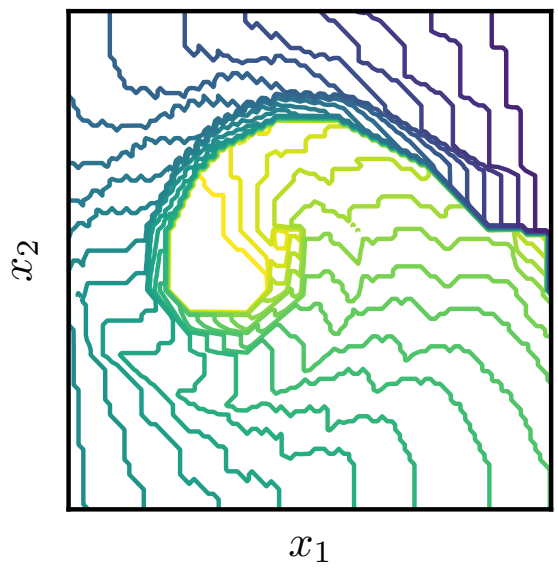
Deep GPs constitute a nice alternative to address these issues!

Motivation for Deep Gaussian Processes

Target function



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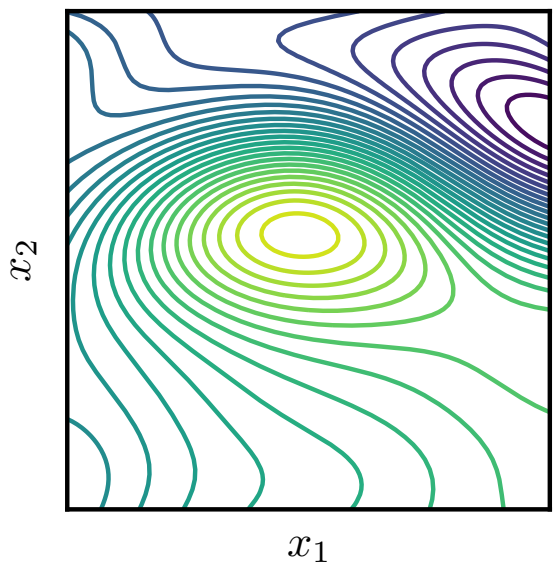

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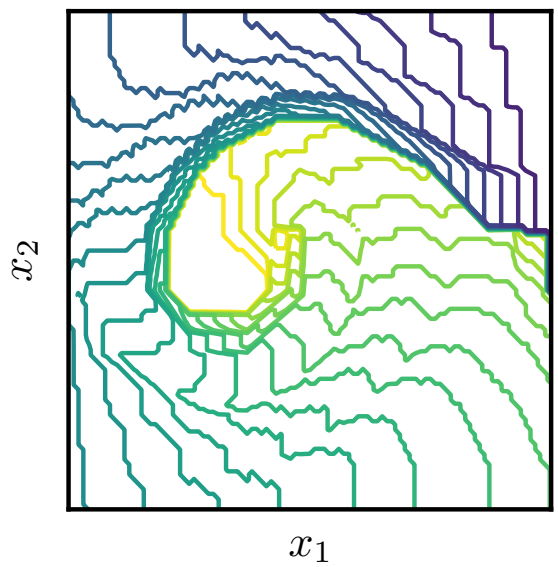

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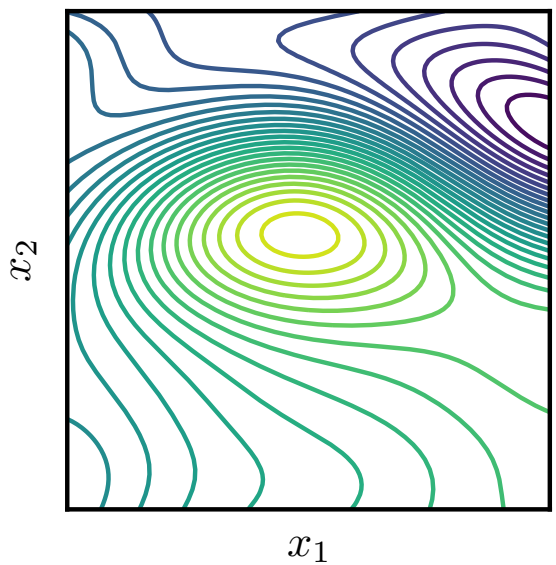

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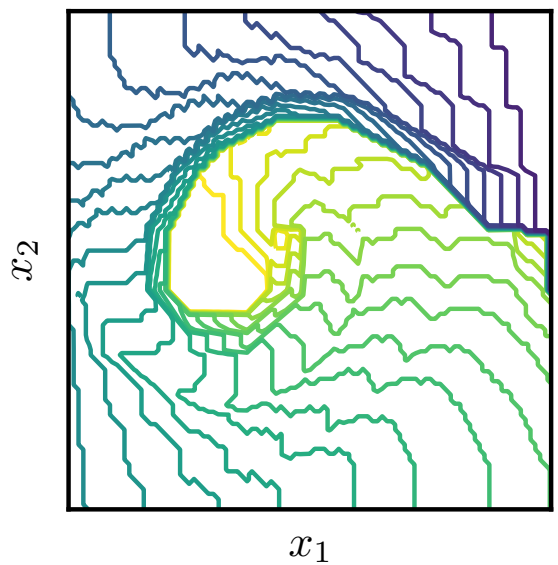
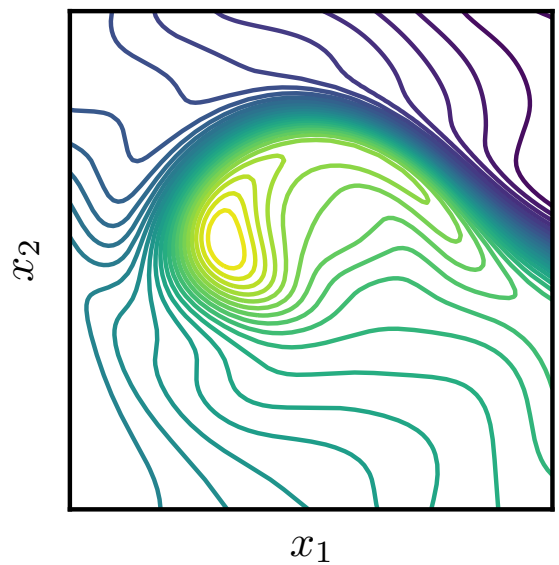
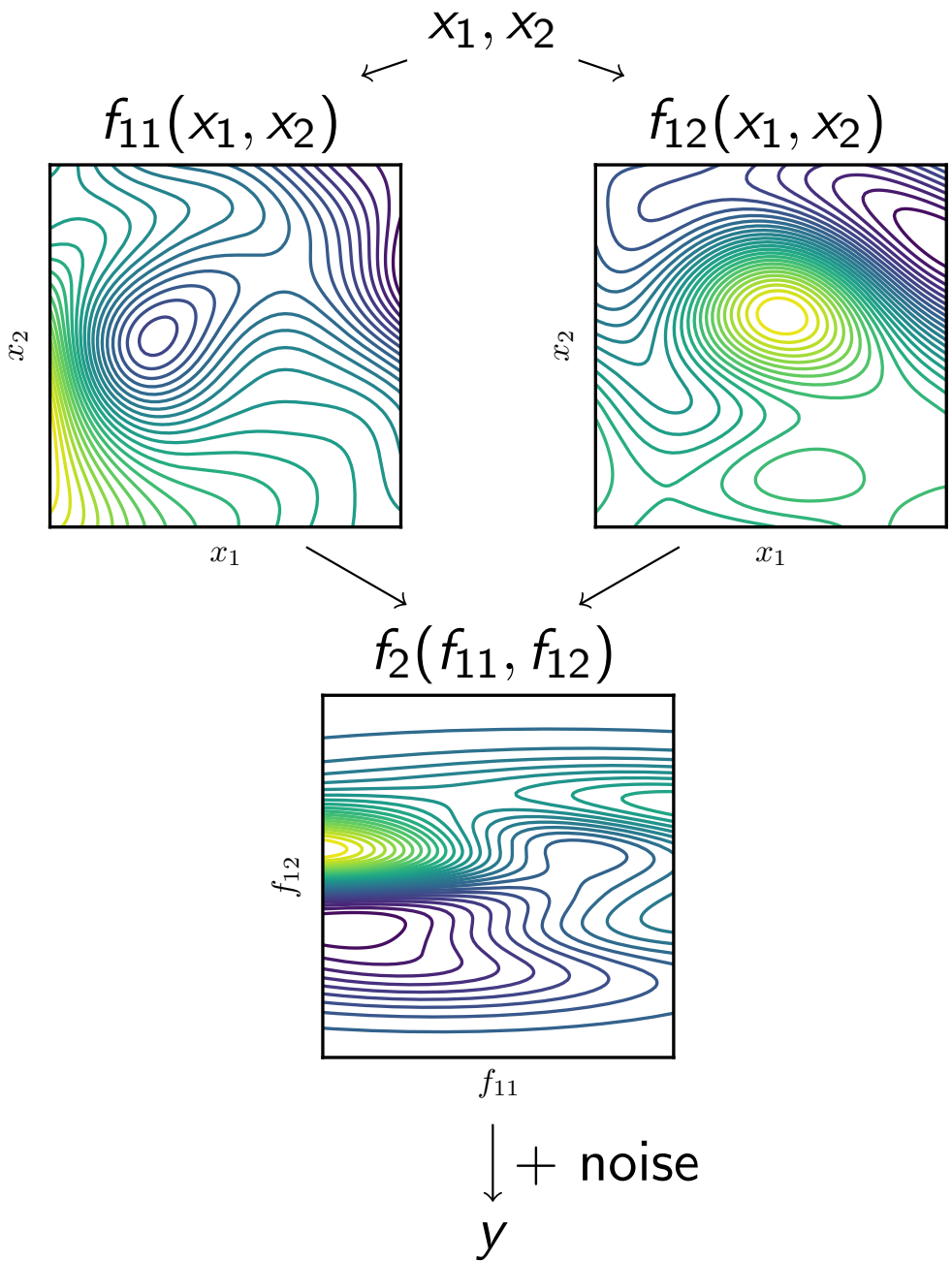


DGP fit



How do deep GPs work?



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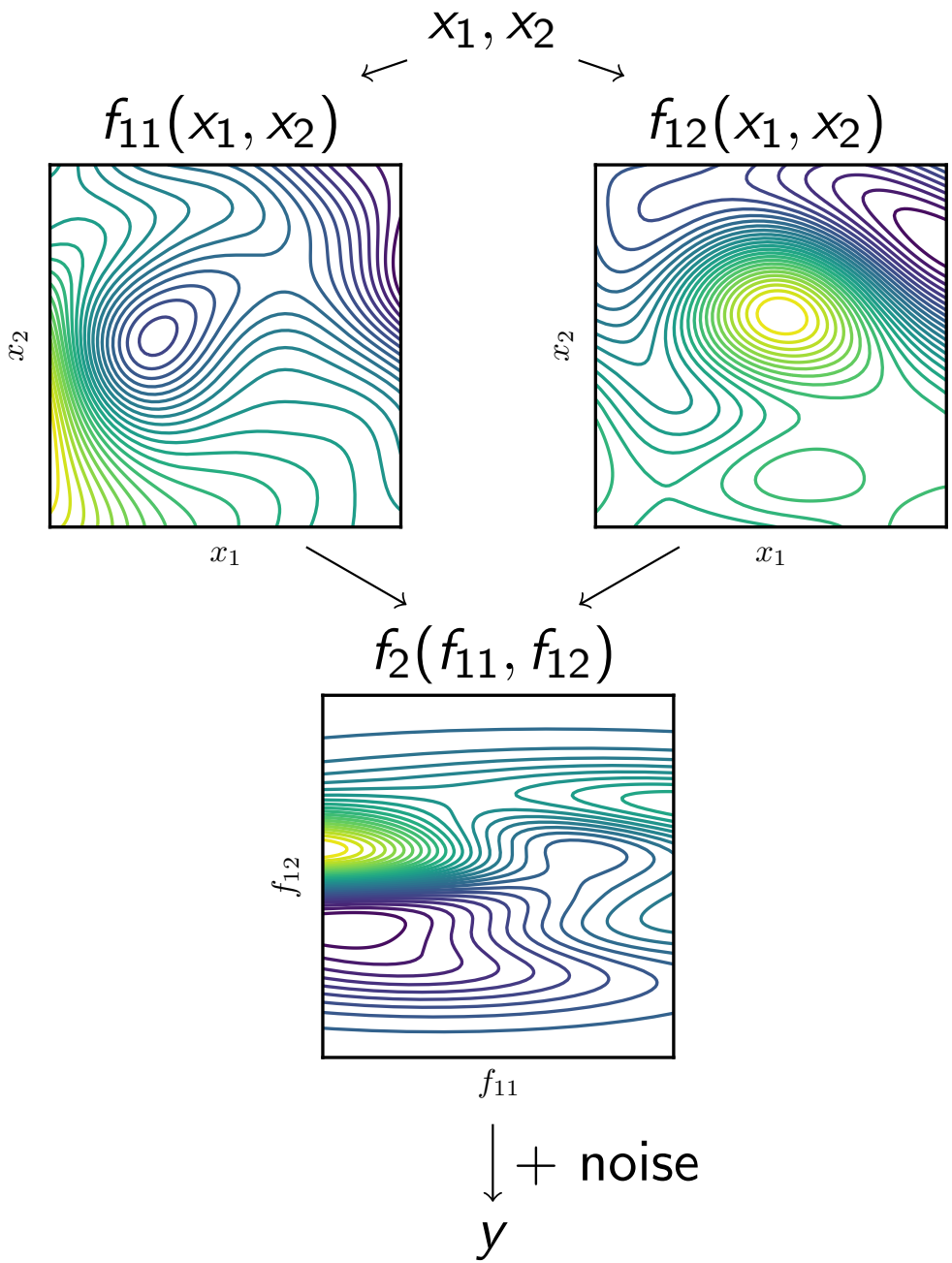

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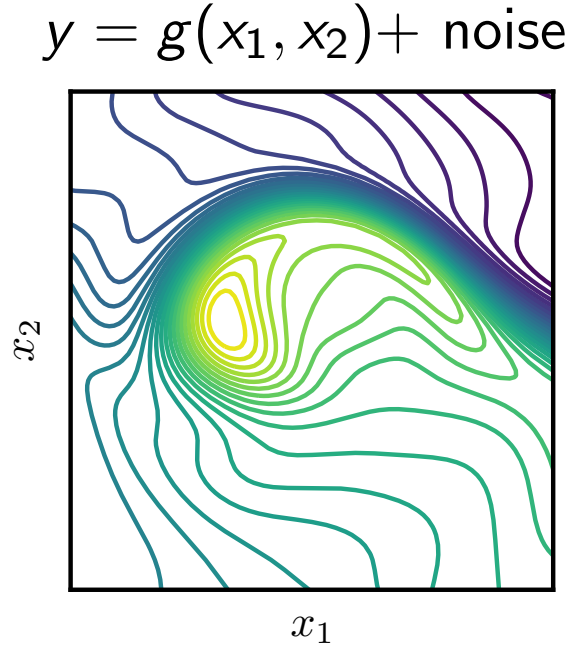

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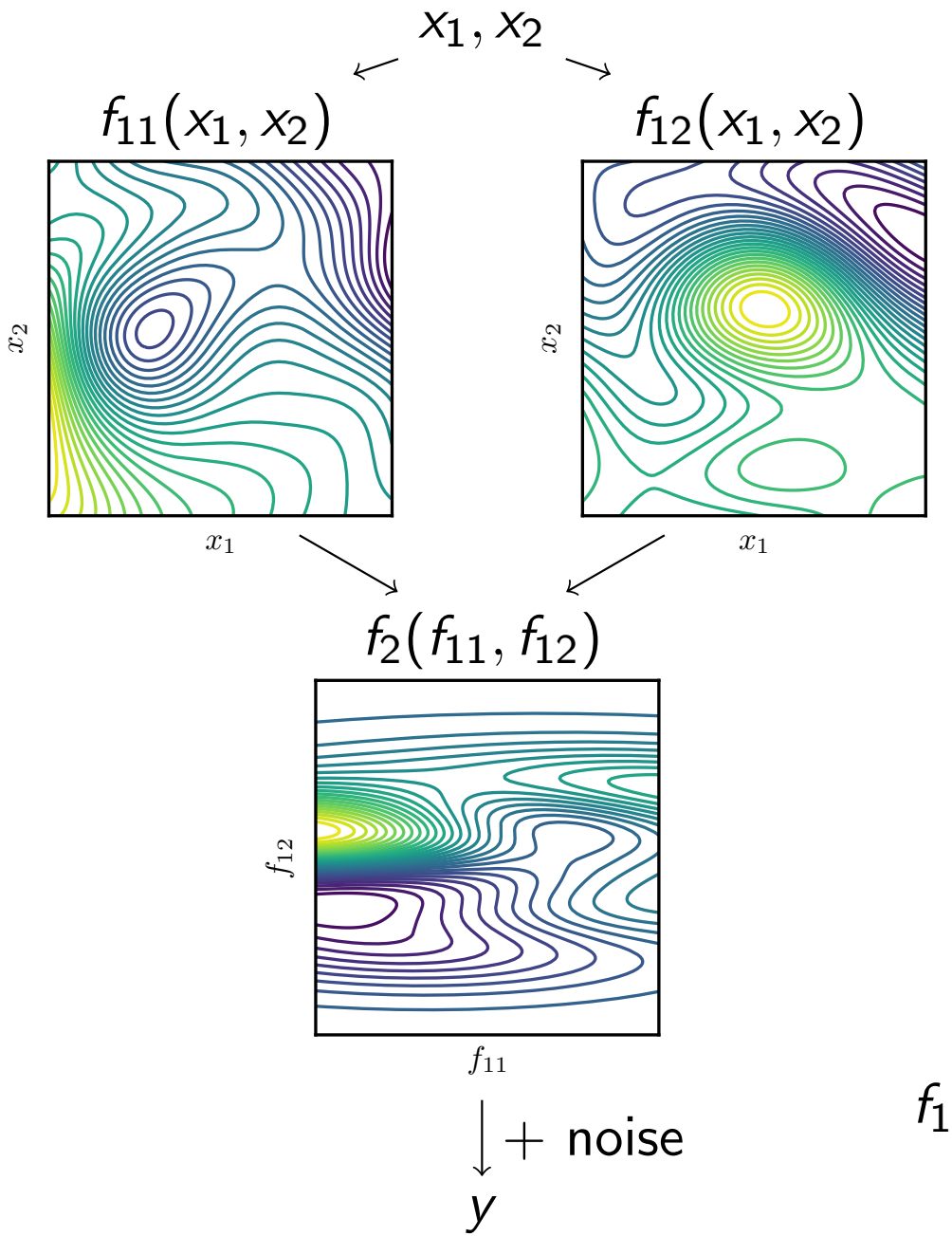

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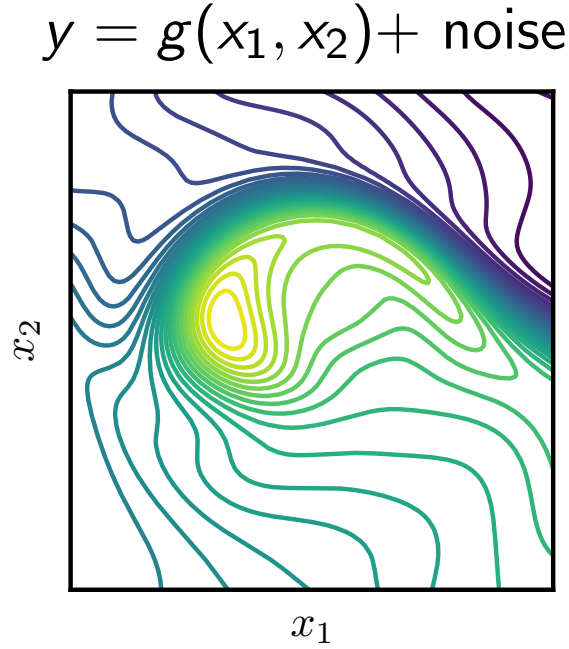
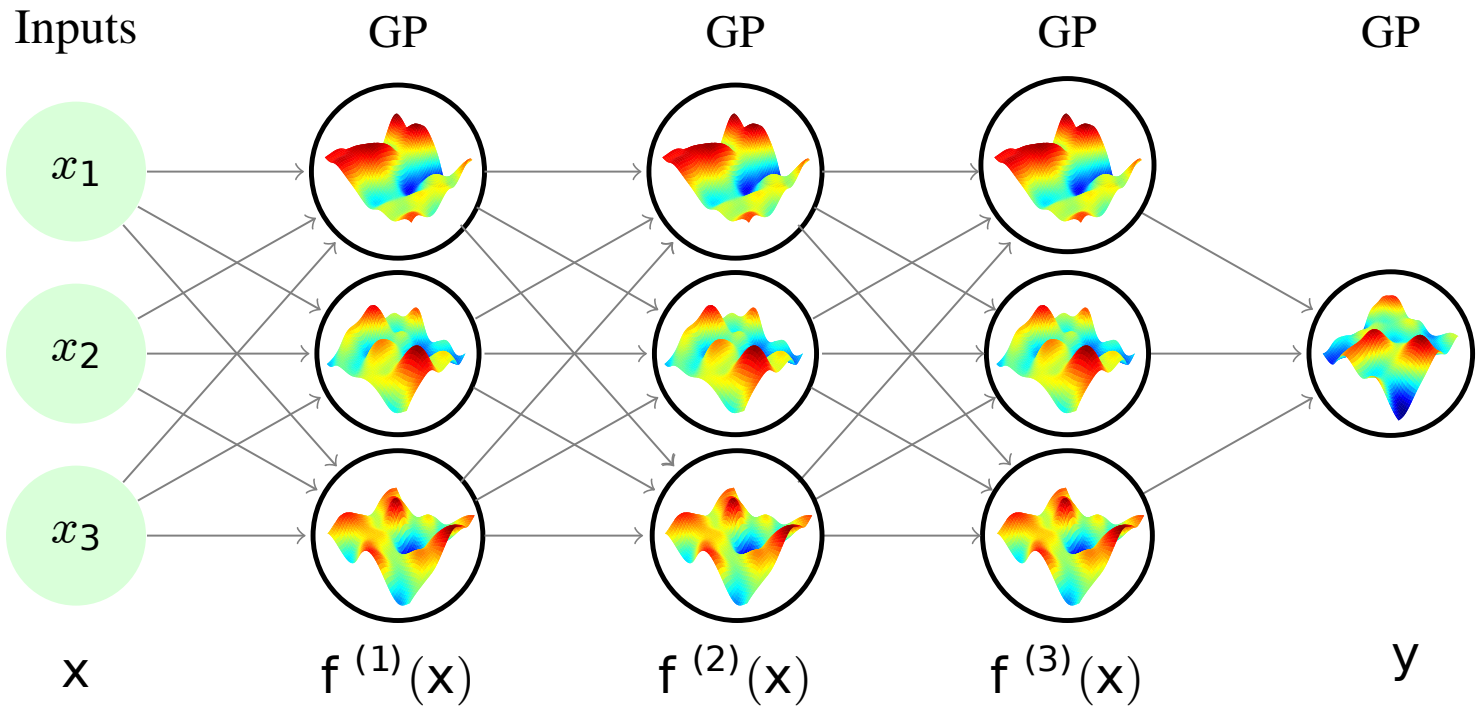


$$f_{11}, f_{12}, f_2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$$

Deep GPs as Deep Neural Networks



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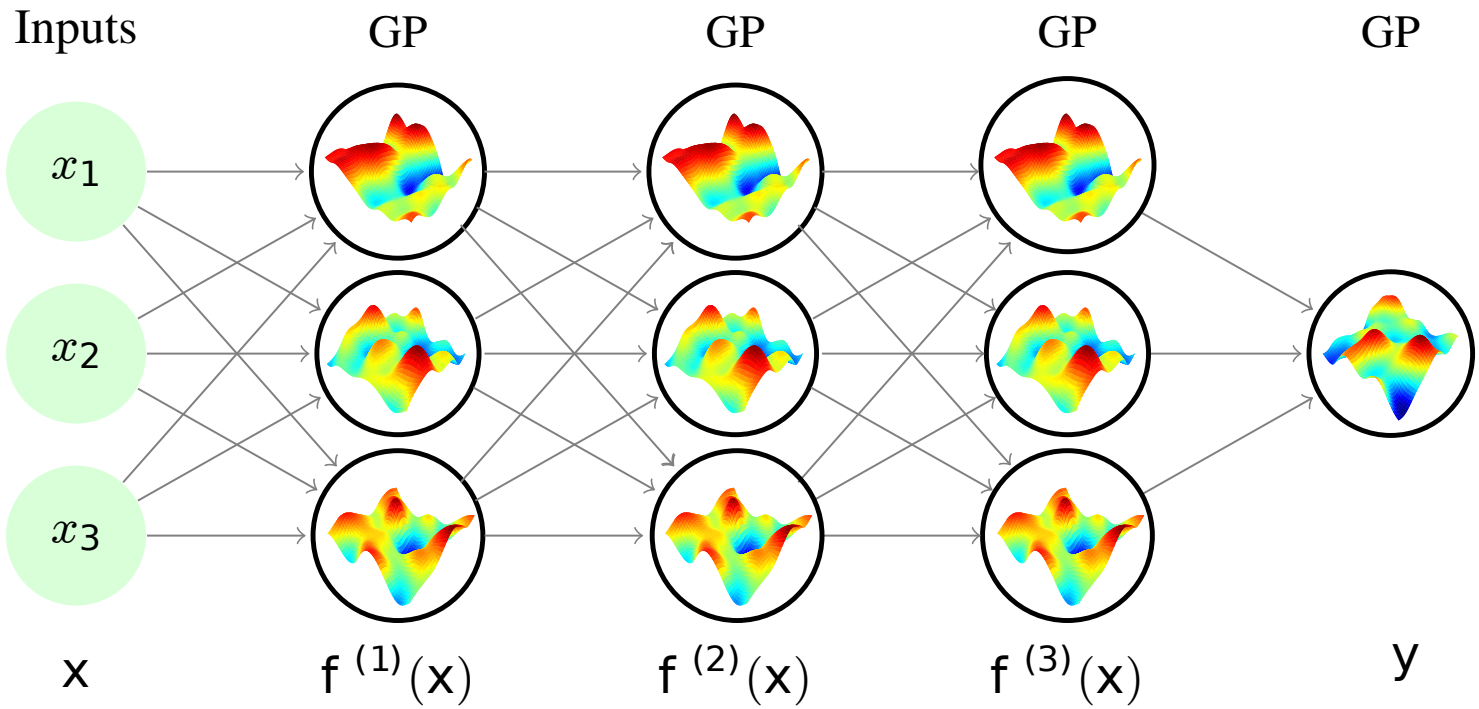

DGPs have a small number of very flexibile units at each layer!

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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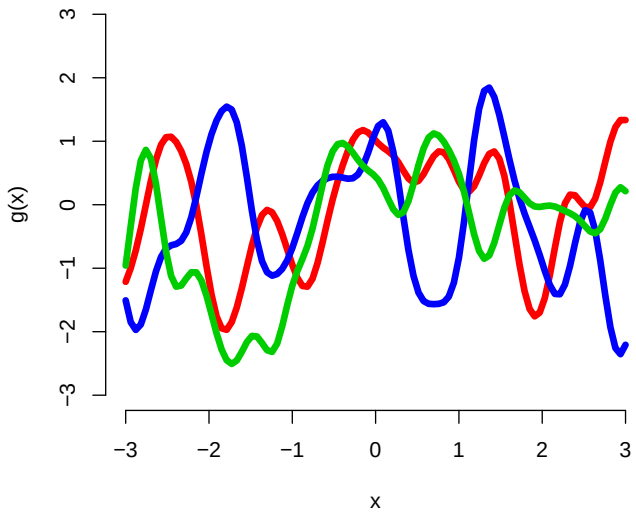

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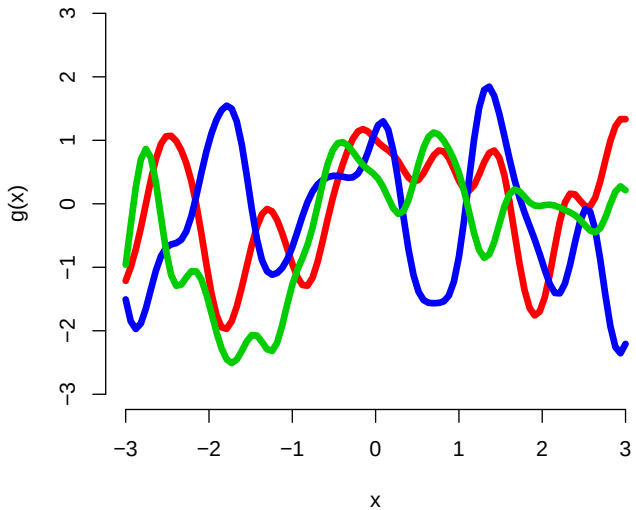

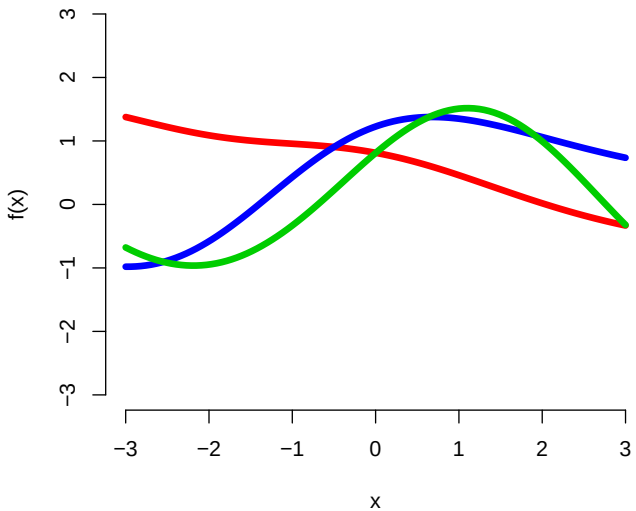

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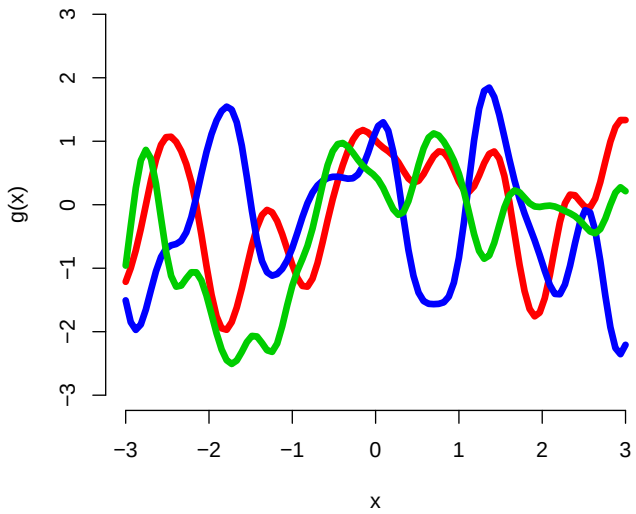

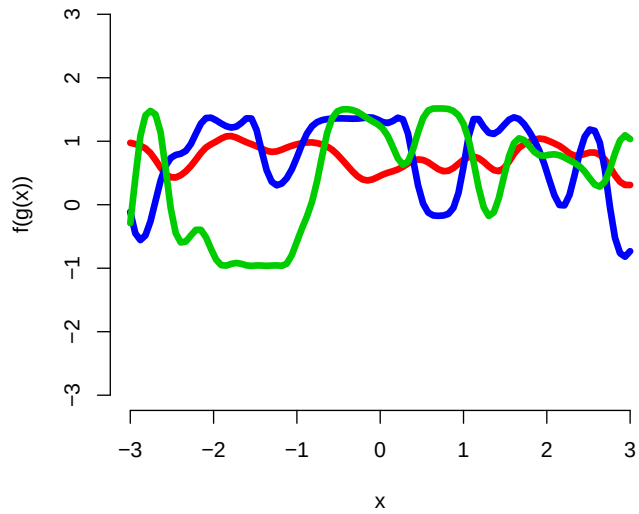

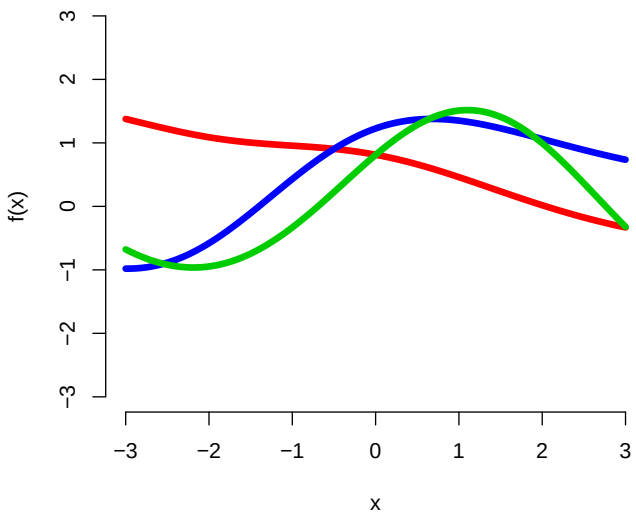

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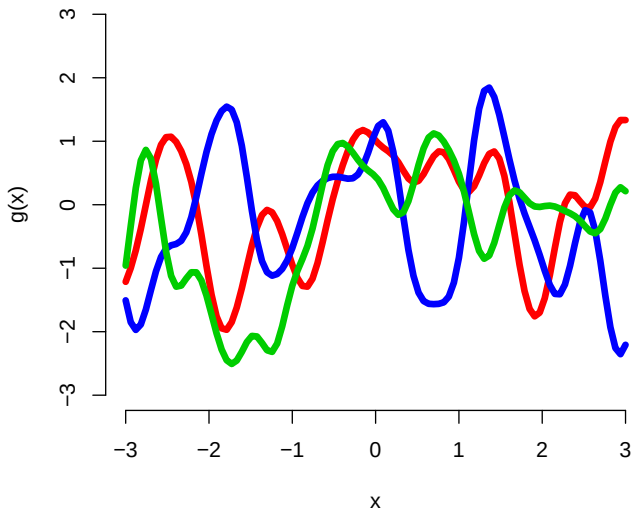
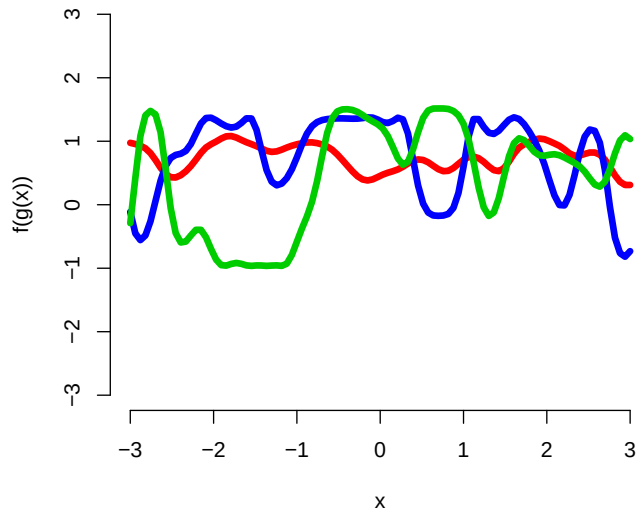
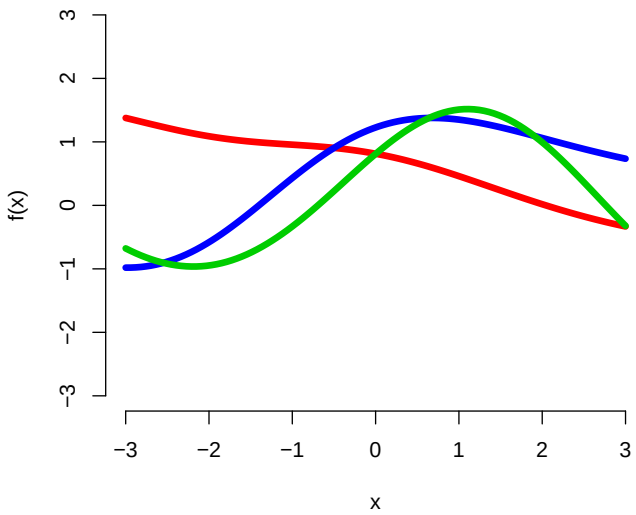
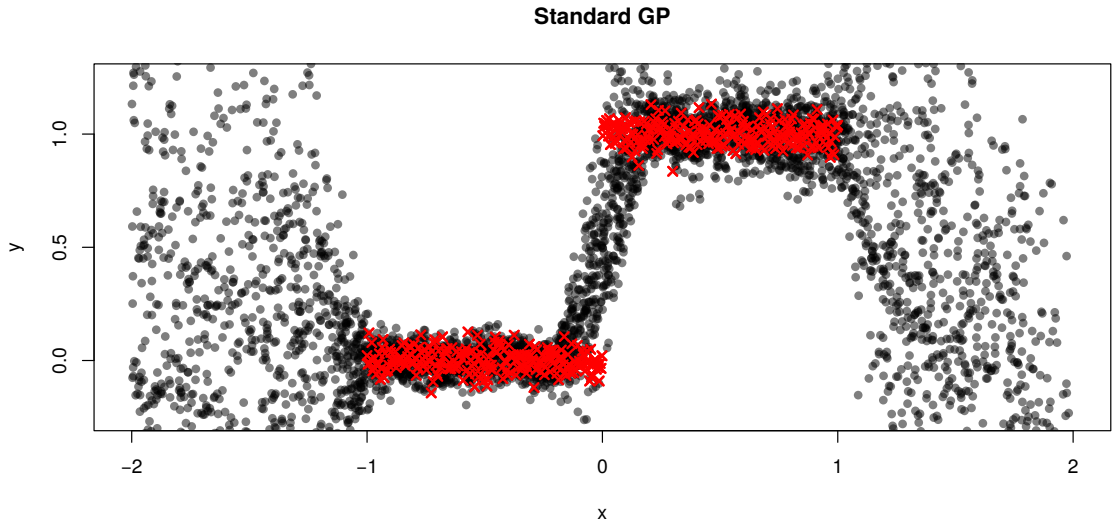






Deep GPs perform automatic covariance function design!

Deep GP Predictive Distribution



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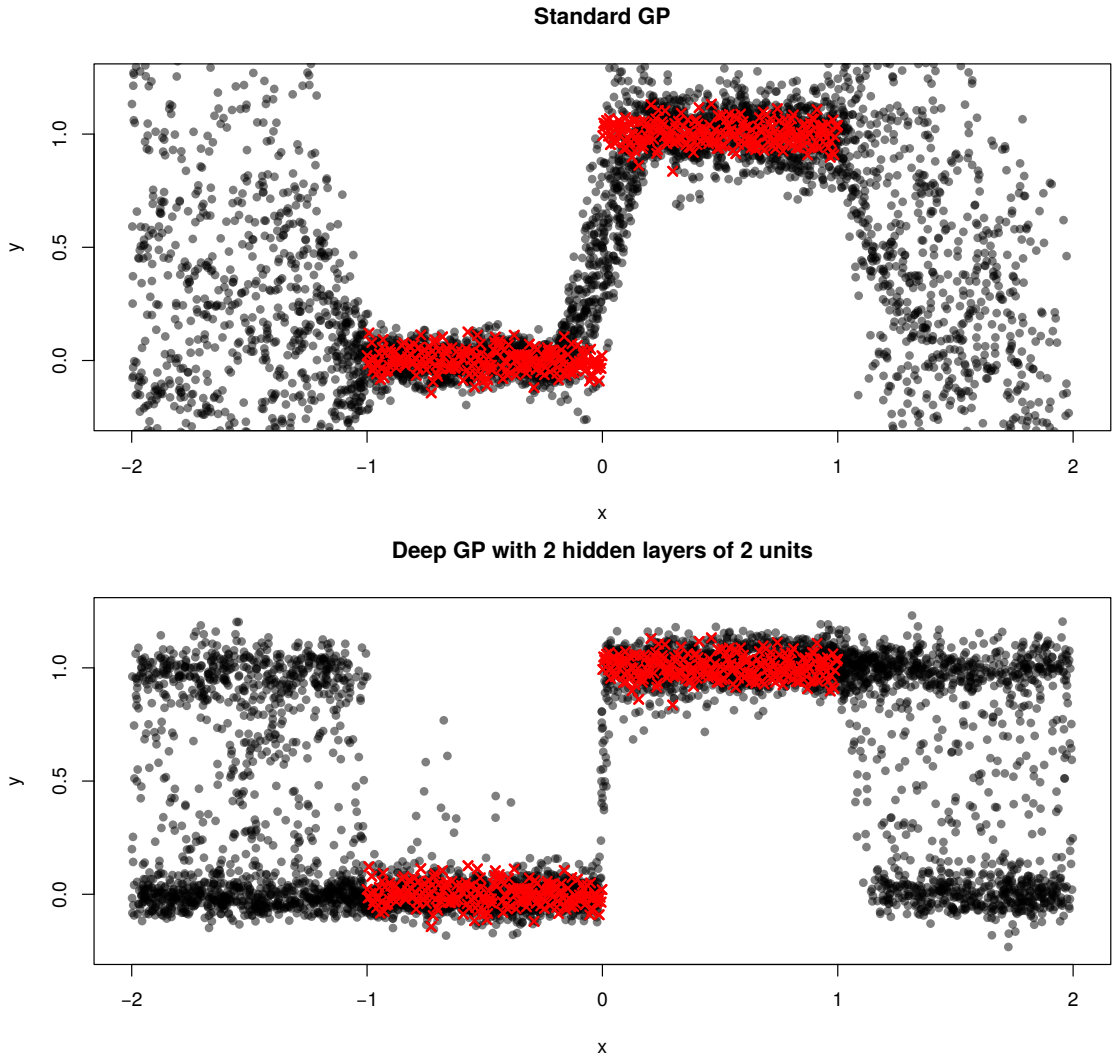

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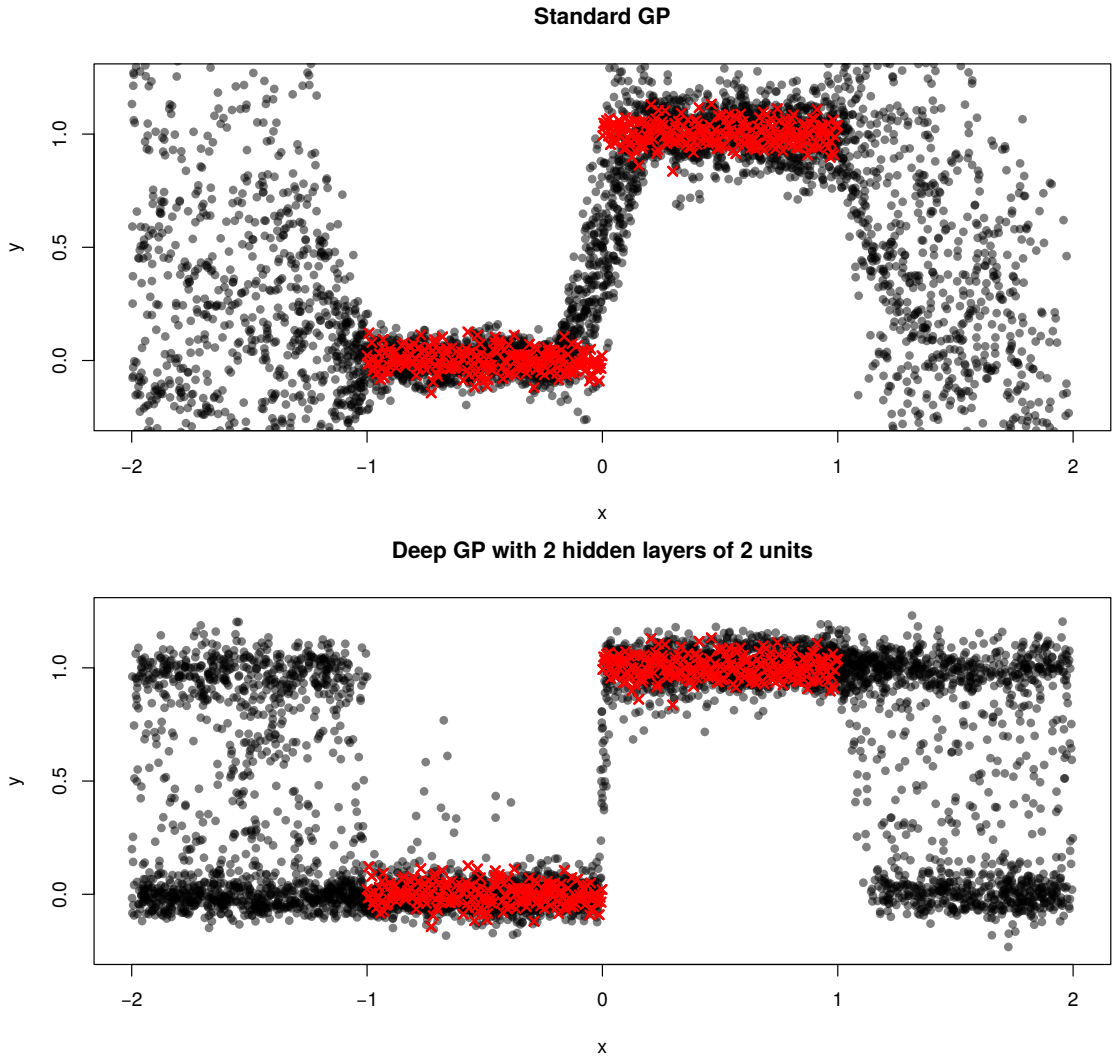

In a deep GP the predictive distribution needs not be Gaussian!

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- Require complicated approximate inference methods.
- High computational cost of approximate inference.

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

$$m^\star = \Sigma_{f^\star,\mathbf{u}}\Sigma_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\,,$$
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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, $f(\mathbf{x}^\star)$ is fully specified!

Deep GPs Joint Distribution

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

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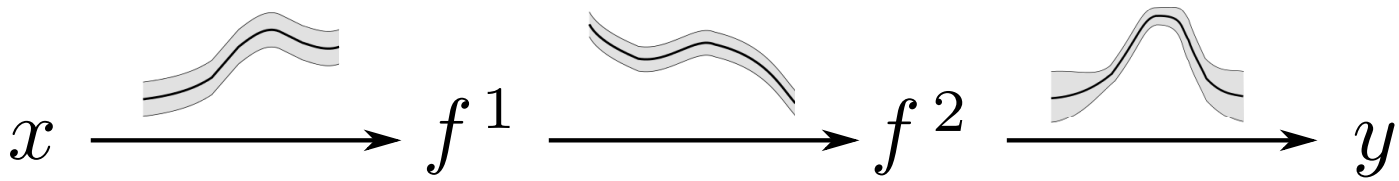
Ideally we would like to make inference about $\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^L$!

Challenges of Approximate Inference for DGPs



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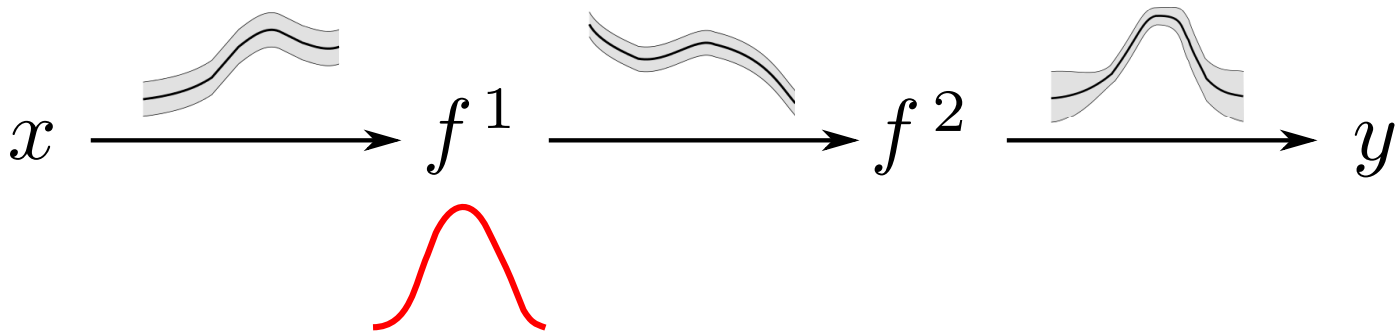

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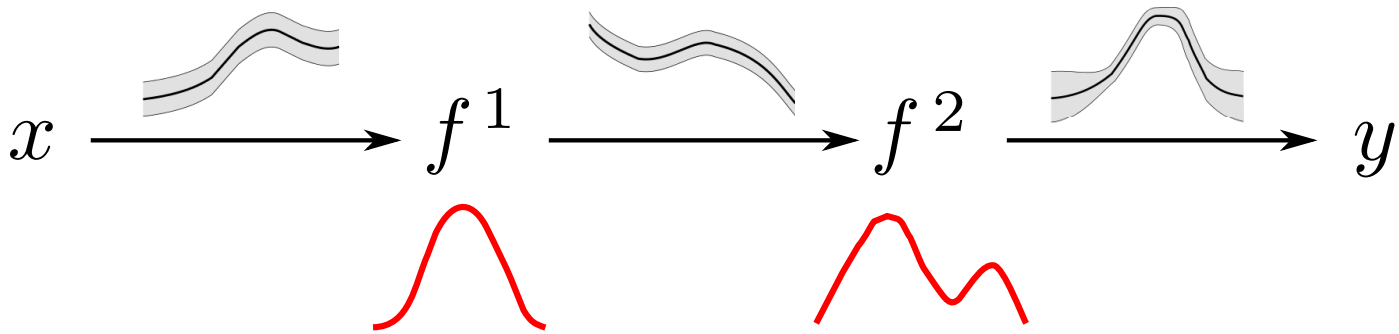

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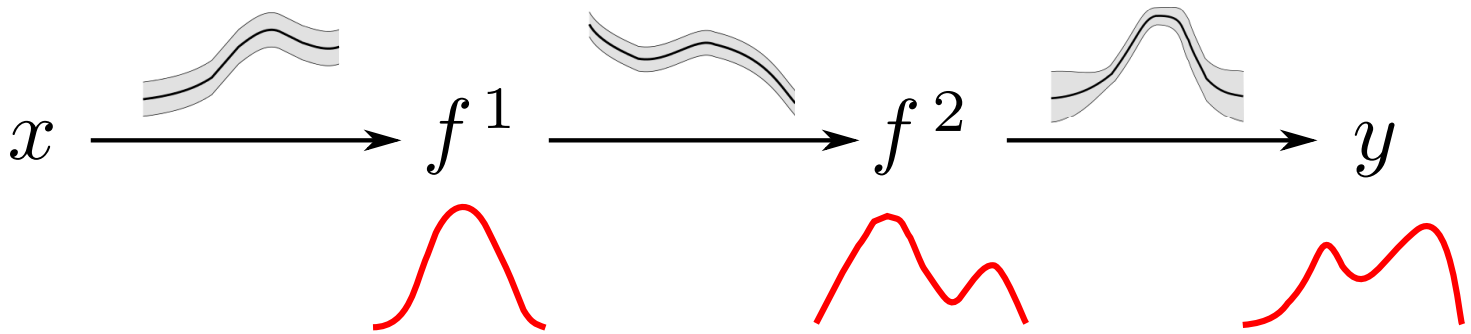

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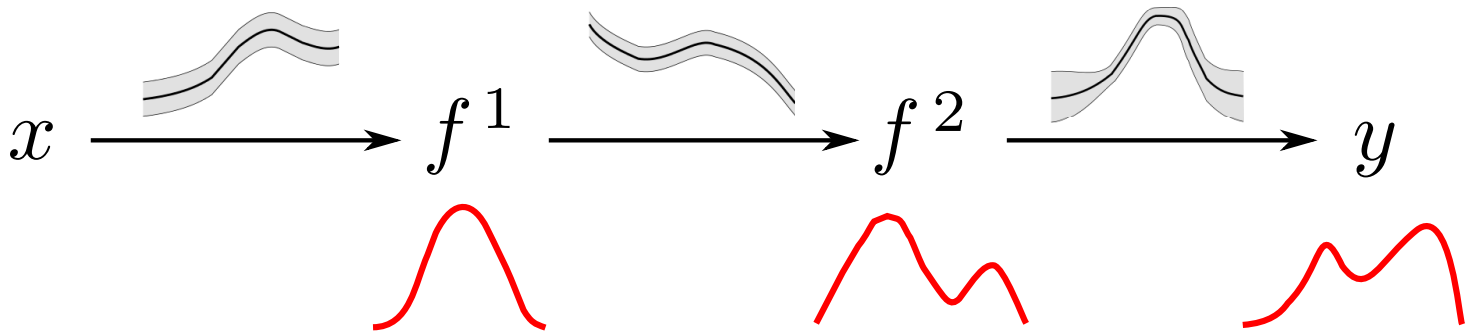

The predictive distribution after the first layer is non Gaussian!

Methods for Training DGPs

- Using VI and an analytic lower bound.

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- Using VI and an analytic lower bound.
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- Using stochastic variational inference.
- By minimizing alpha divergences.

Analytic ELBO via Variational Inference

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For this, noisy versions of the variables at each layer **but last** are introduced:

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with $\boldsymbol{\Lambda}_l$ a diagonal matrix for $l = 1, \ldots, L-1$.

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The joint distribution is now:

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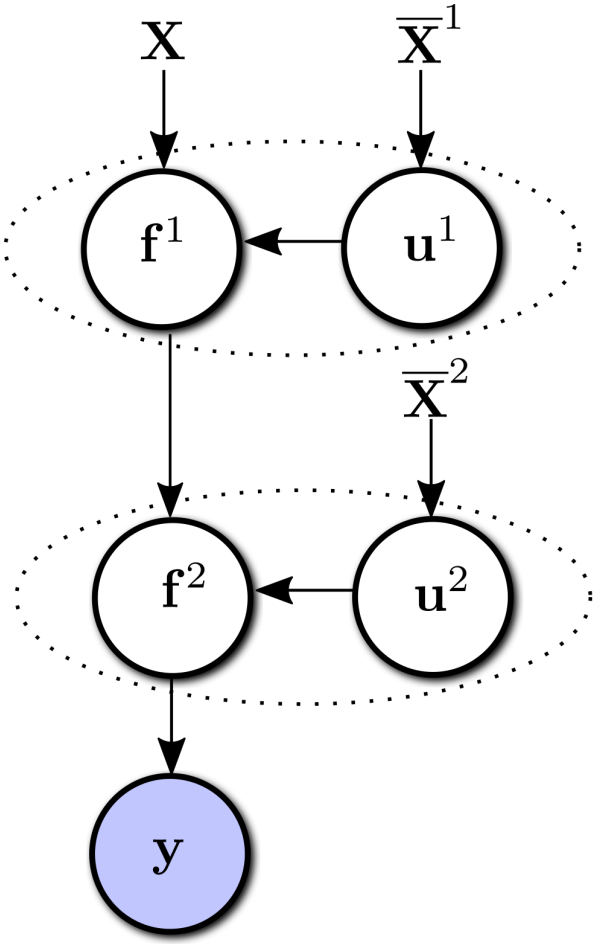
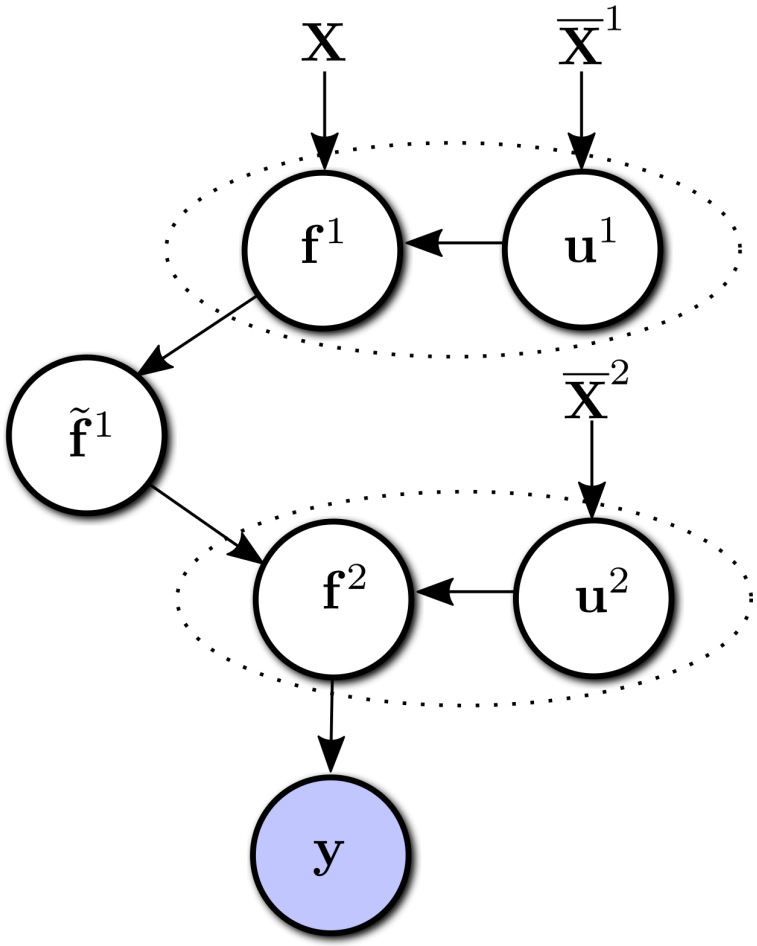
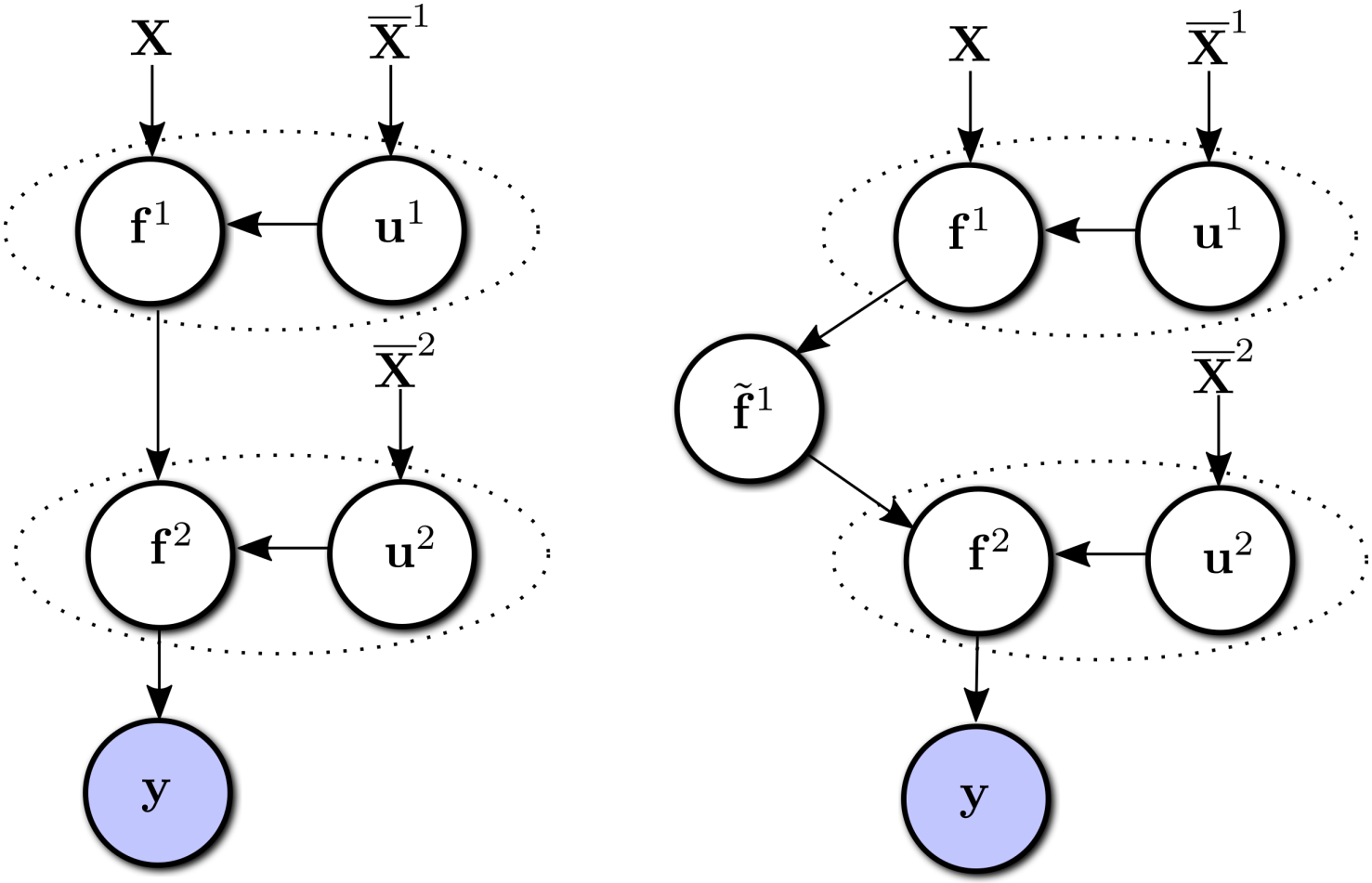
$$\underbrace{p(\mathbf{f}^L|\mathbf{u}^L, \overline{\mathbf{X}}^L)p(\mathbf{u}^L|\overline{\mathbf{X}}^L) \prod_{l=1}^{L-1} p(\tilde{\mathbf{f}}^l|\mathbf{f}^l)p(\mathbf{f}^l|\mathbf{u}^l, \overline{\mathbf{X}}^l)p(\mathbf{u}^l|\overline{\mathbf{X}}^l)}_{\text{Deep GP prior}}$$

Original Graphical Model and Extended





Original Graphical Model and Extended



Both models are equivalent, but this setting simplifies inference!

Analytic ELBO via Variational Inference

The posterior approximation q considered assumes independence among layers!

Analytic ELBO via Variational Inference

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Posterior approximation:

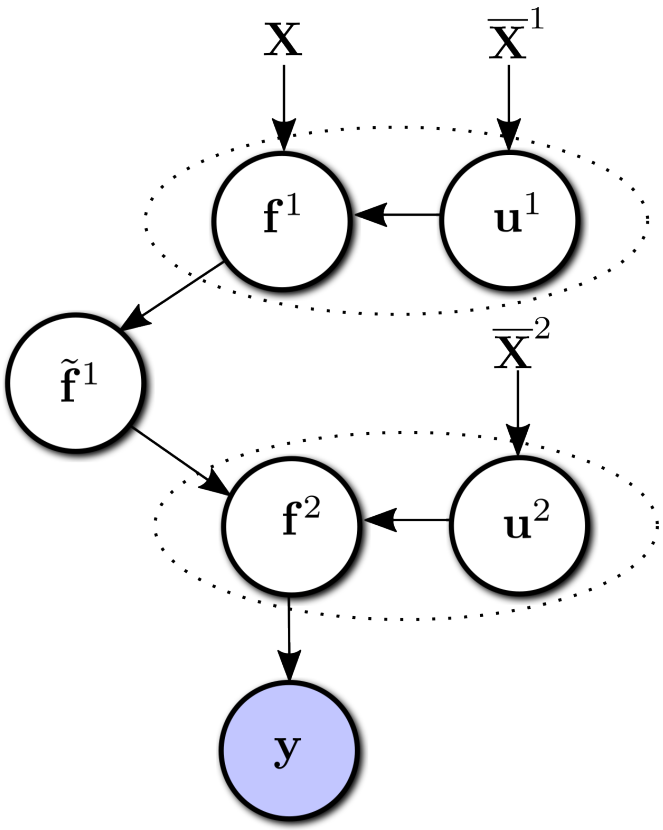
$$q(\{\mathbf{u}^l, \mathbf{f}^l, \tilde{\mathbf{f}}^l\}_{l=1}^L) = q(\mathbf{u}^L) p(\mathbf{f}^L | \mathbf{u}^L, \overline{\mathbf{X}}^l) \prod_{l=1}^{L-1} q(\mathbf{u}^l) q(\tilde{\mathbf{f}}^l) p(\mathbf{f}^l | \mathbf{u}^l, \overline{\mathbf{X}}^l)\,,$$

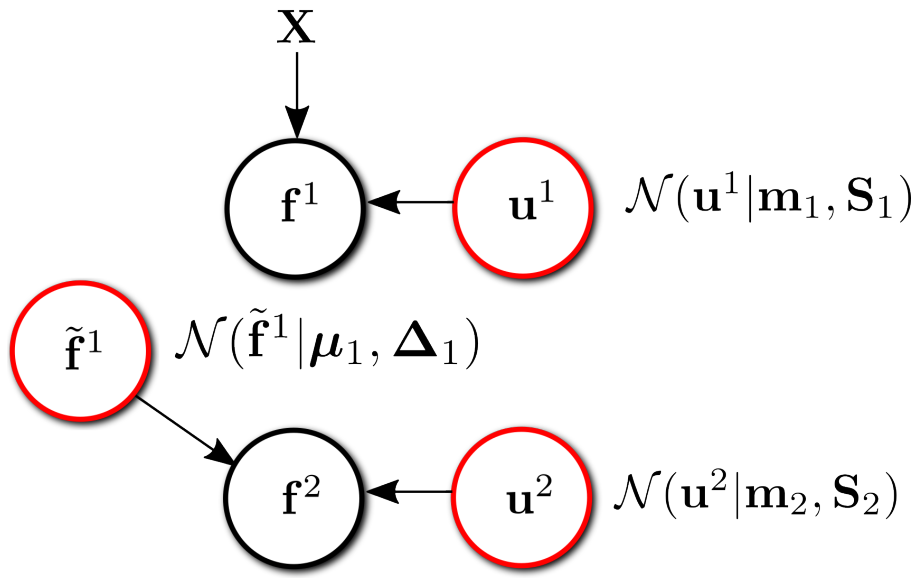
where the input to the layer $l+1$ is $\tilde{\mathbf{f}}^l$ and

$$q(\mathbf{u}^l) = \mathcal{N}(\mathbf{u}^l | \mathbf{m}_l, \mathbf{S}_l)\,, \qquad q(\tilde{\mathbf{f}}^l) = \mathcal{N}(\tilde{\mathbf{f}}^l | \boldsymbol{\mu}_l, \boldsymbol{\Delta}_l)\,,$$

with $\boldsymbol{\Delta}_l$ a diagonal matrix.

Graphical Model and Approximate Distribution





Analytic Variational Inference for DGPs

Minimizes KL$(q(\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^L, \{\tilde{\mathbf{f}}^l\}_{l=1}^{L-1}) | p(\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^L, \{\tilde{\mathbf{f}}^l\}_{l=1}^{L-1} | \mathbf{y}))$

(Damianou, 2013)

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

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

$$= \sum_{i=1}^N \mathbb{E}_q[\log p(y_i|f_i^L)] + \sum_{l=1}^{L-1} \left[\mathbb{E}_q[\log p(\tilde{\mathbf{f}}^l|\mathbf{f}^l)] + H[q(\tilde{\mathbf{f}}^l)] \right]$$

$$- \sum_{l=1}^L \mathrm{KL}(q(\mathbf{u}^l)|p(\mathbf{u}^l)).$$

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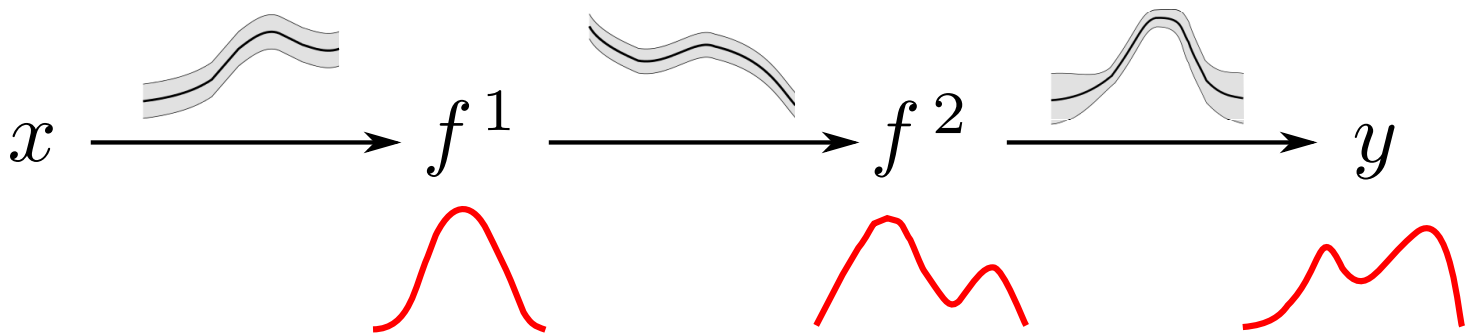
Which can be evaluated in closed-form (form some cov. functions) and maximized to find q and good model hyper-parameters!

(Damianou, 2013)

Predictive Distribution via Monte Carlo Sampling



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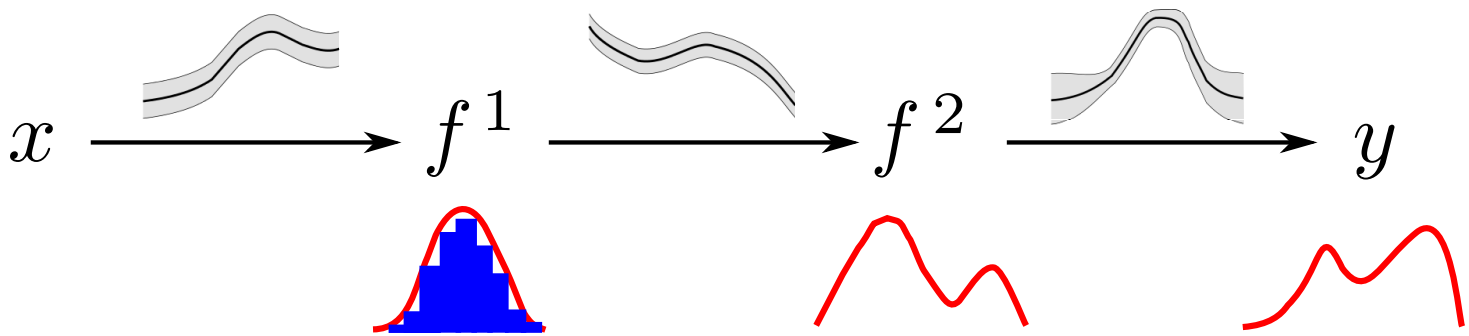

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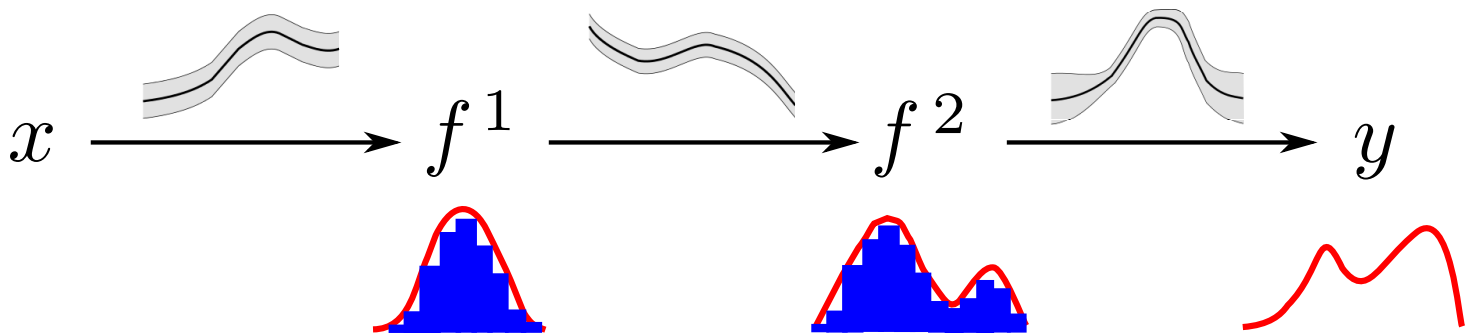

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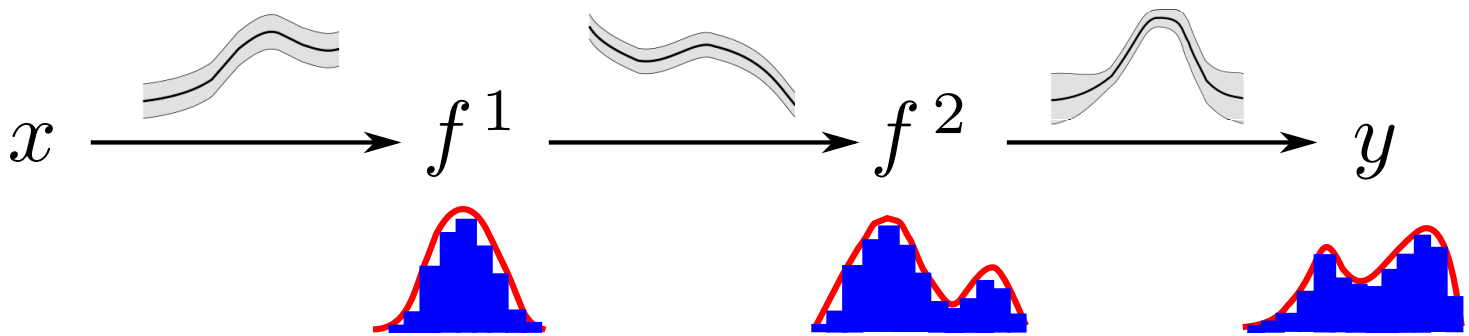

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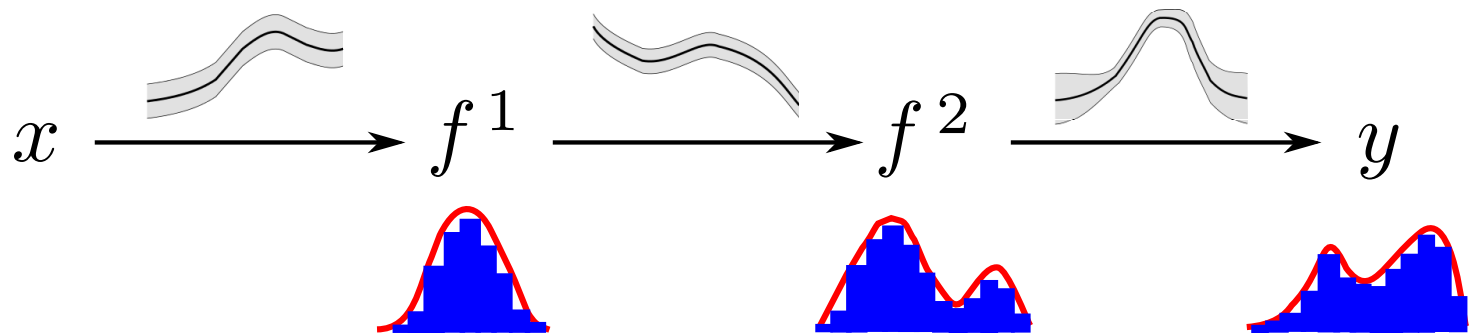
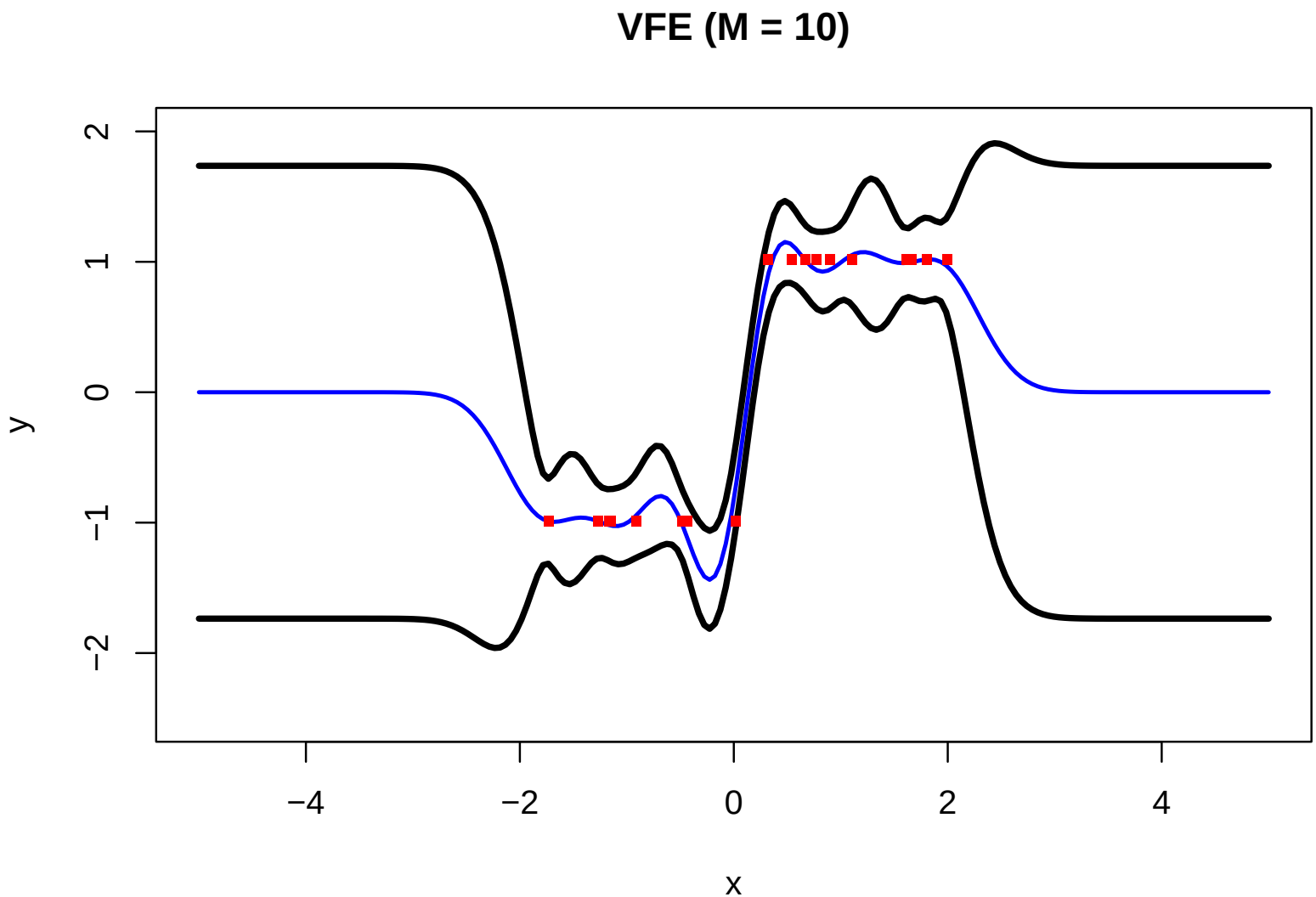


For a particular fixed input, the predictive distribution of each layer is Gaussian!

DGPs Tractable Bound: Illustrative Example



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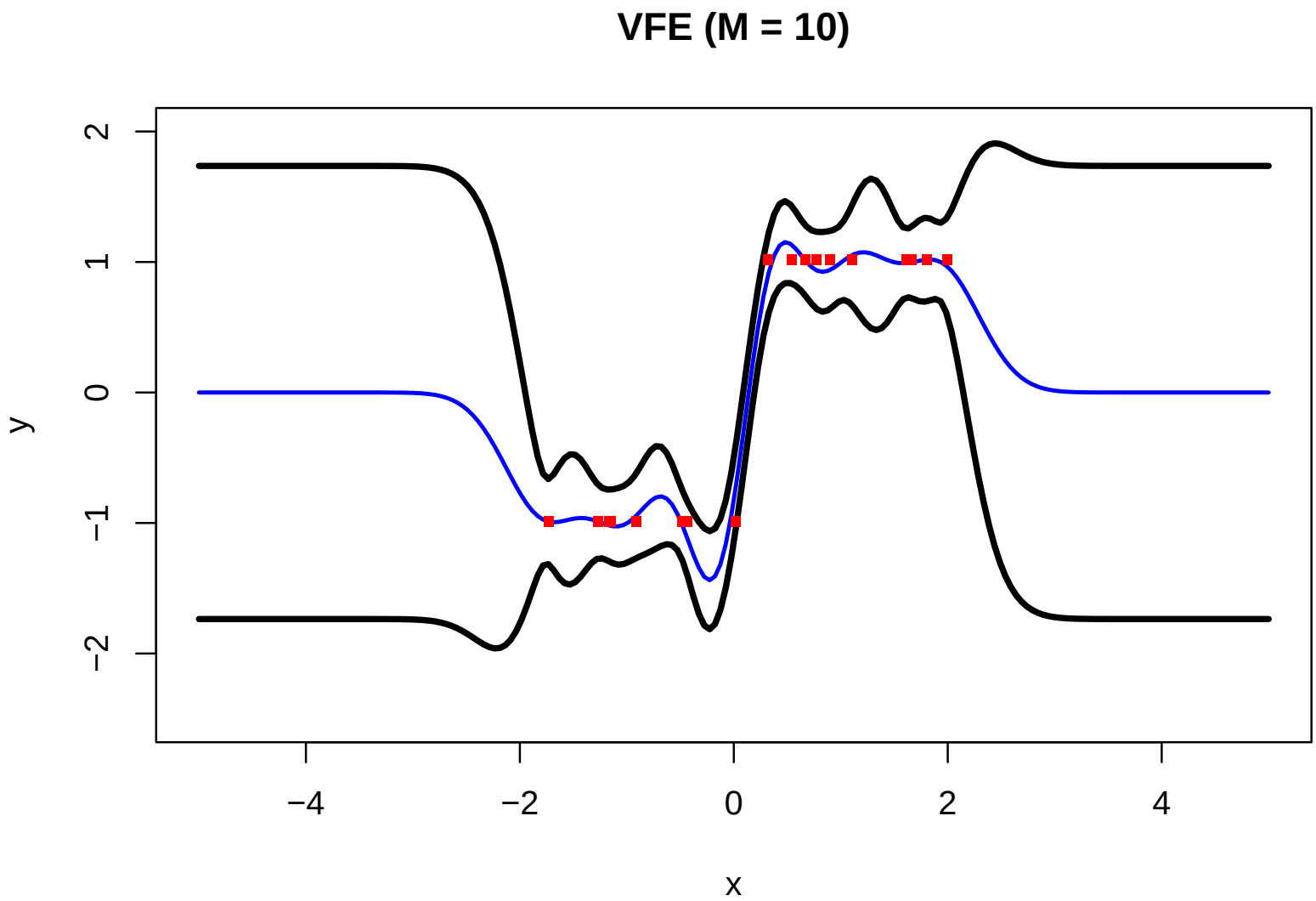

The VFE sparse GP reduces the length-scale to explain the data!

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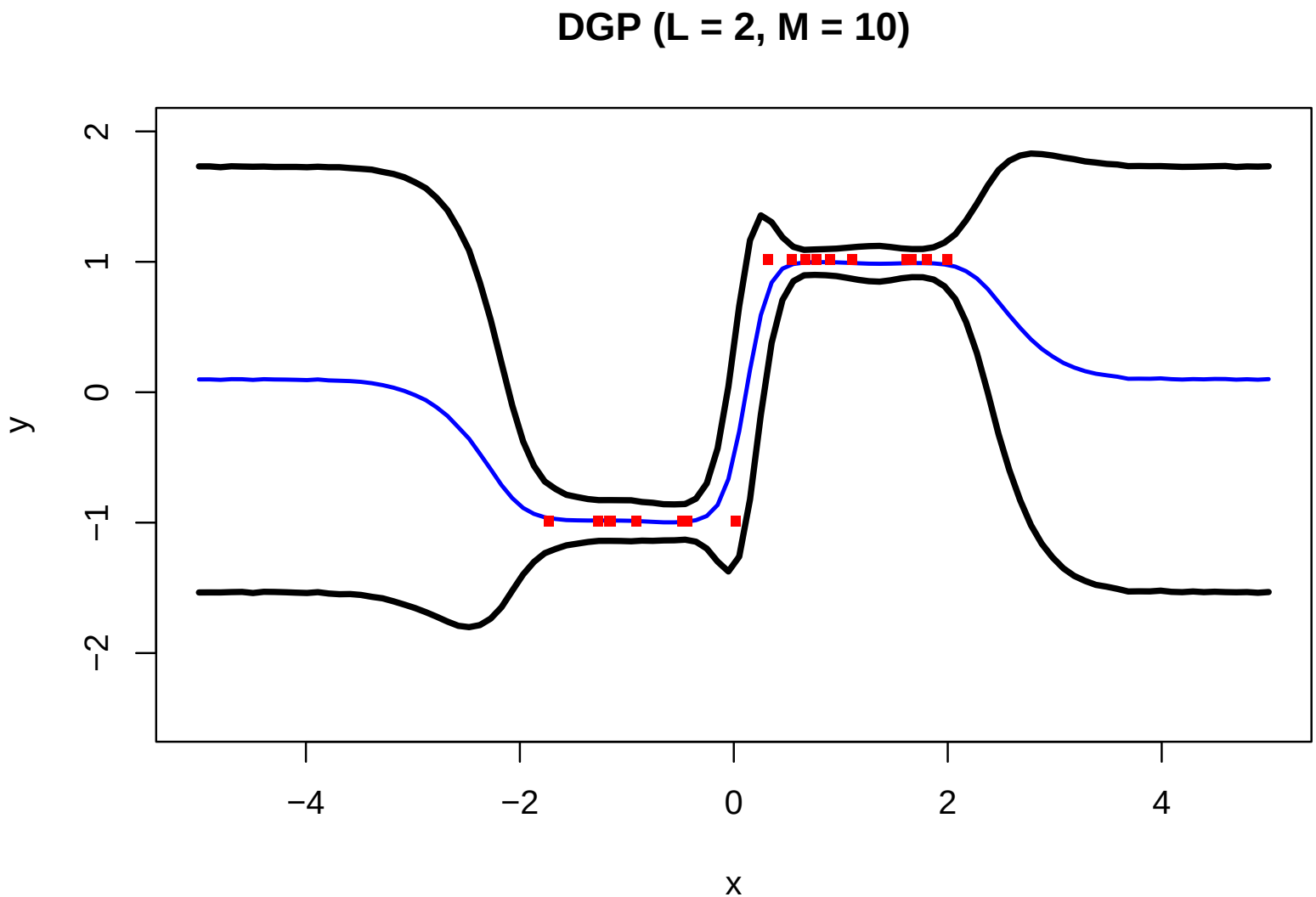

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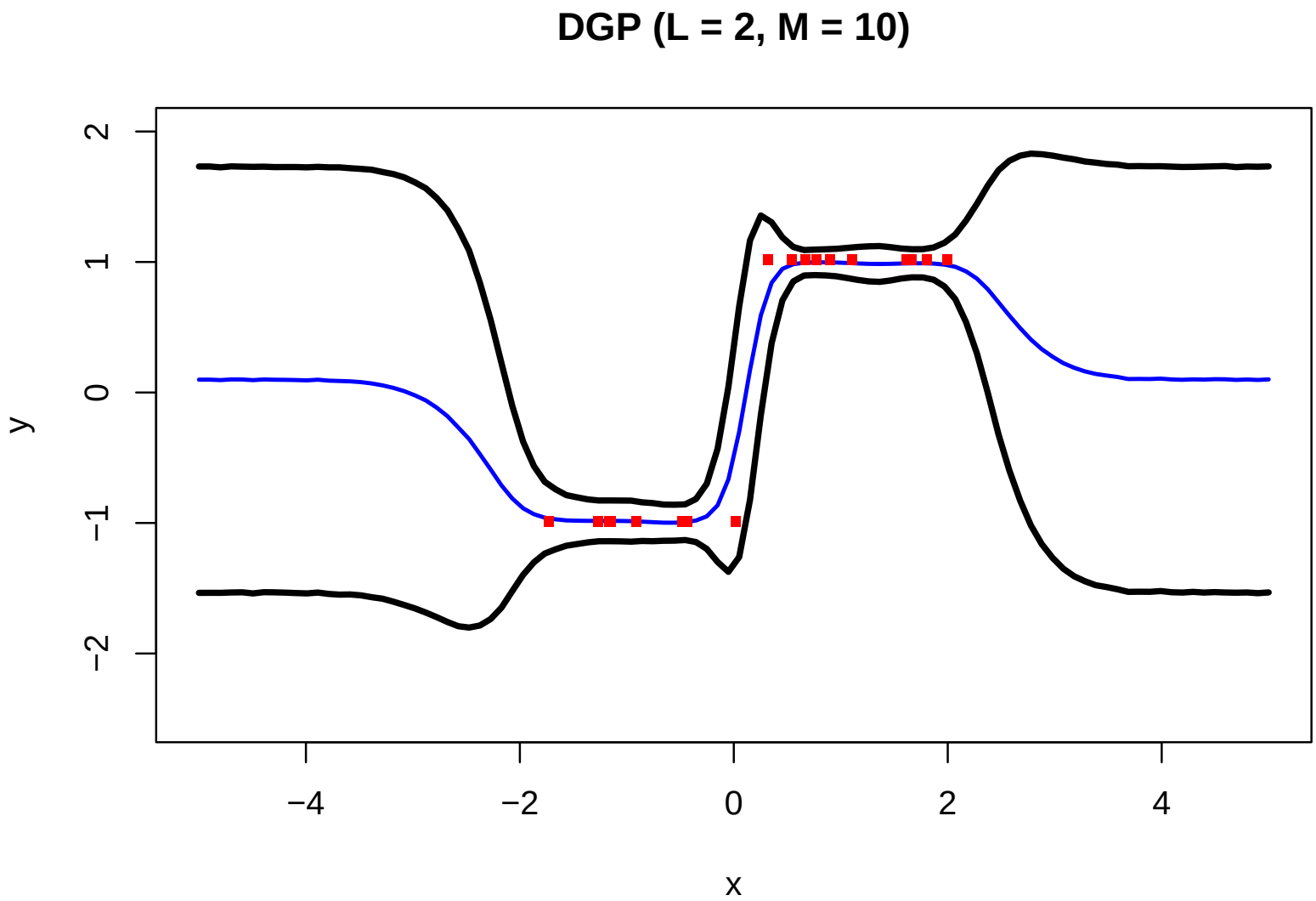
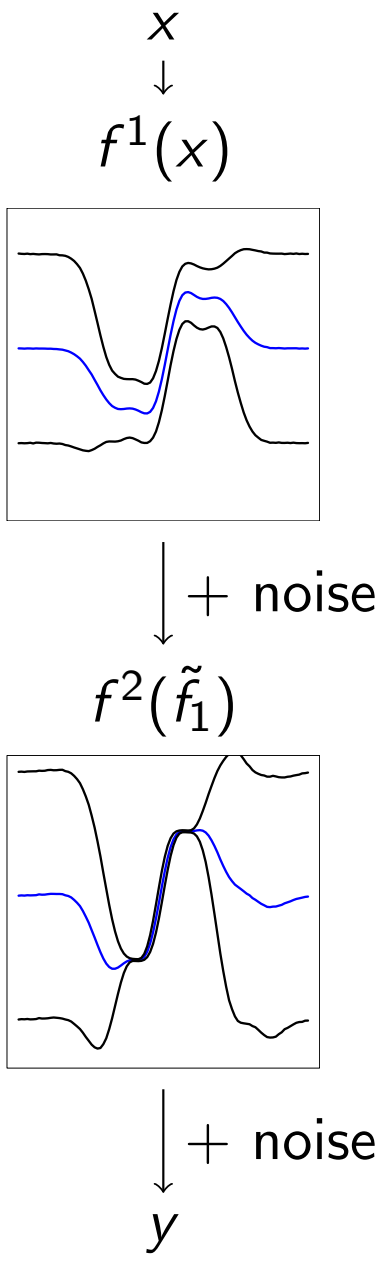


The DGP provides a more sensible predictive distribution!

DGPs Tractable Bound: Illustrative Example

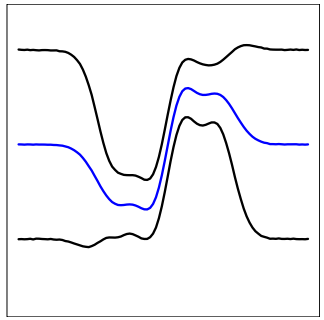


DGPs Tractable Bound: Illustrative Example

x

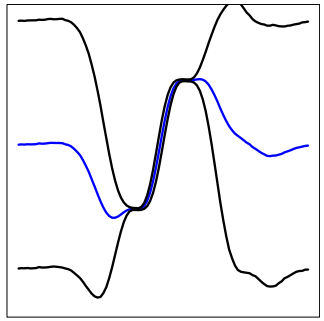
$\downarrow$

$f^1(x)$



$\downarrow$ + noise

$f^2(\tilde{f}_1)$

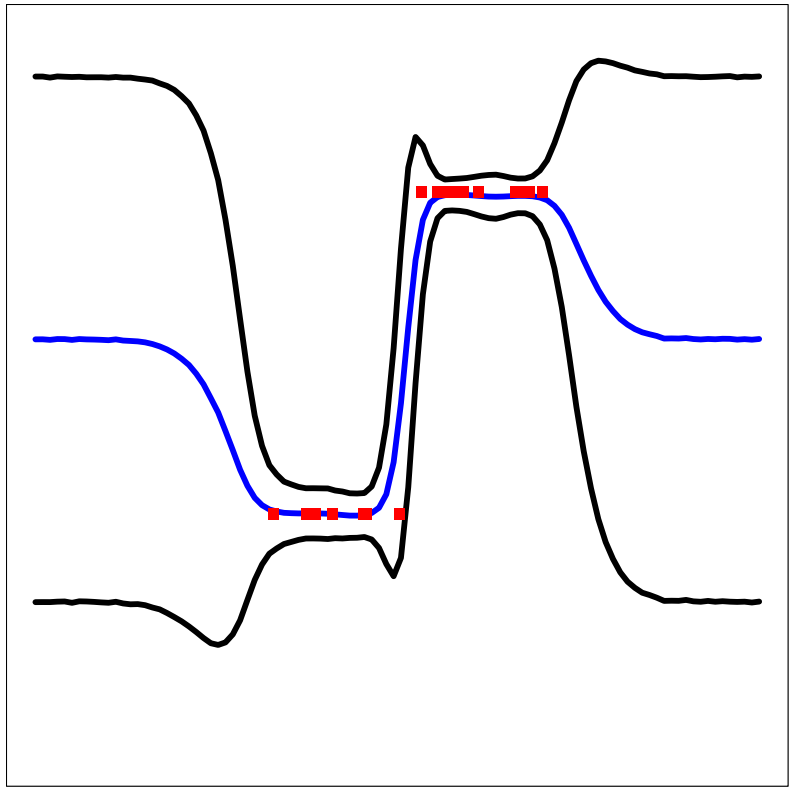


$\downarrow$ + noise

y

$\equiv$

$y = f^2(f^1(x) + \text{noise}) + \text{noise}$



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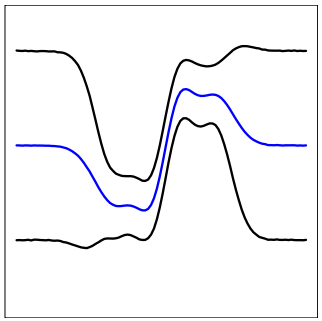

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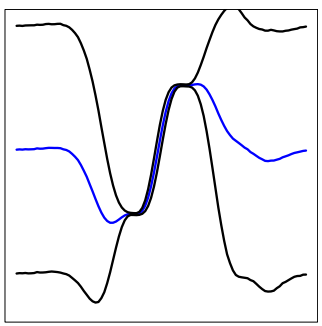

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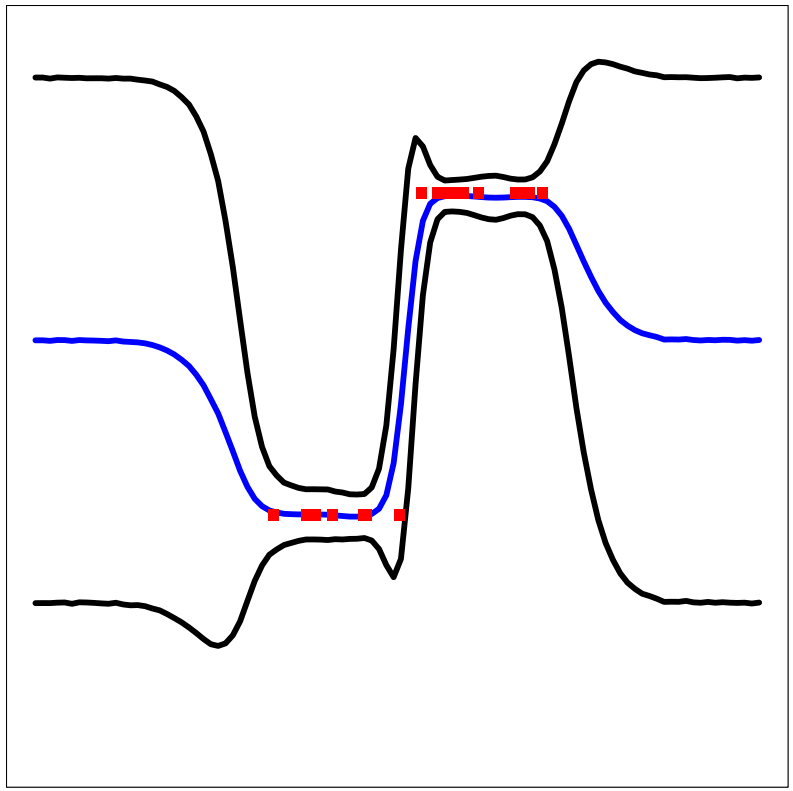

$f^1, f^2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$

Limitations of DGPs via Tractable VI Bound

- The posterior approximation q assumes independence between layers inputs and outputs.

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- The tractable VI bound is limited to certain covariance functions, *e.g.*, the squared exponential covariance function.
- The original method did not consider mini-batch training and scales linearly with N, which makes infeasible addressing large problems.

DGPs and Approximate Expectation Propagation

Features:

- Does not assume independence between inputs and outputs in each layer in the approximate distribution q.

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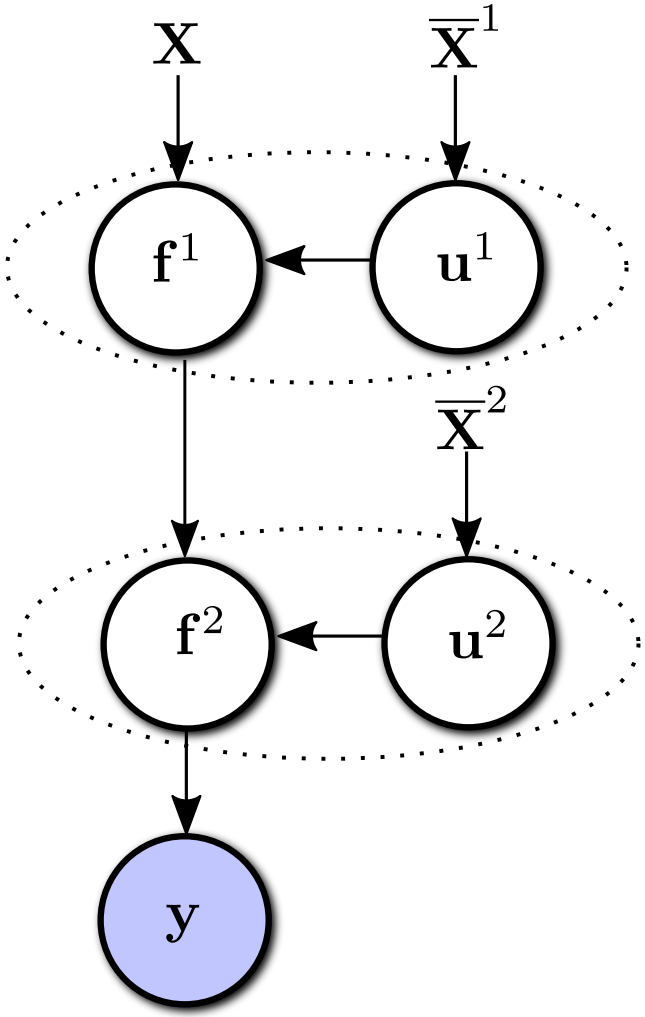
- Uses the FITC approximation for tractable scaling and allows for mini-batch training. Thus, the model is changed.
- Relies on a modified version of EP to estimate the approximate distribution q using standard optimization techniques.
- The intractable predictive distribution at each layer is approximated by a Gaussian with the same moments.

(Bui et al., 2016)

Alternative Graphical Model



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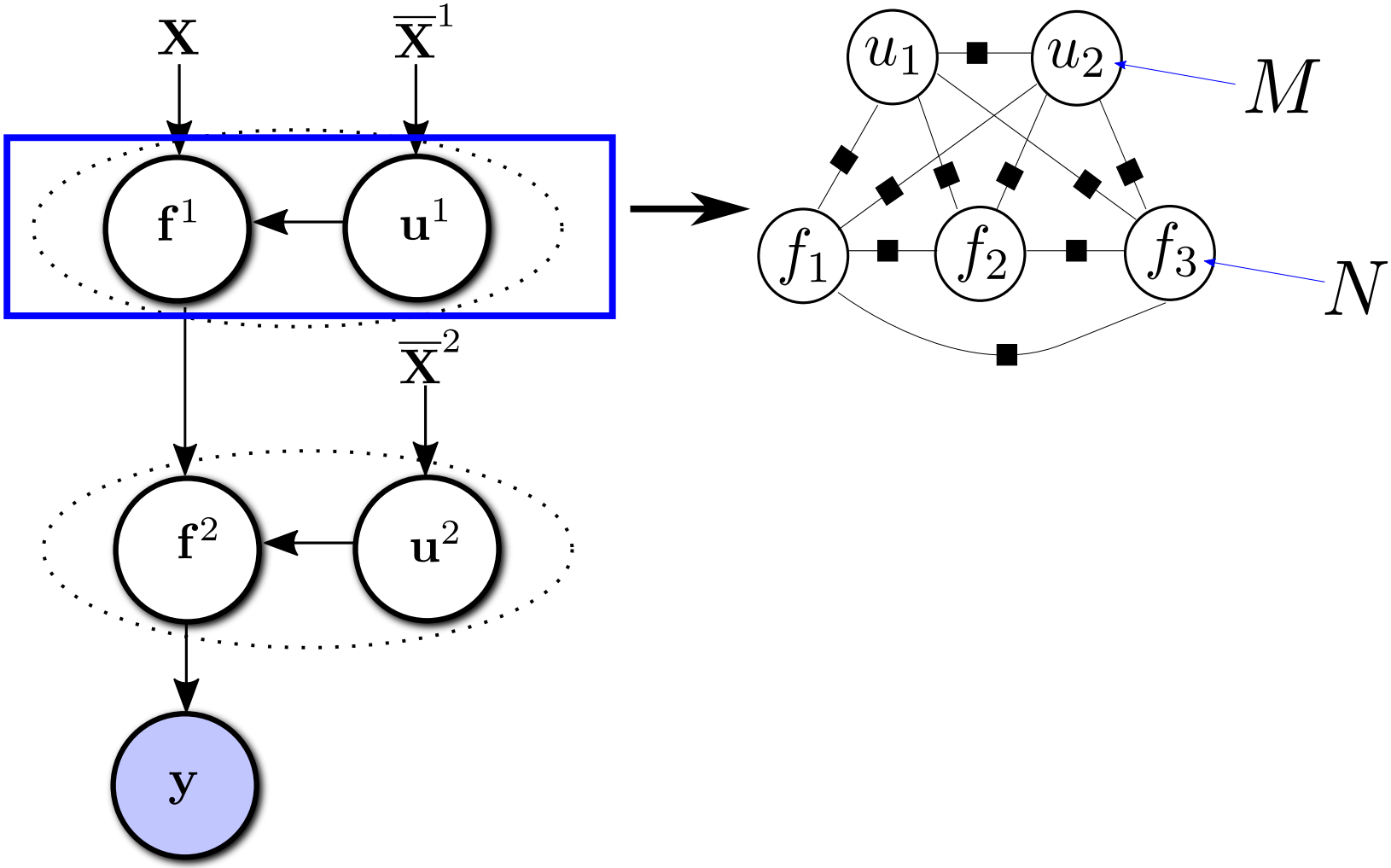

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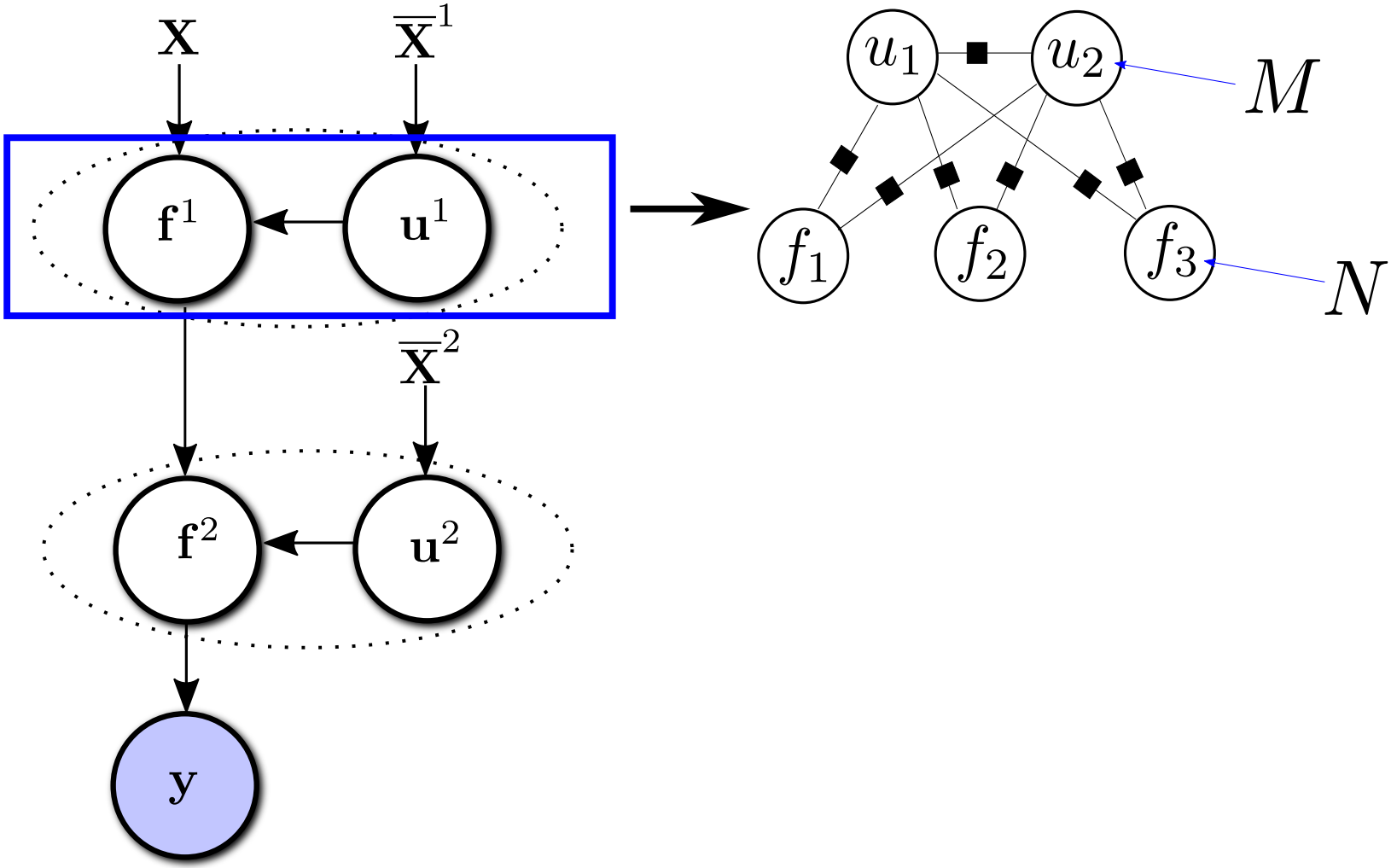

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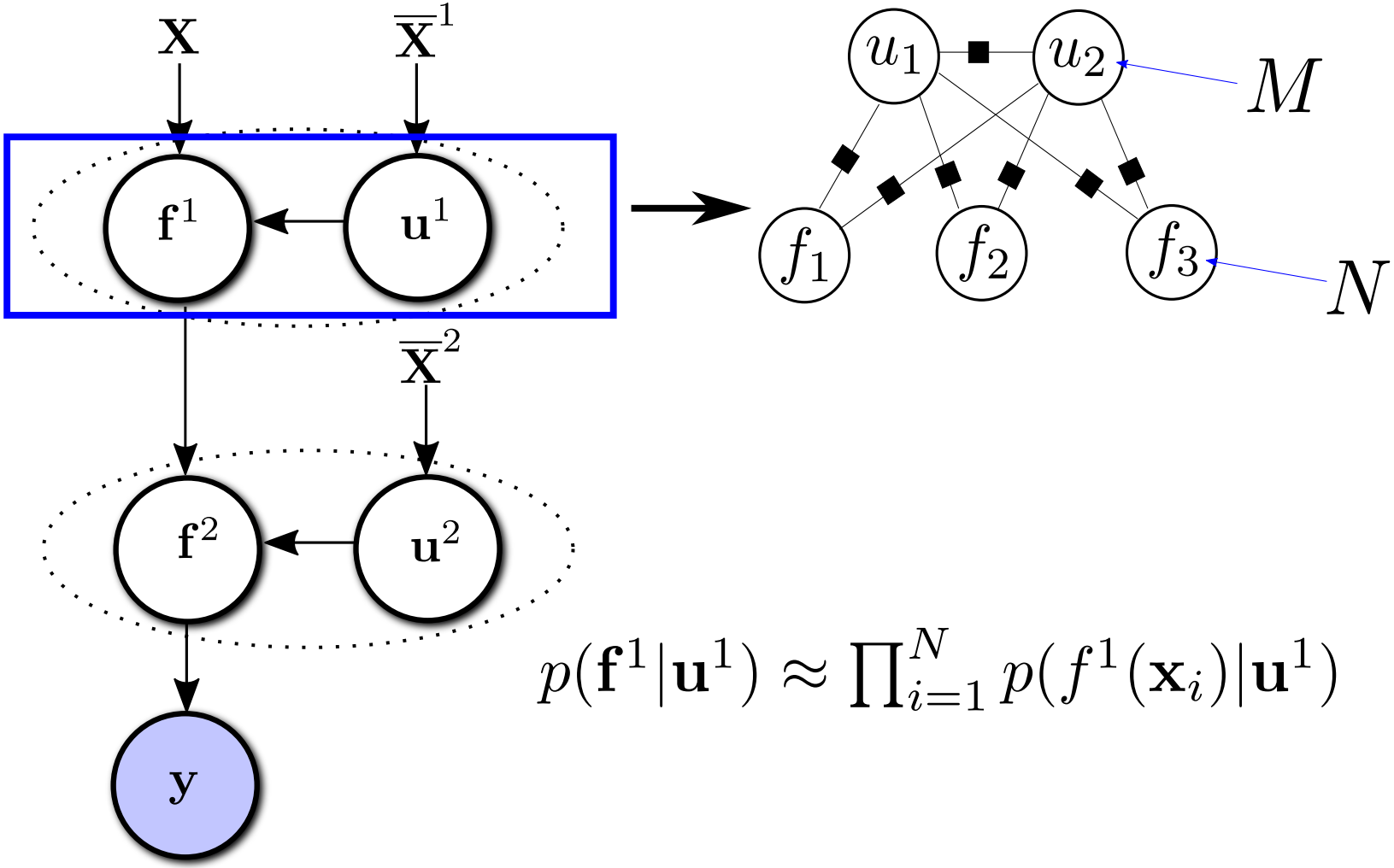
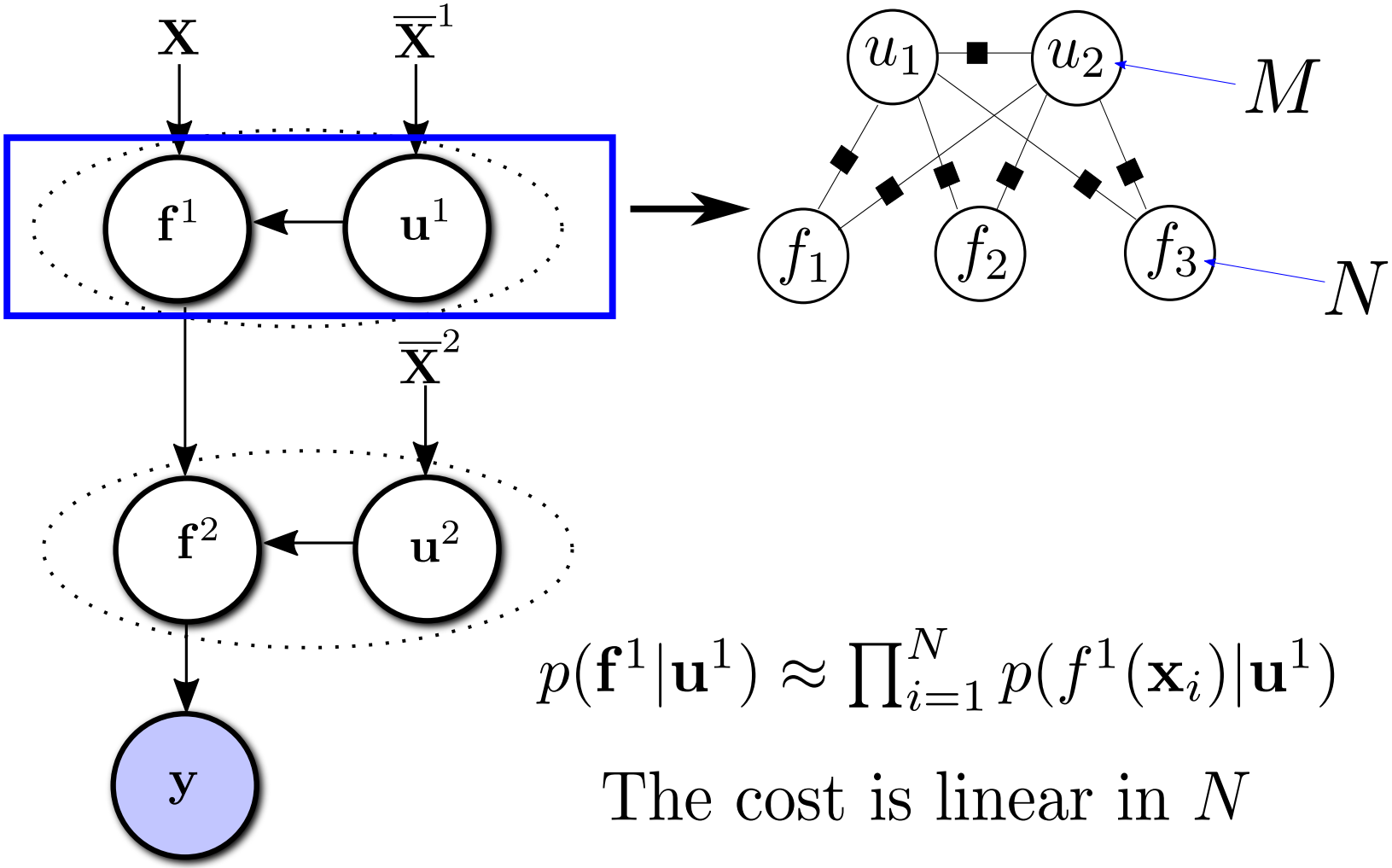


$$p(\mathbf{f}^1|\mathbf{u}^1) \approx \prod_{i=1}^{N} p(f^1(\mathbf{x}_i)|\mathbf{u}^1)$$

Alternative Graphical Model



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

The cost is linear in N

Approximate Deep GP Joint Distribution

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

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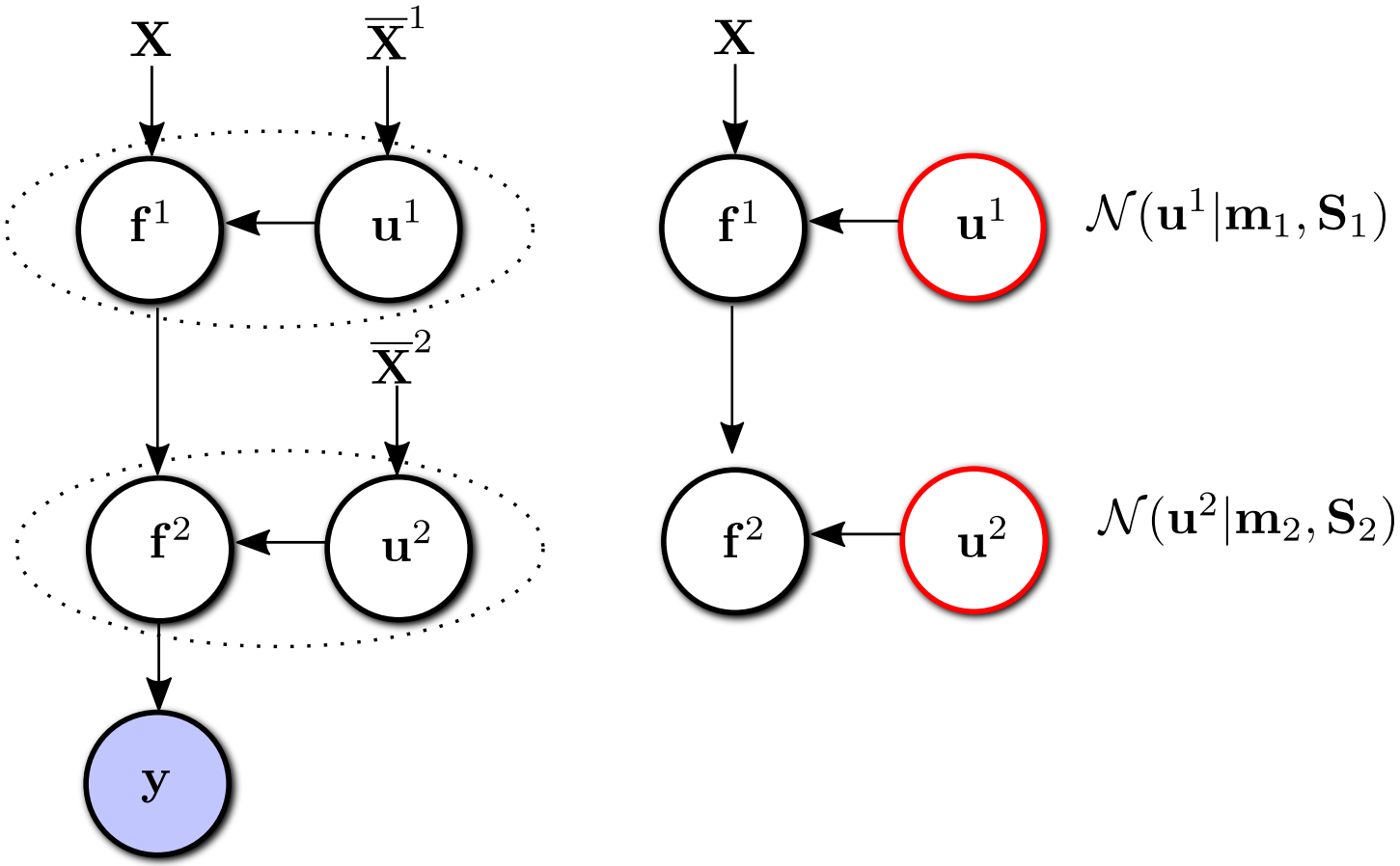
The FITC approximation enforces $\tilde{p}(\mathbf{f}^l|\mathbf{u}^l, \overline{\mathbf{X}}^l)$ to factorize across the N data instances!

Graphical Model and Approximate Distribution



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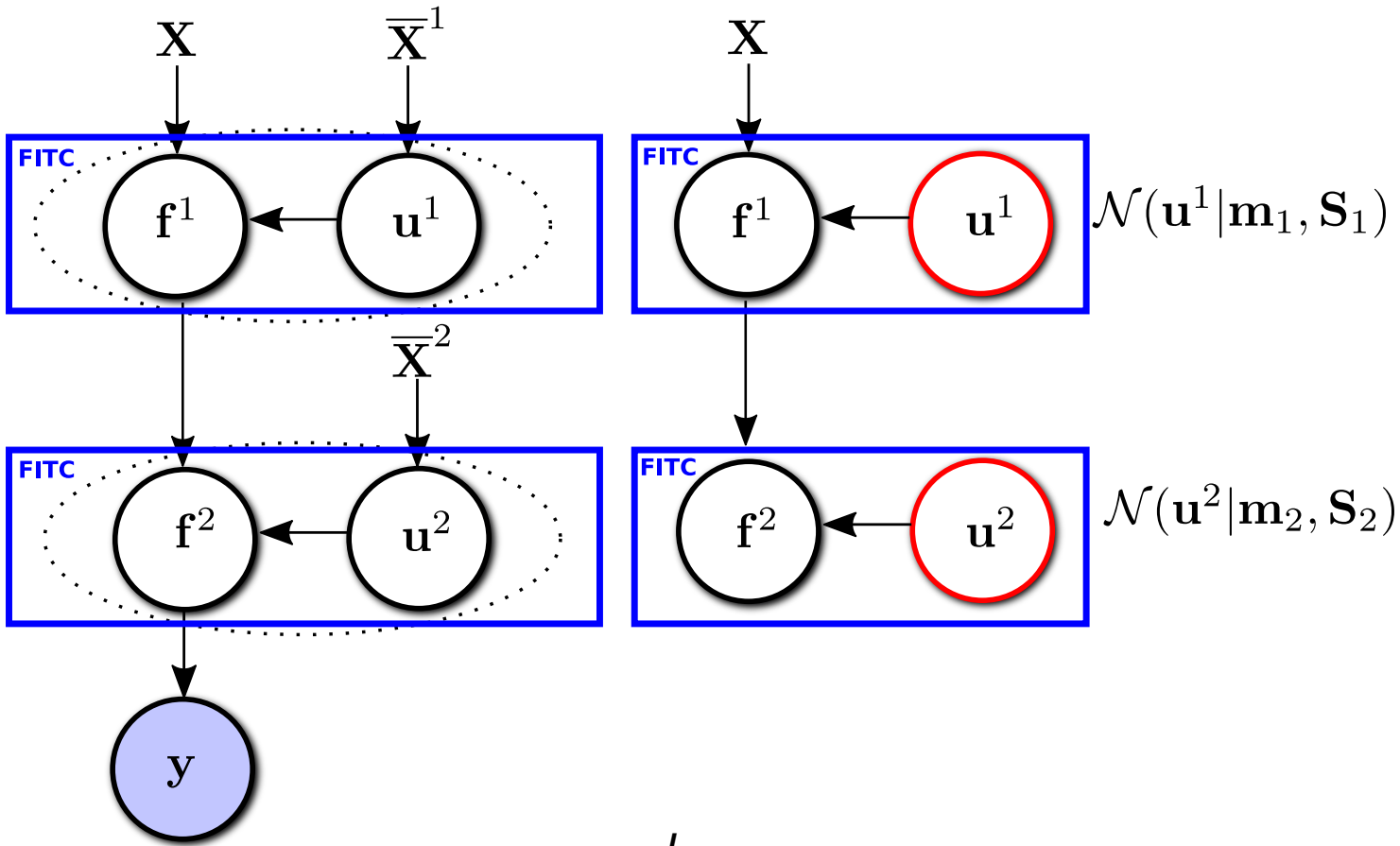

$$q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) = \prod_{l=1}^{L} \tilde{p}(\mathbf{f}^{l-1}|\mathbf{u}^l)\, q(\mathbf{u}^l)$$

- Fixed and factorizing across data
- Tunable Gaussian

Graphical Illustration of EP for DGPs

Approximates $p(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L | \mathbf{y}) \propto \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \prod_{i=1}^N p(y_i | f_i^L)$ with

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$$p(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L|\mathbf{y}) \propto \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \quad p(y_1|f_1^L) \quad p(y_2|f_2^L) \quad p(y_3|f_3^L)$$

$$\approx \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_1(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_2(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_3(\{\mathbf{u}^l\}_{l=1}^L) \propto q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$$

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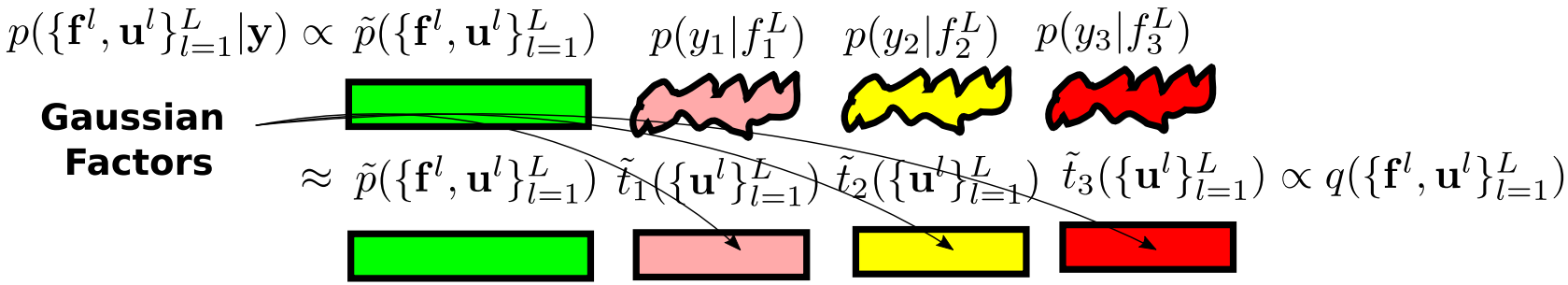

The $\tilde{t}_i$ are tuned by minimizing the KL-divergence $\mathrm{KL}[\hat{p}_i||q] \quad \forall i$,

$$\text{where} \quad \begin{array}{lcll} \hat{p}_i(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) & \propto & p(y_i|f_i^L) & \prod_{j\neq i} \tilde{t}_j(\{\mathbf{u}^l\}_{l=1}^L)\tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \\ q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) & \propto & \tilde{t}_i(\{\mathbf{u}\}_{l=1}^L) & \prod_{j\neq i} \tilde{t}_j(\{\mathbf{u}^l\}_{l=1}^L)\tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \end{array}.$$

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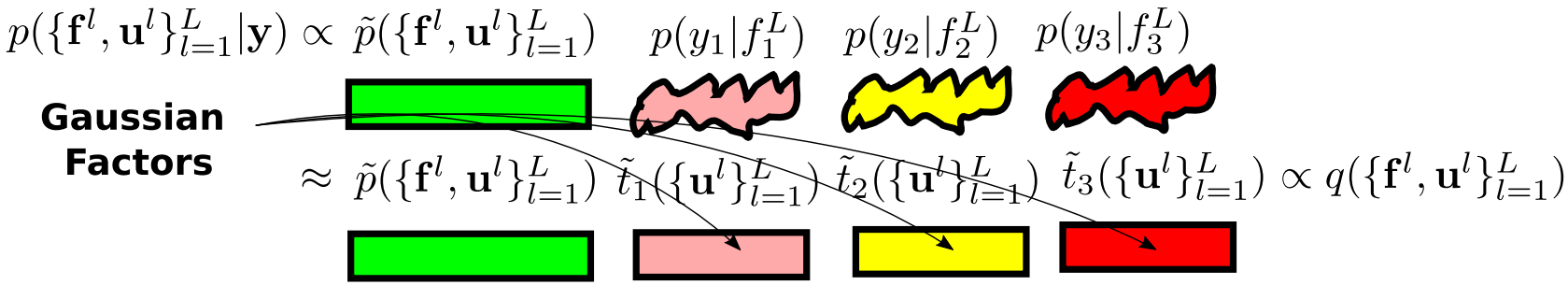

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Since $\tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$ is fixed, we only have to match the moments of $\hat{p}_i$ and q over $\{\mathbf{u}^l\}_{l=1}^L$!

EP as an Optimization Problem

The EP approximation to the **evidence** $p(\mathbf{y})$ is given by:

$$\log Z_{\text{EP}} = g(\boldsymbol{\eta}_q) - g(\boldsymbol{\eta}_{\text{prior}}) + \sum_{i=1}^{N} \log Z_i + g(\boldsymbol{\eta}_q) - g(\boldsymbol{\eta}_q^{\setminus i})$$

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Approximate Expectation Propagation

$$p(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L|\mathbf{y}) \propto \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \quad p(y_1|f_1^L) \quad p(y_2|f_2^L) \quad p(y_3|f_3^L)$$

$$\approx \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_1(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_2(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \propto q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$$

We tie the approximate factors!

$$\approx \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \propto q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$$

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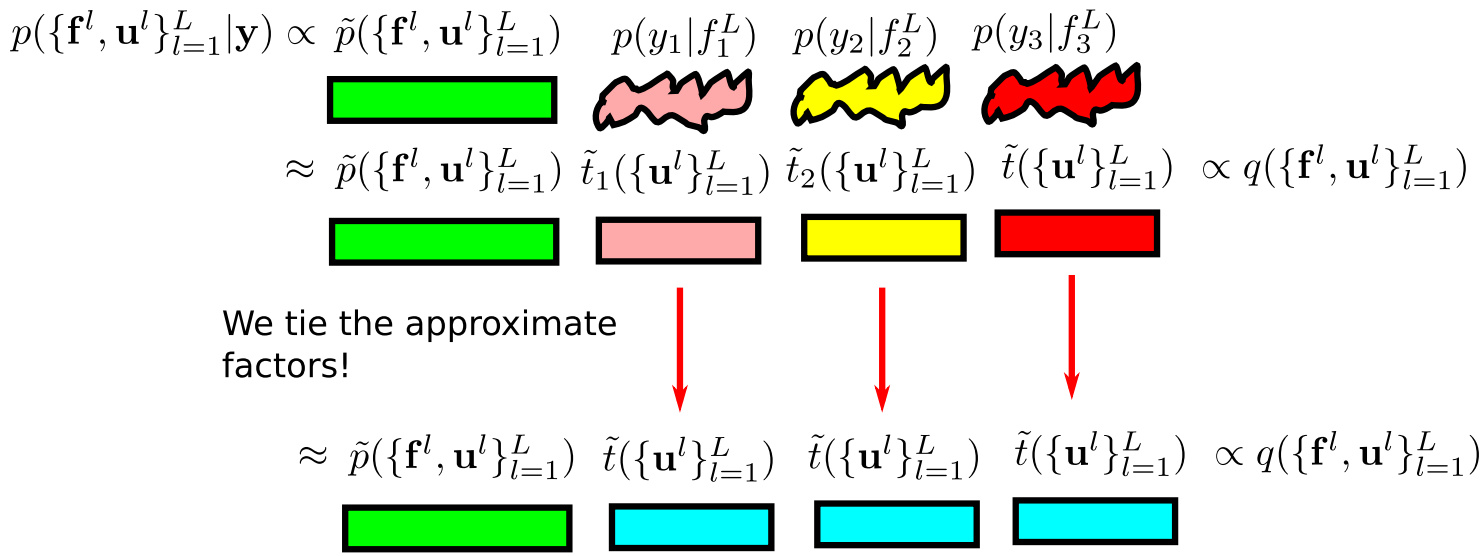

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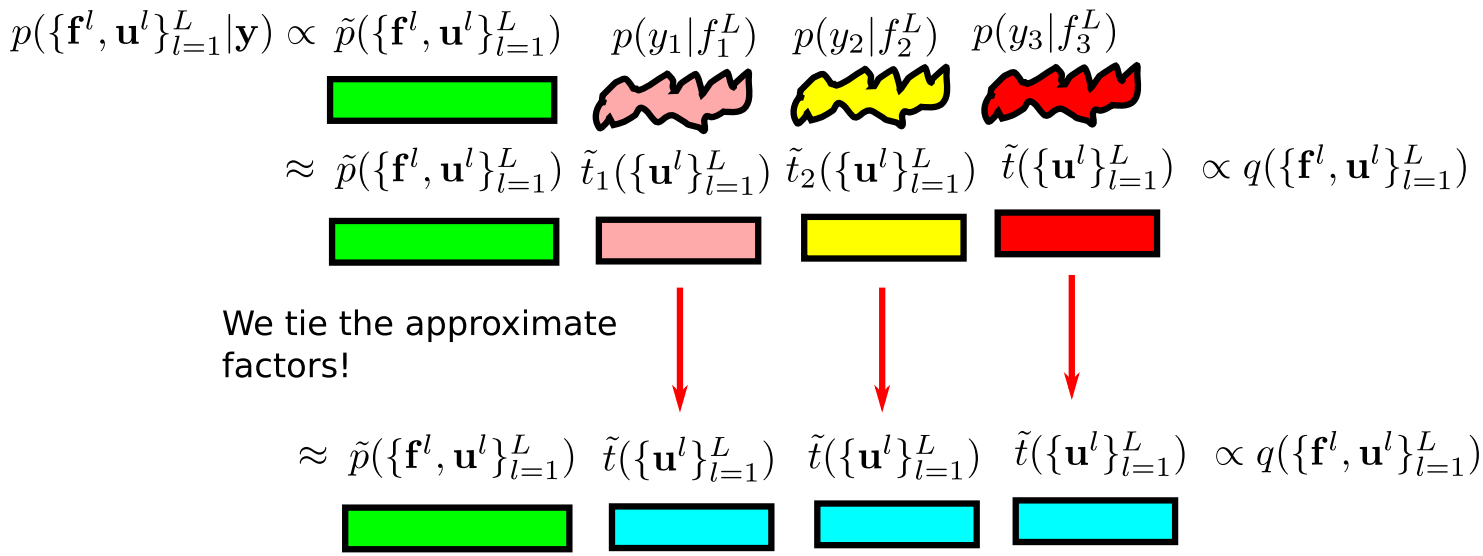

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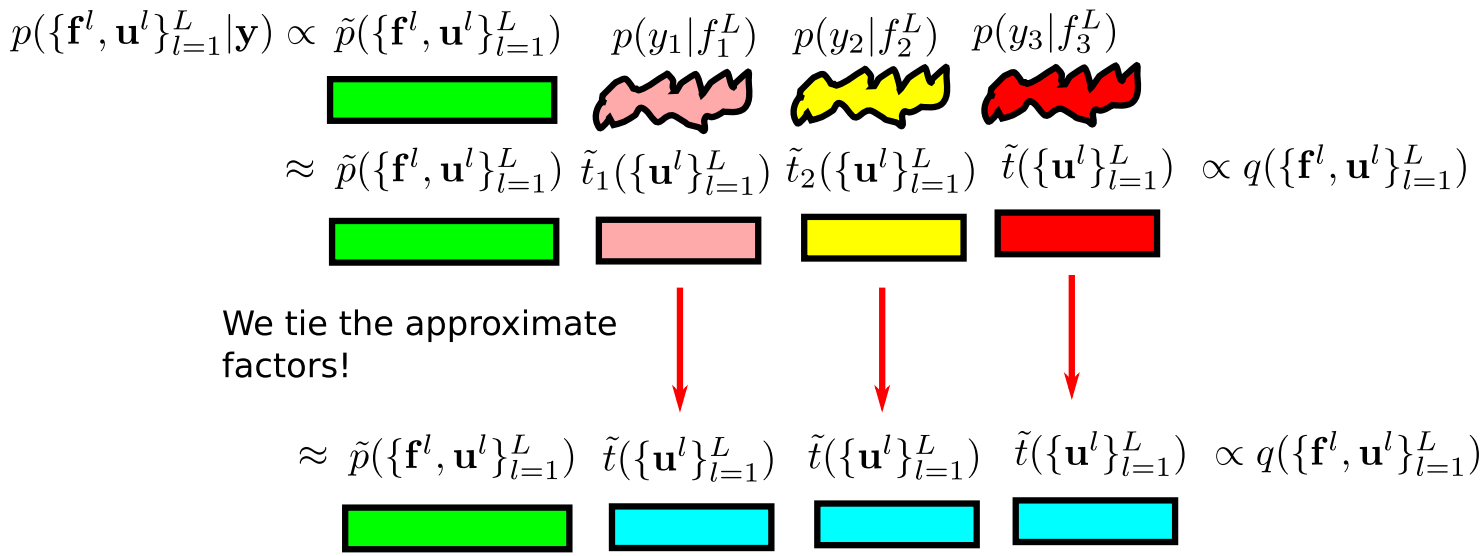

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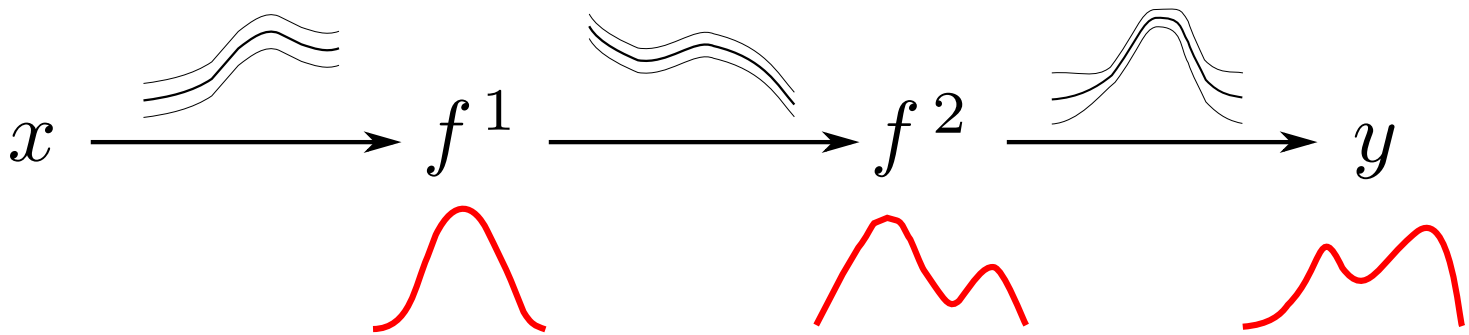

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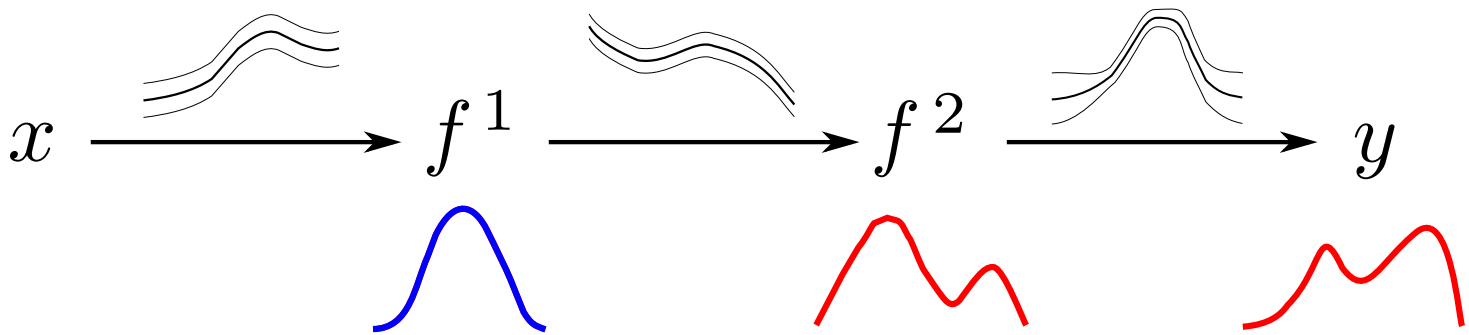

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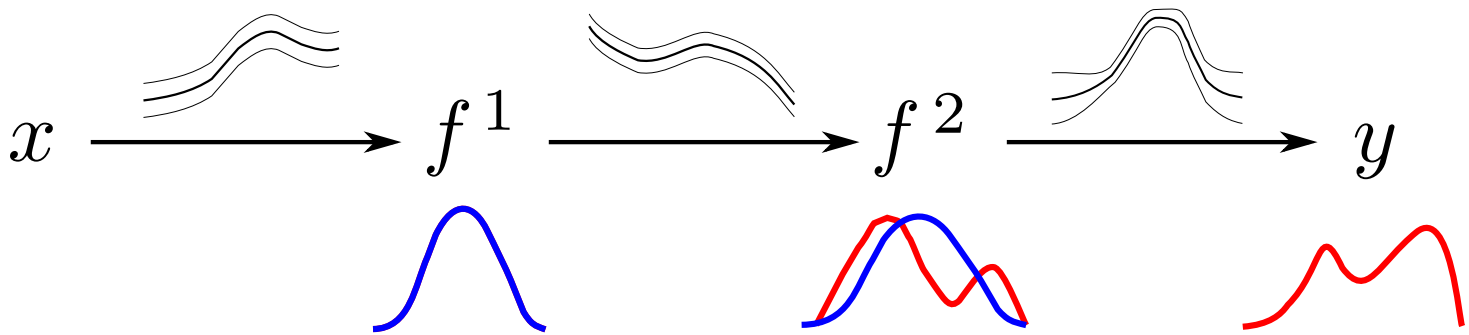

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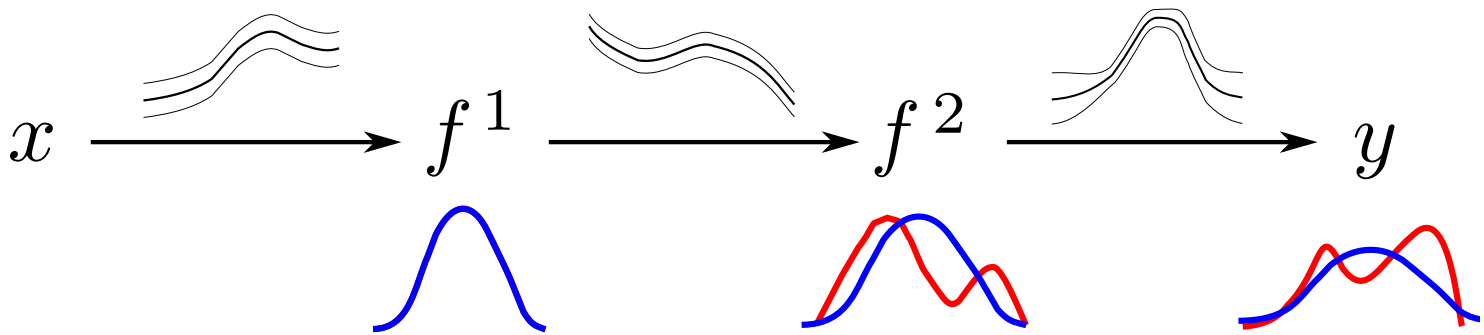

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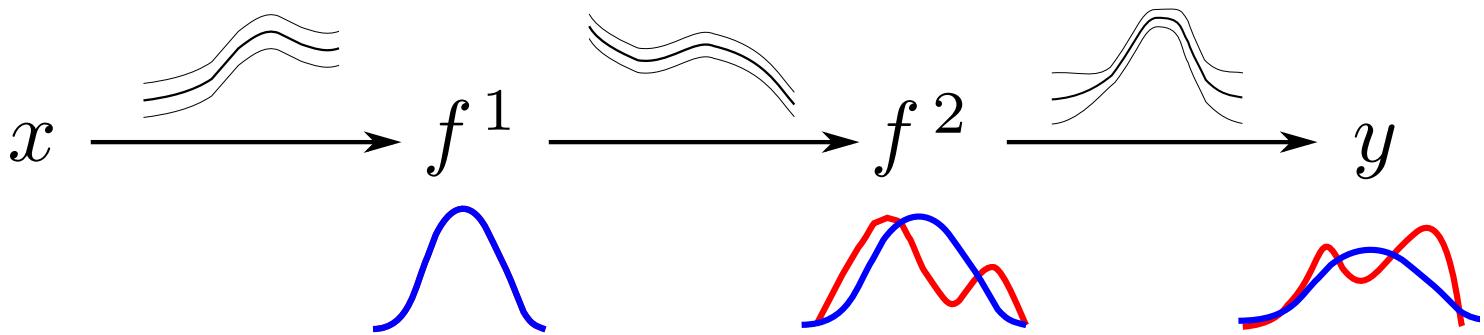
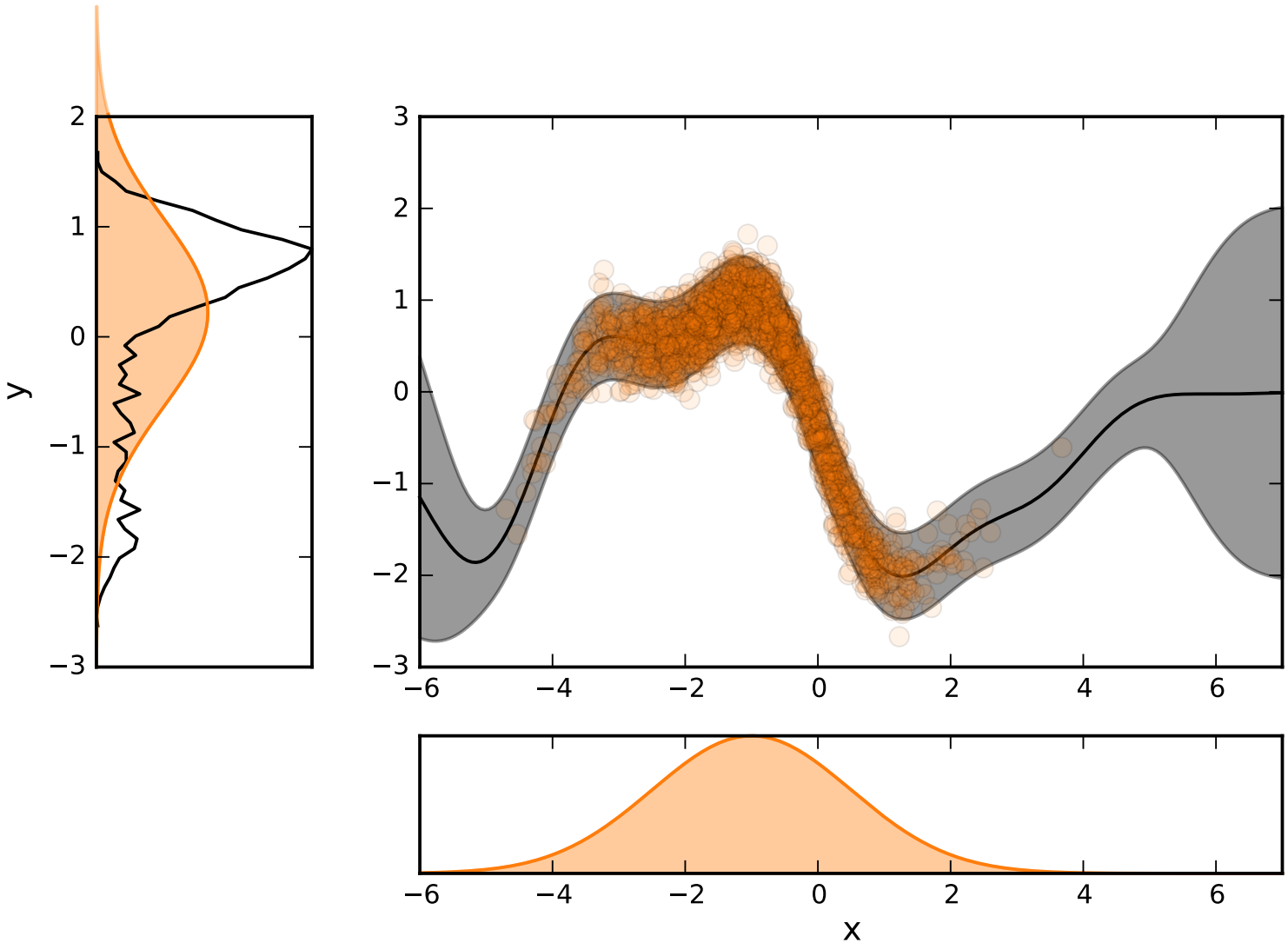
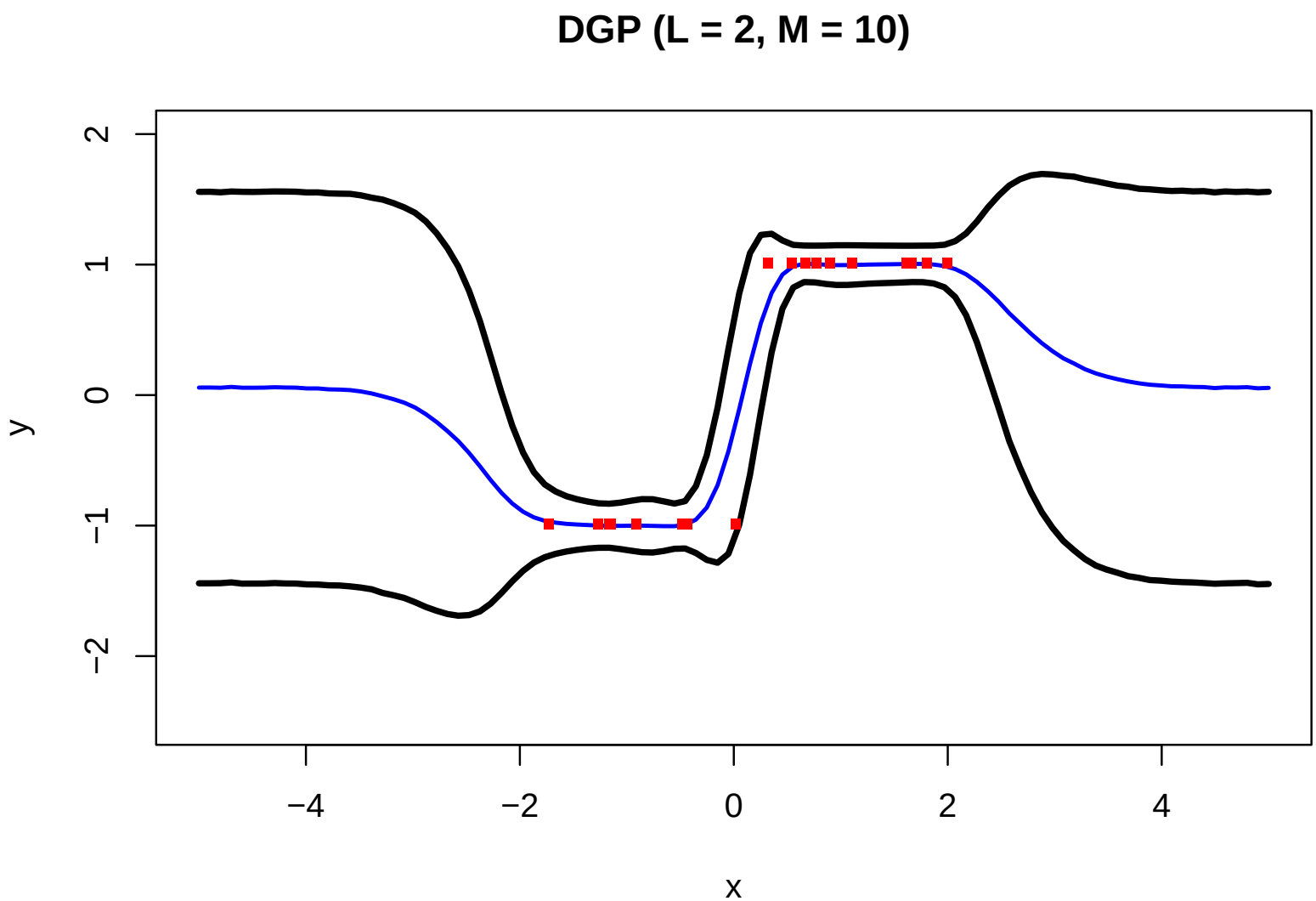


Doable for certain covariance functions, e.g., the squared exponential!

Gaussian Projection Example



Approx. EP for DGPs: Illustrative Example



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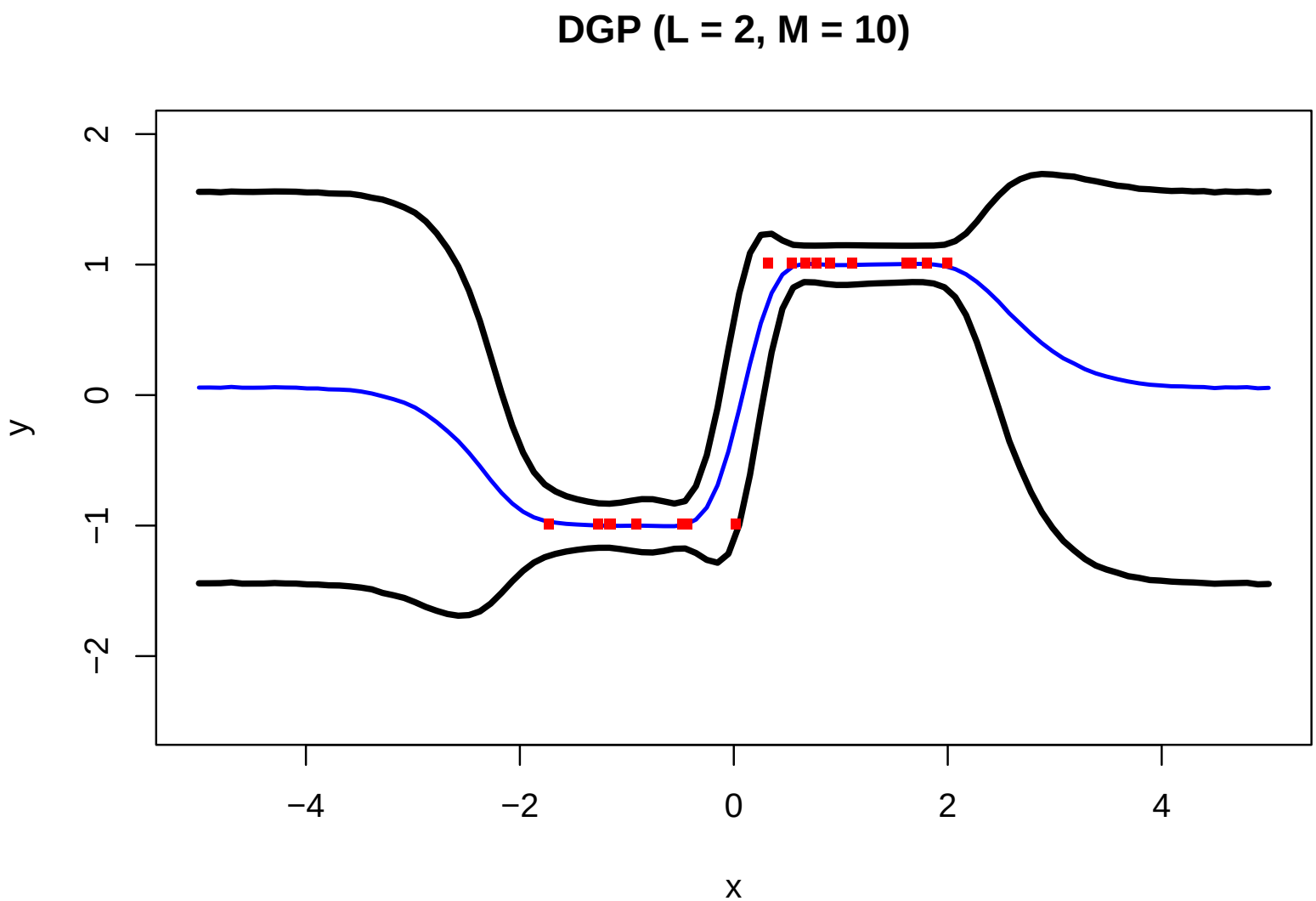

The AEP method provides a similar predictive distribution to the previous method!

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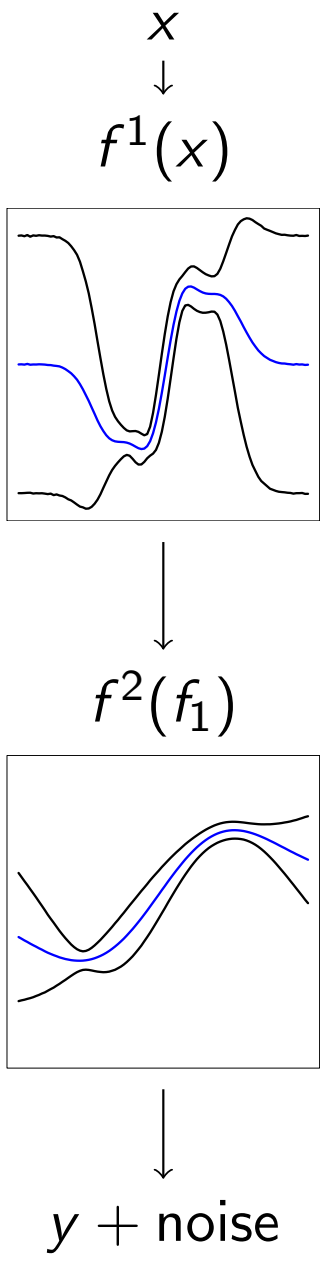

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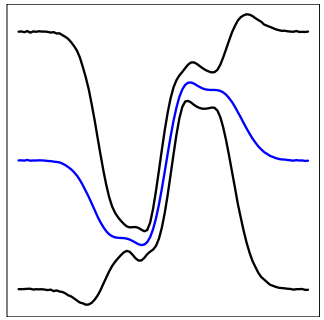
x

$\downarrow$

$f^1(x)$



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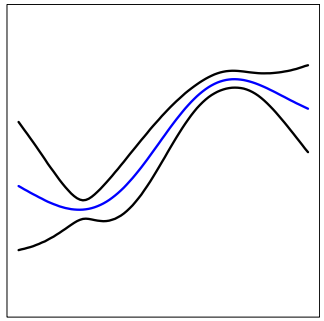
$f^2(f_1)$

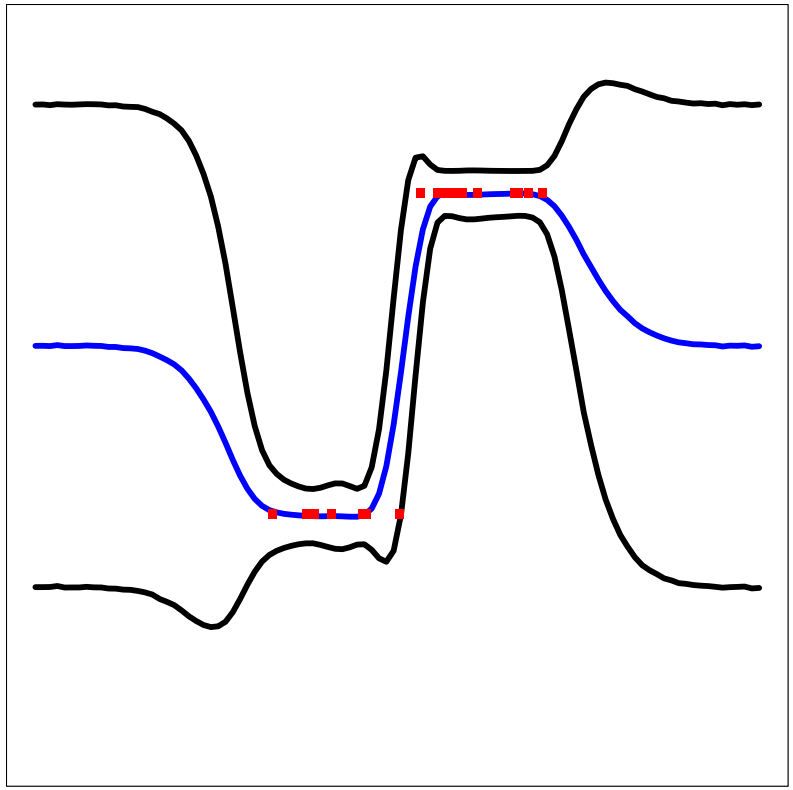


$\downarrow$

$y + \text{noise}$

$\equiv$

$y = f^2(f^1(x)) + \text{ noise}$



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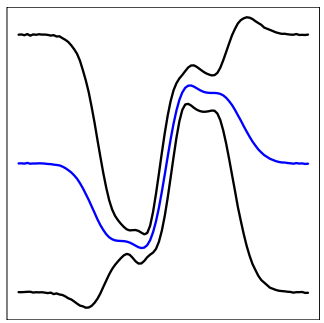

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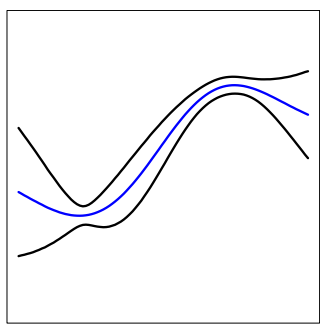

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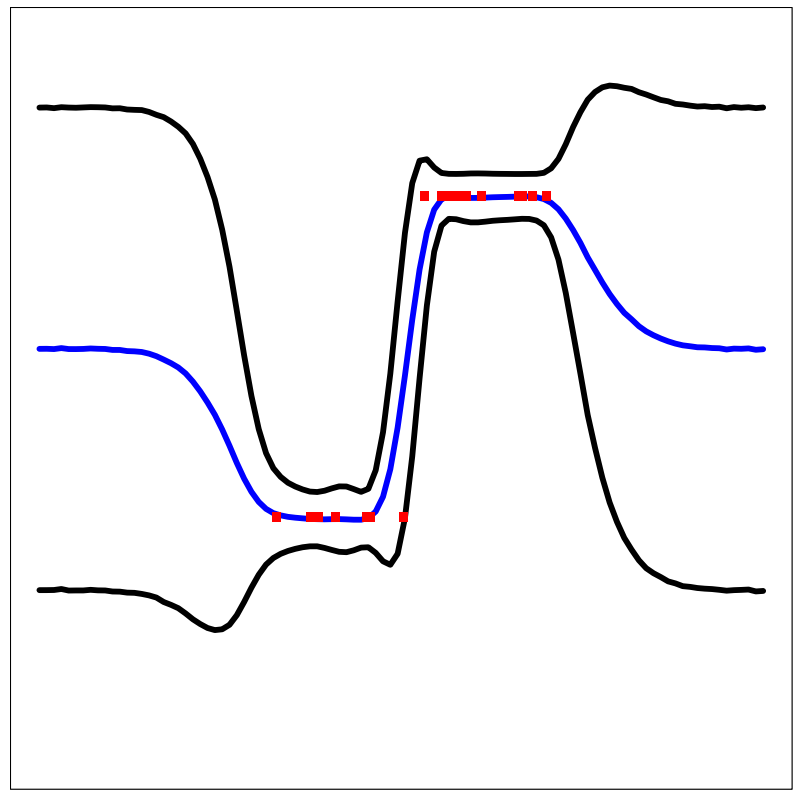

$f^1, f^2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$

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- It is limited to certain covariance functions, *e.g.*, the squared exponential covariance function.
- It modifies the deep GP prior and hence the model, by introducing the FITC approximation.

Doubly Stochastic Variational Inference for DGPs

Features:

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(Salimbeni, 2017)

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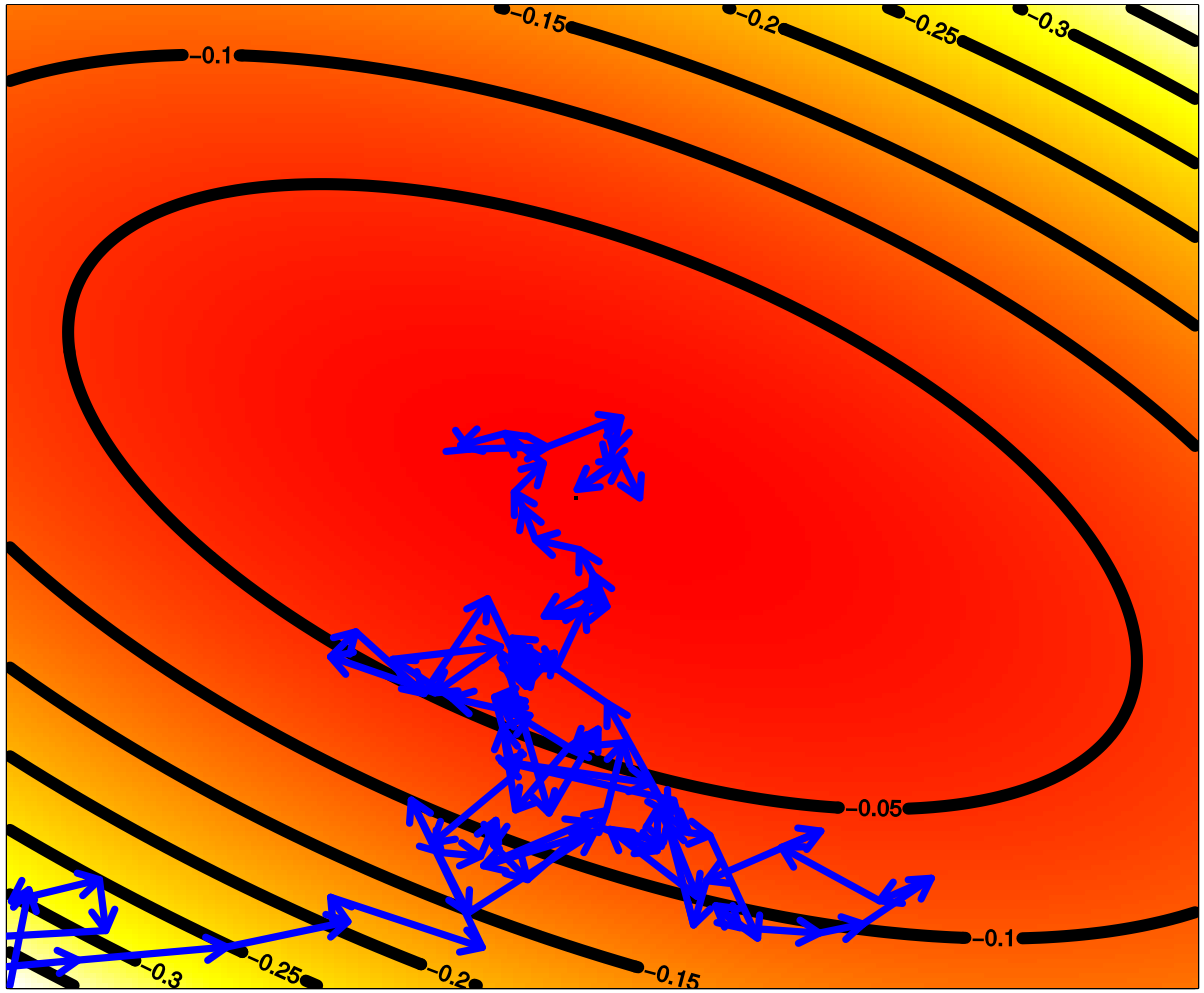
\end{aligned}$$

This is an unbiased estimate of the gradient and can be plugged in any stochastic optimization algorithm!

Stochastic Optimization



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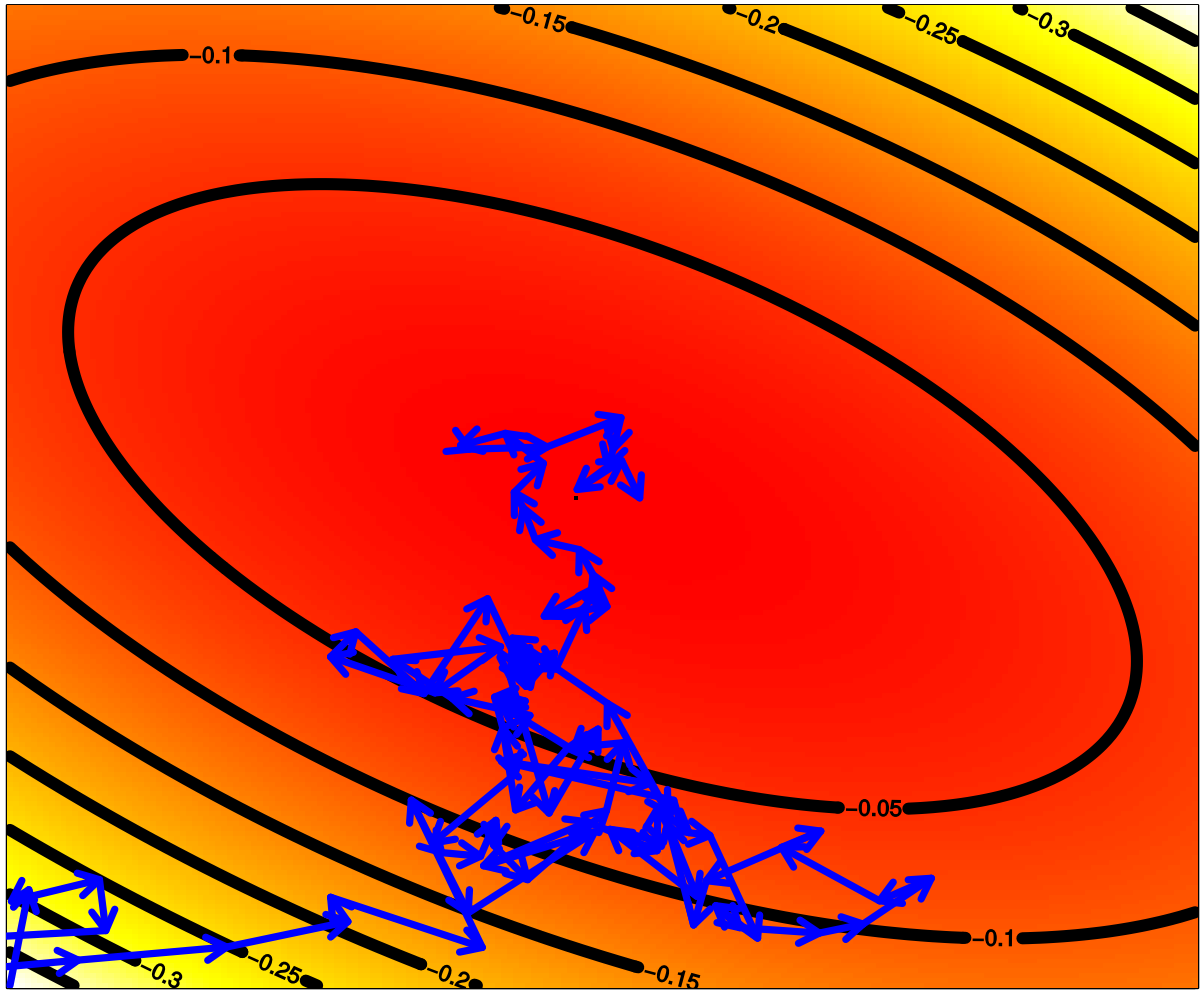

To converge to a local neighborhood of the optimum stochastic methods only require an unbiased estimate of the gradient!

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This other estimator has less variance and leads to better results!

Deep GPs Joint Distribution

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

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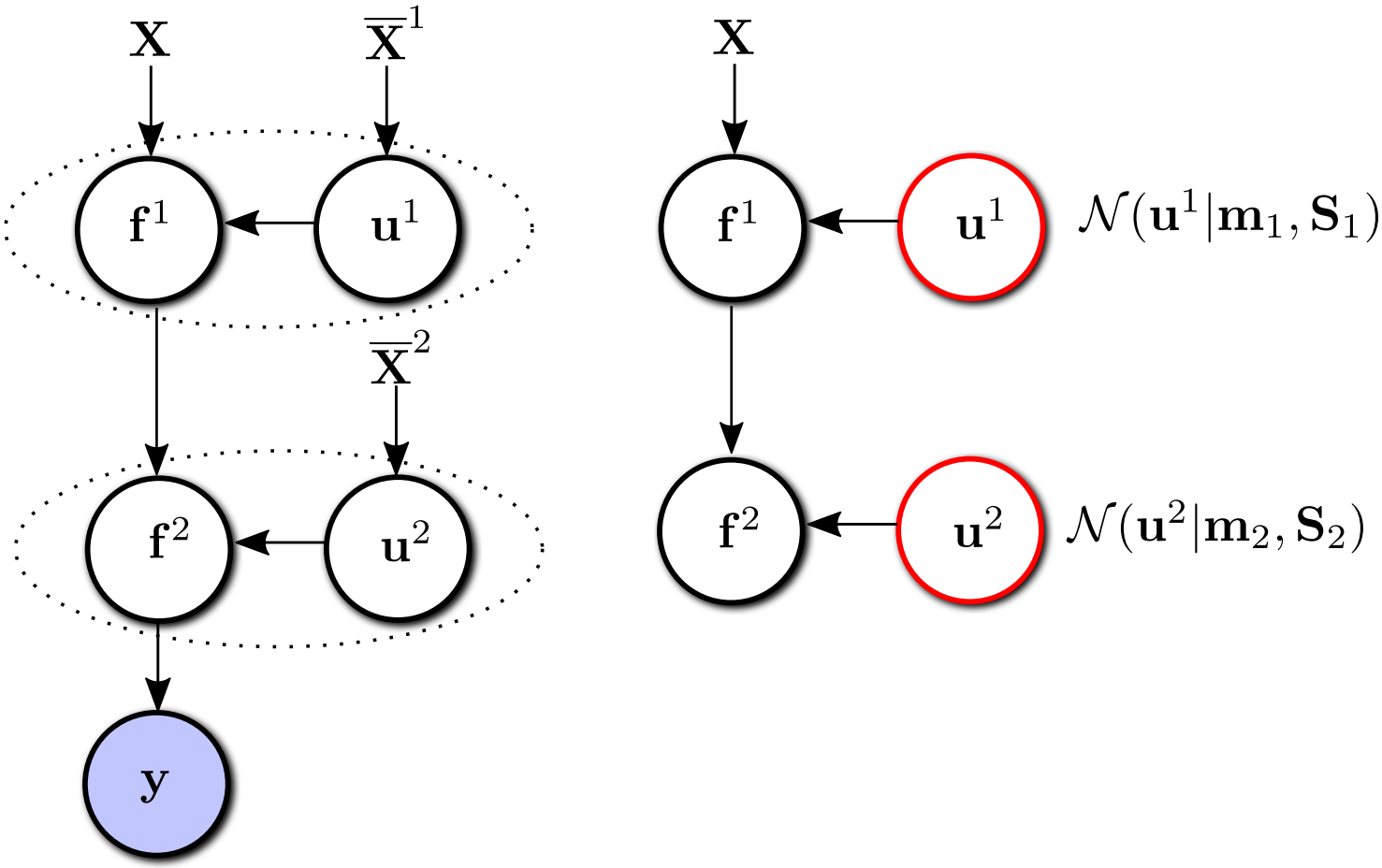
No change in the model is made at all!

Graphical Model and Posterior Approximation



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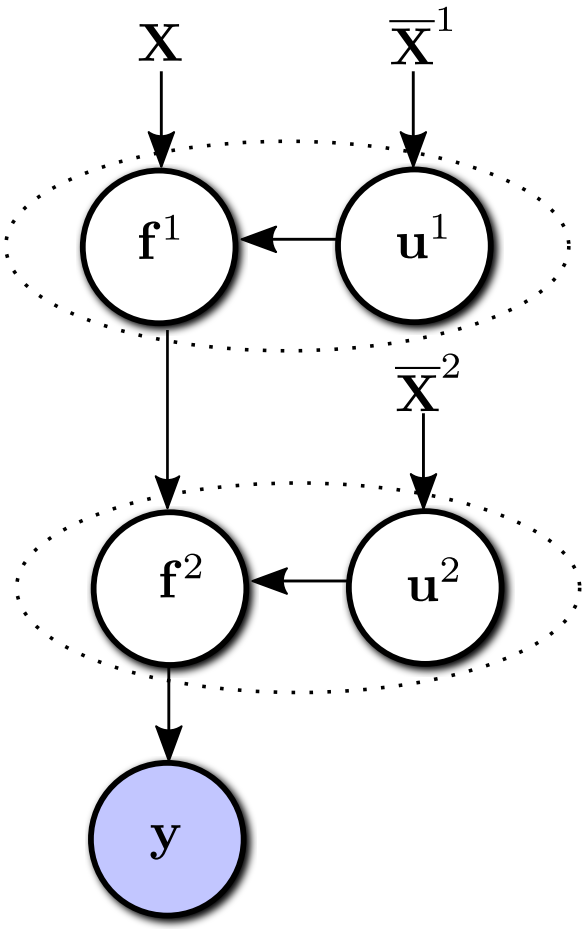

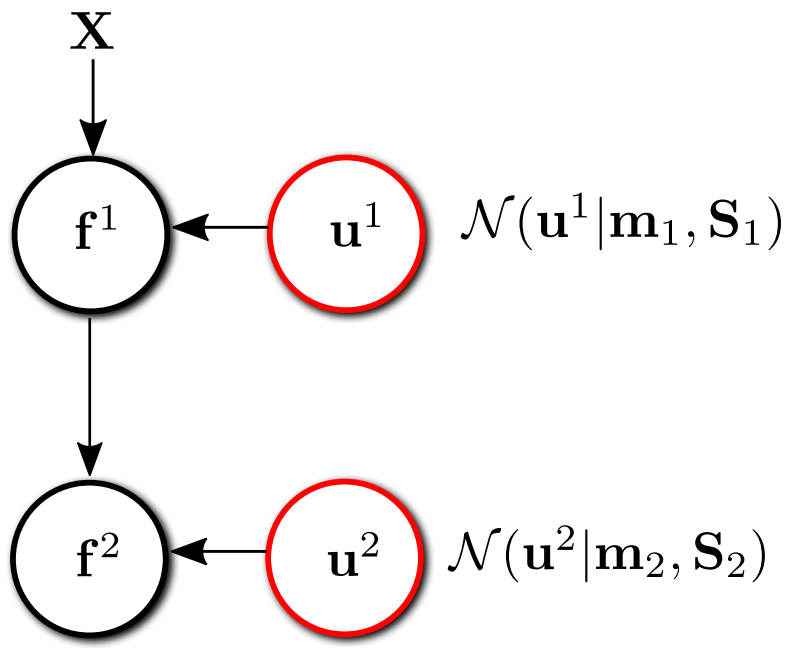

$$q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) = \prod_{l=1}^{L} p(\mathbf{f}^l|\mathbf{u}^l)\, q(\mathbf{u}^l)$$

- 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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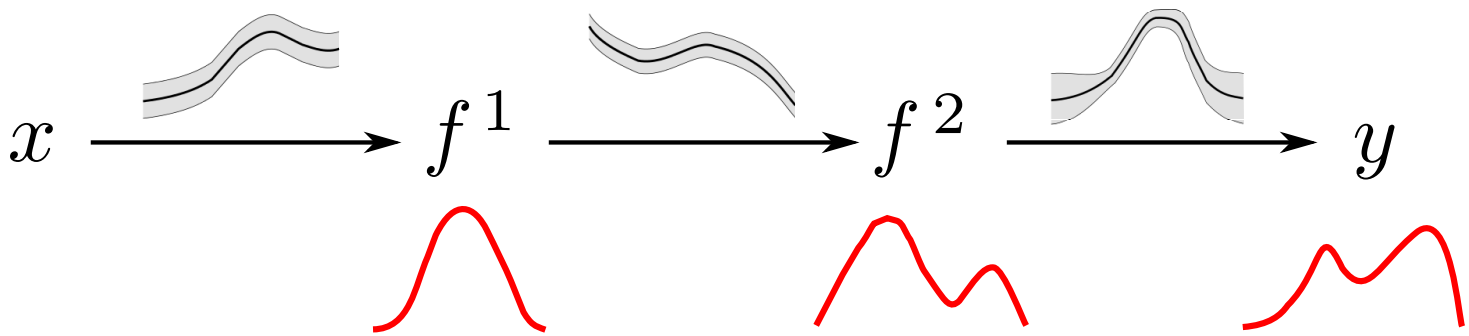
- The expectations can be approximated by Monte Carlo.
- Suitable for mini-batch training by subsampling the data.

(Salimbeni, 2017)

Predictive Distribution via Monte Carlo Sampling



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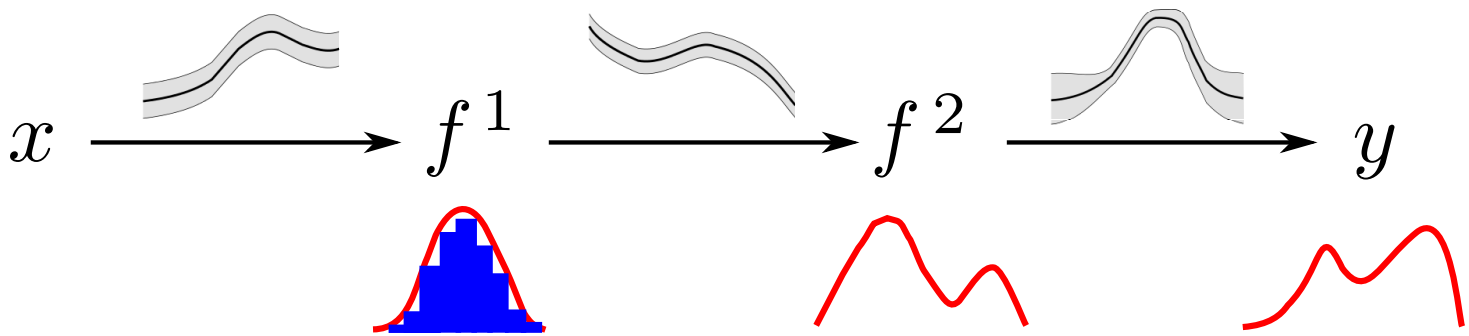

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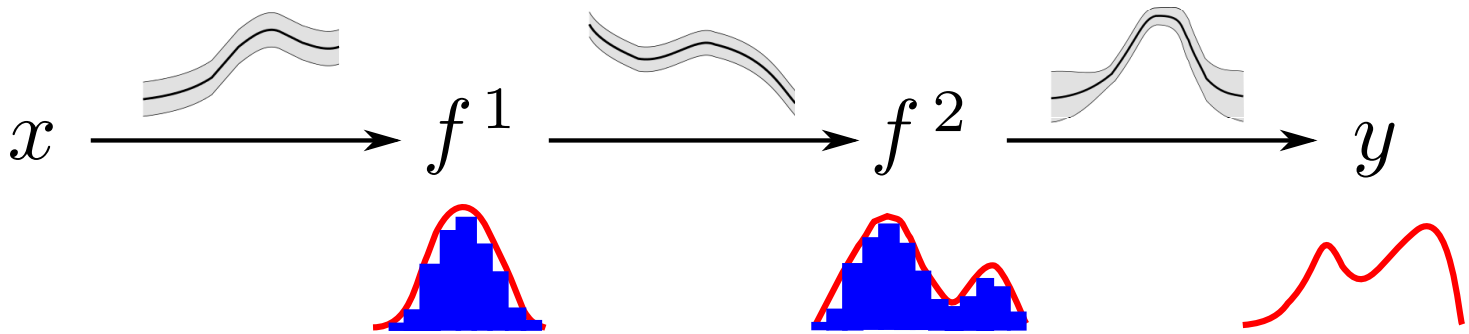

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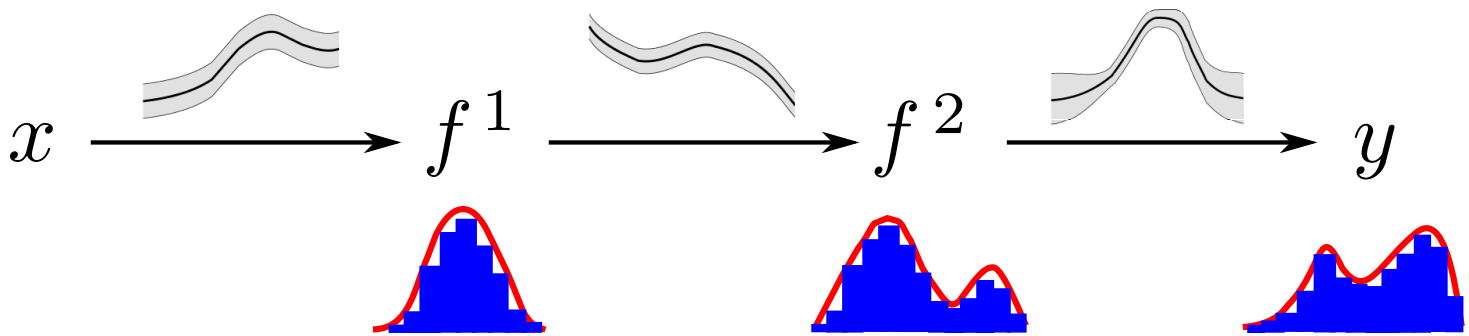

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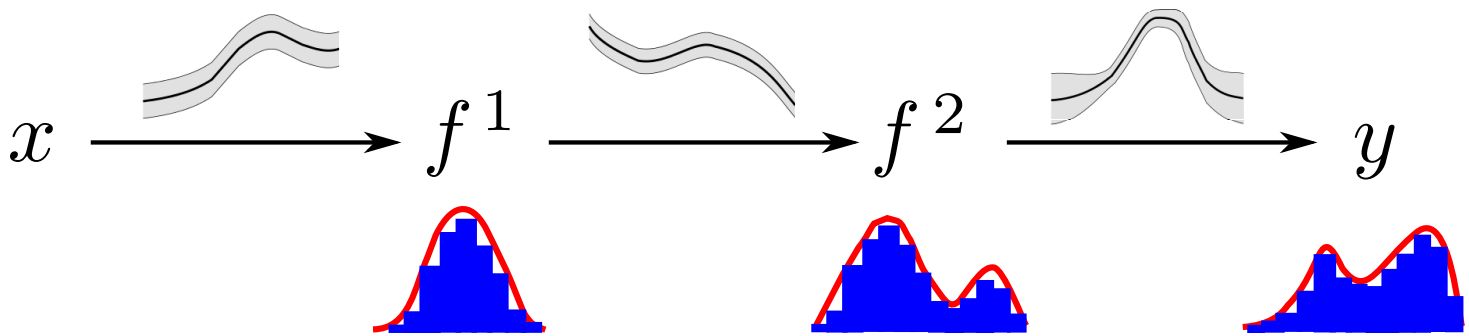
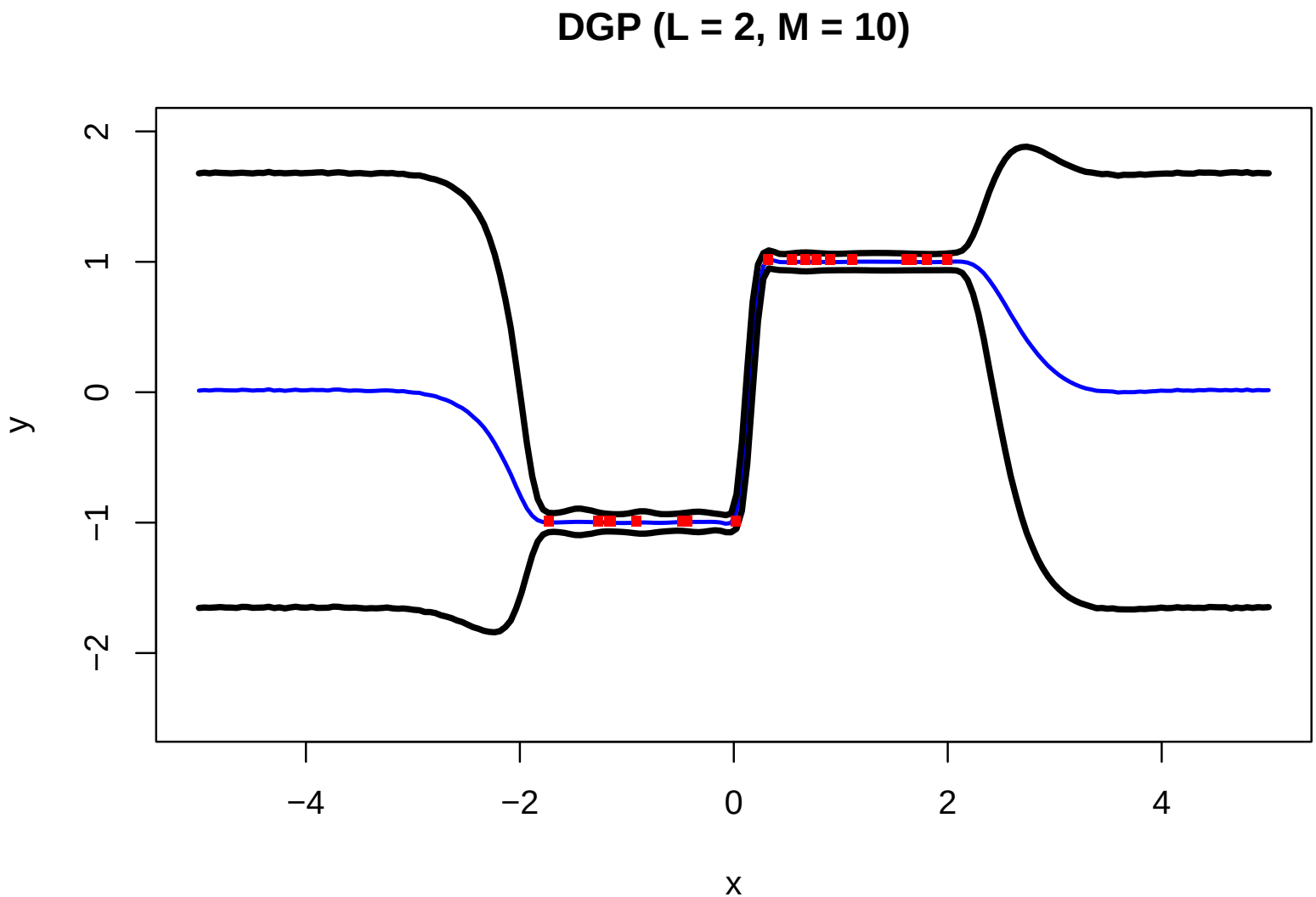


Used not only for testing, but also during training, unlike the previous methods!

DSVI for DGPs: Illustrative Example



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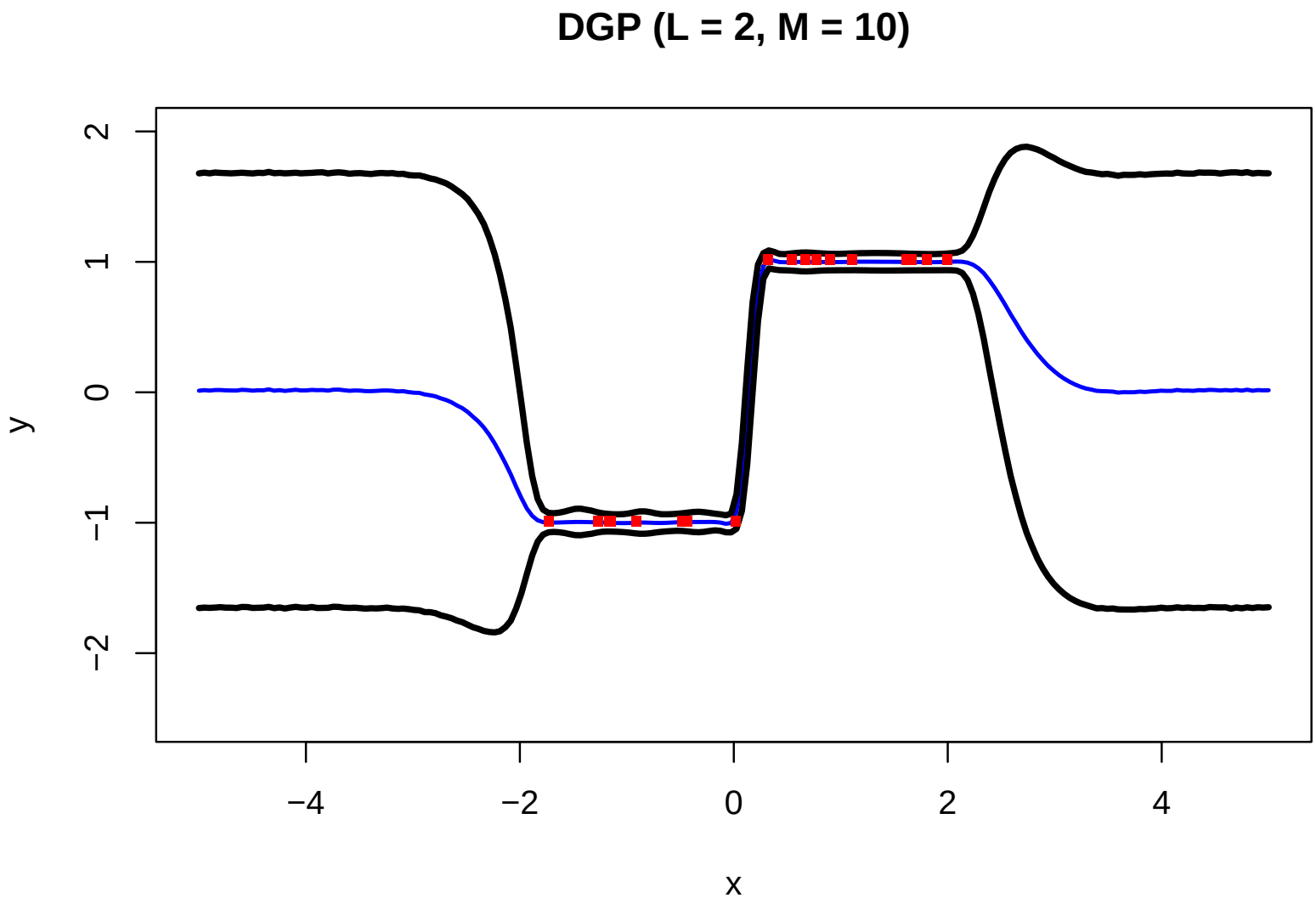


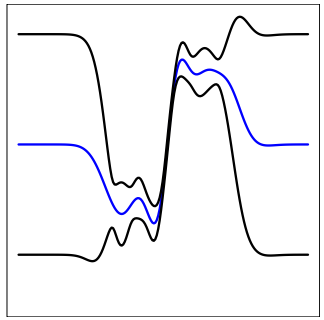
DSVI provides better results than the previous methods!

DSVI for DGPs: Illustrative Example

x

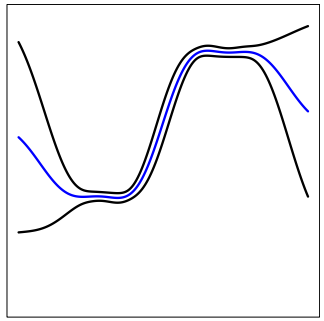
$\downarrow$

$f^1(x)$



$\downarrow$

$f^2(f_1)$



$\downarrow$

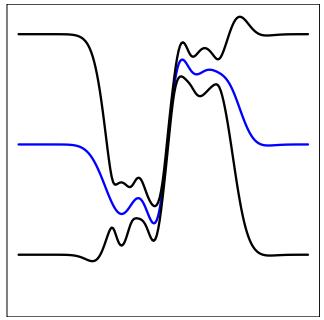
$y + \text{noise}$

DSVI for DGPs: Illustrative Example

x

$\downarrow$

$f^1(x)$



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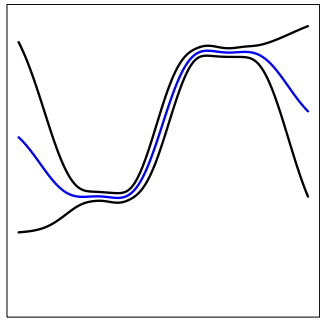
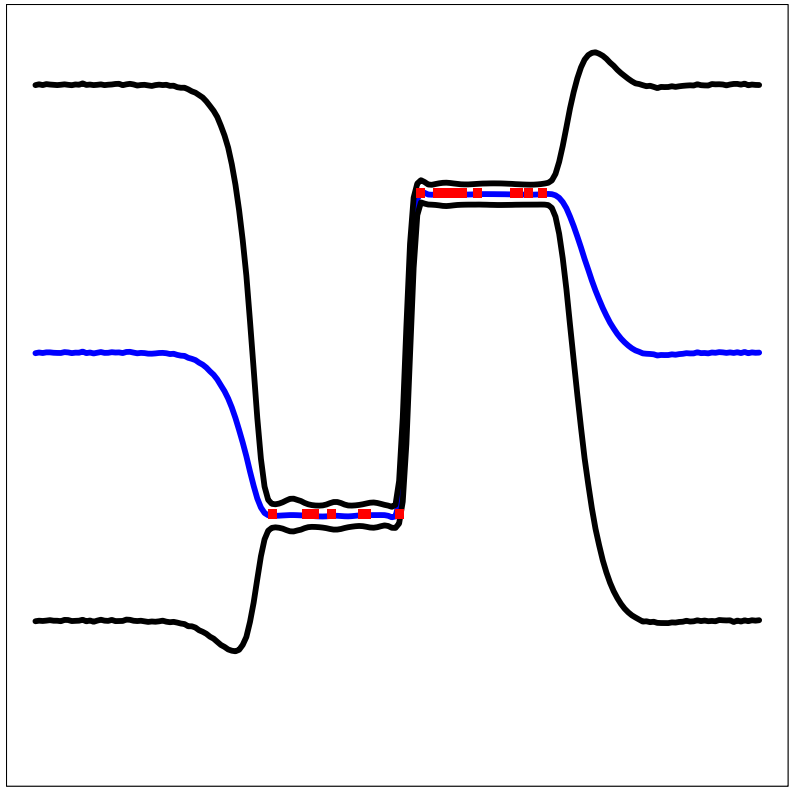


$\downarrow$

$y + \text{noise}$

$\equiv$

$y = f^2(f^1(x)) + \text{noise}$



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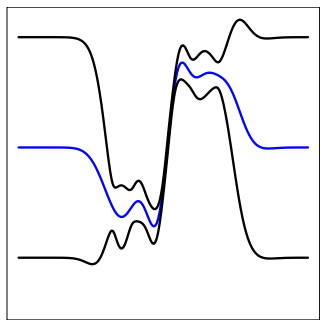

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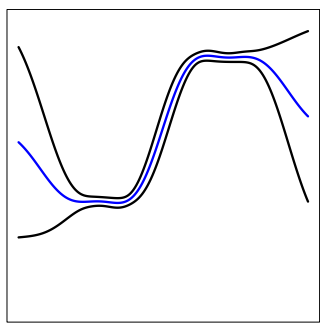

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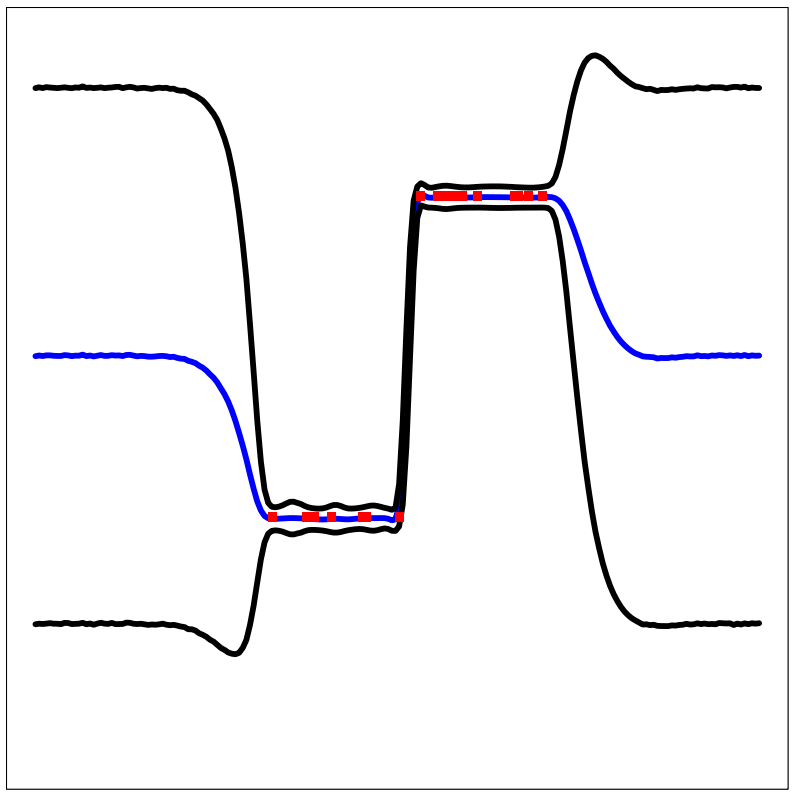
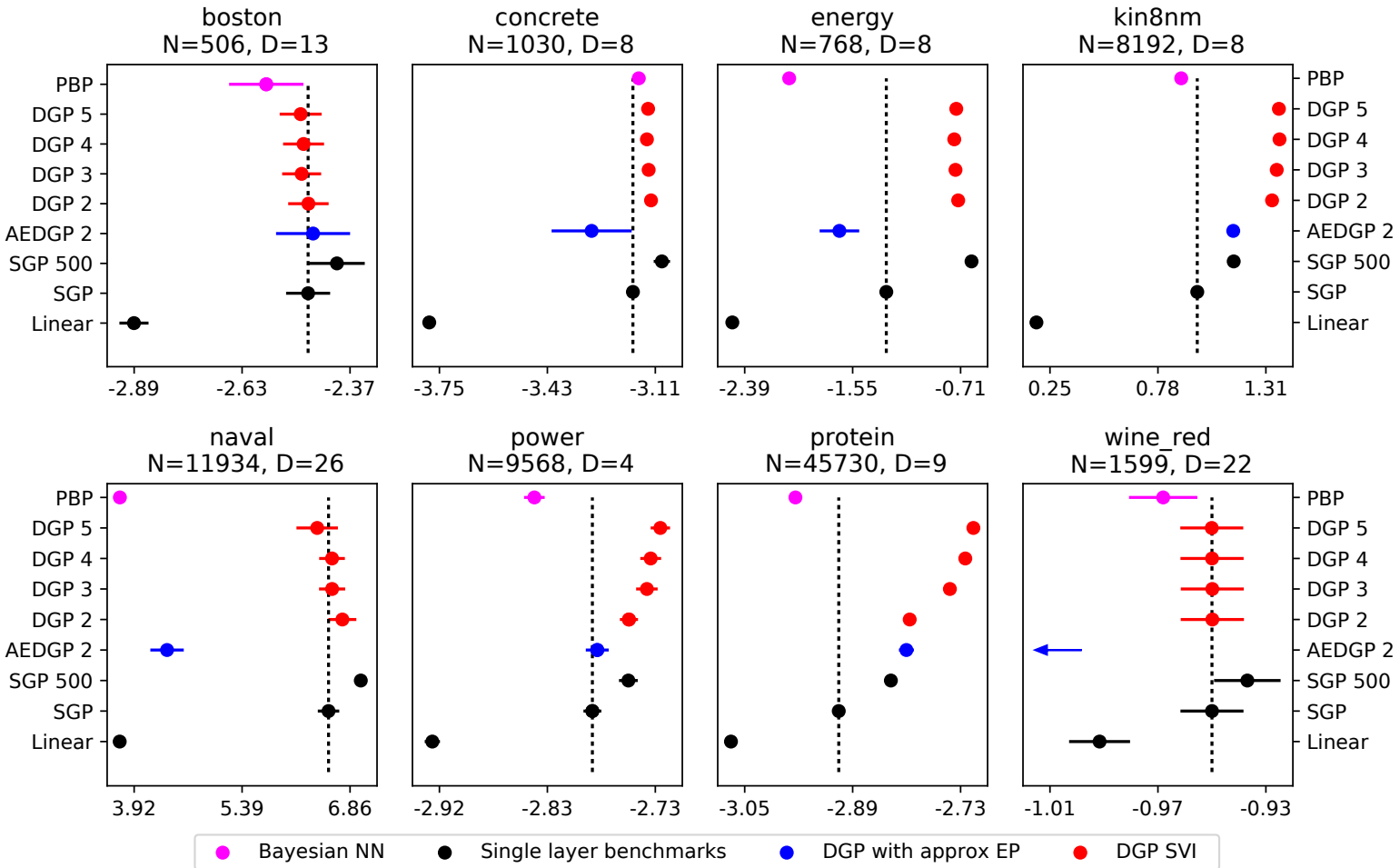


$f^1, f^2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$

DGPs via DSVI: LL Experimental Results



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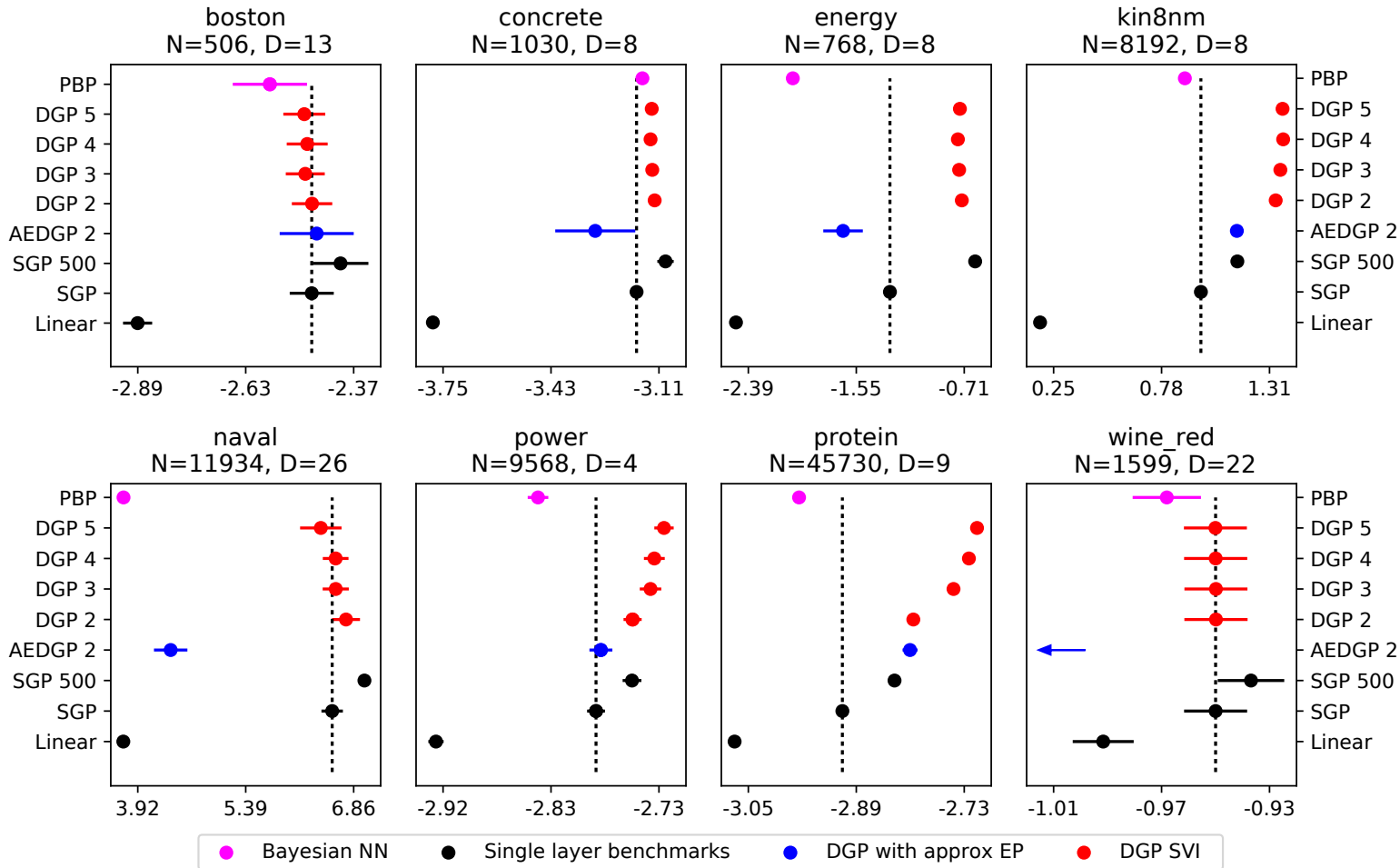

DGPs perform similar or better than the sparse GP and adding more layers does not seem to overfit!

(Salimbeni, 2017)

Run the first cells of the notebook to fit a DGP using DSVI and complete task 1!

Limitations of DSVI for DGPs

DSVI and the approximate EP method for training DGPs target different divergences: $\mathrm{KL}[q|p]$ and $\mathrm{KL}[p|q]$!

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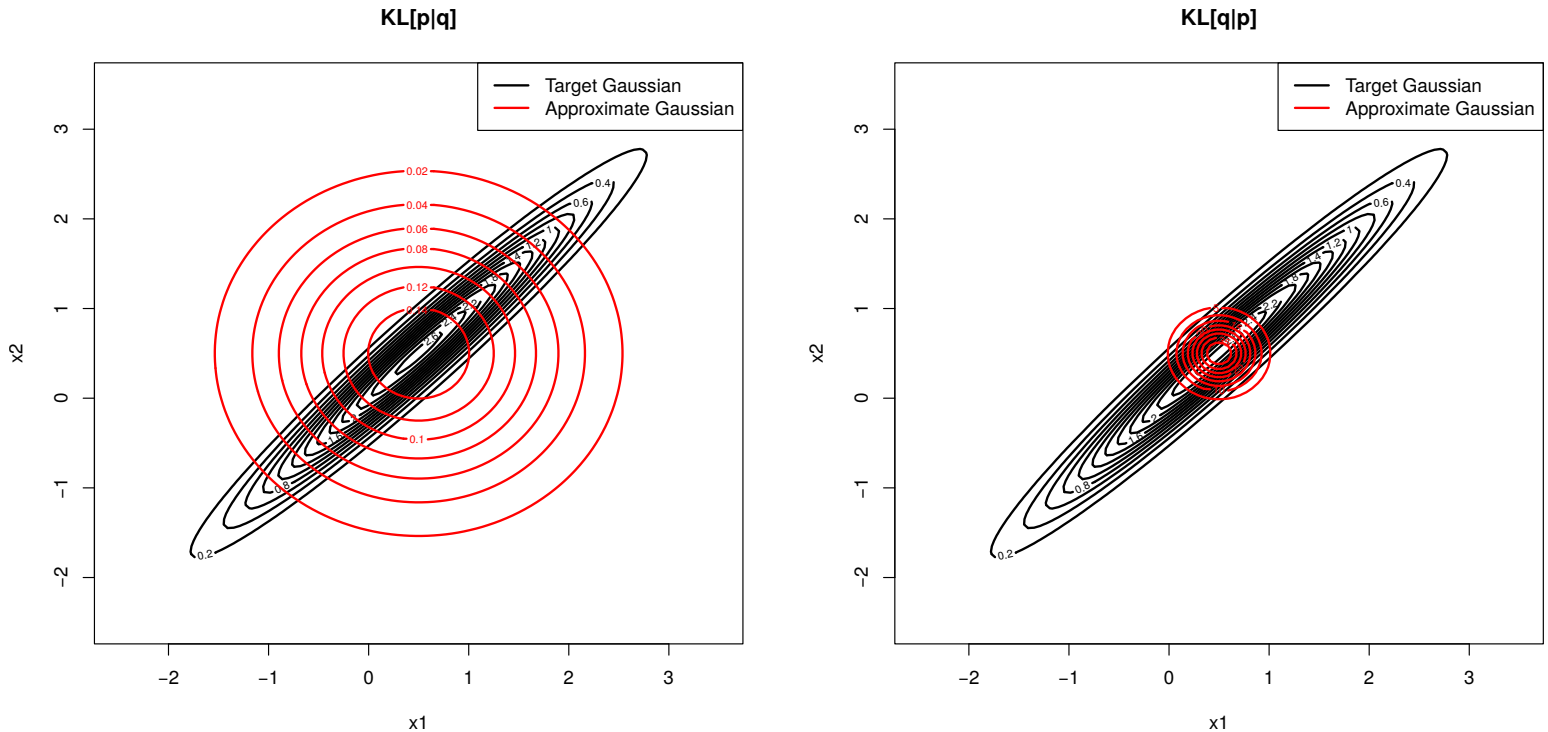

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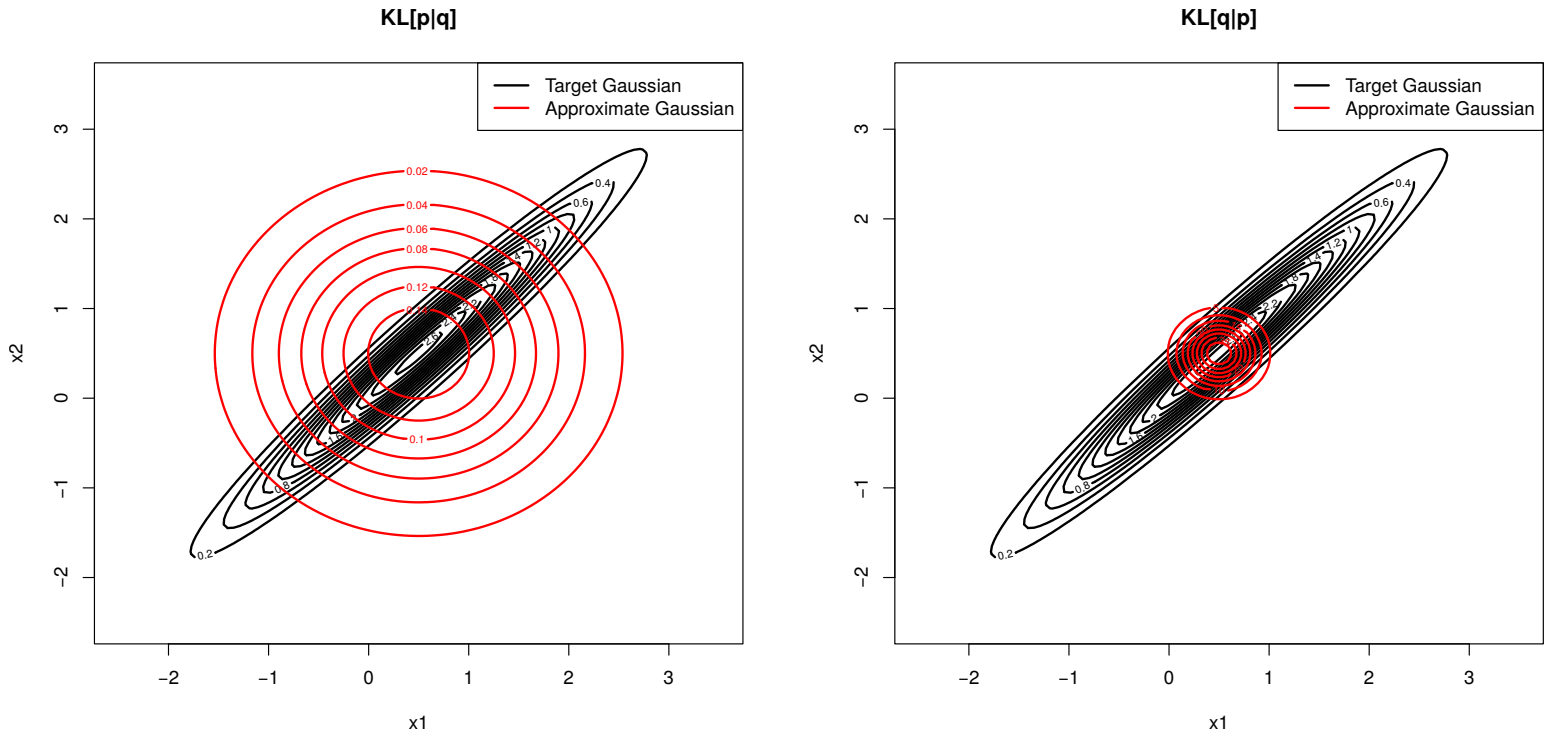

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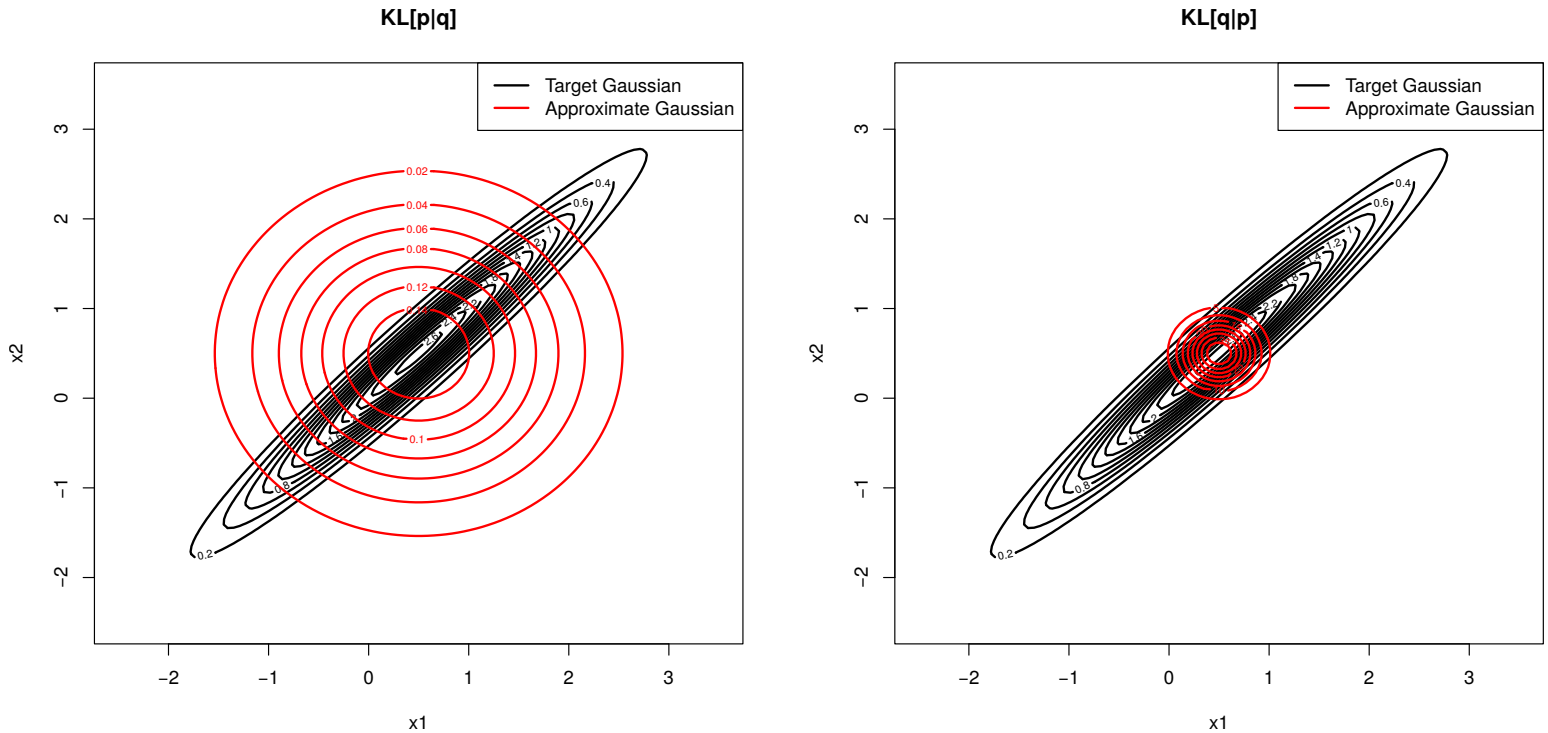

KL$[q|p]$ may result in too compact approximations while KL$[p|q]$ may put mass in regions with no posterior density. Can we have something in between?

Alpha Divergence

$$D_\alpha(p||q) = \frac{\int_{\boldsymbol{\theta}} \left(\alpha p(\boldsymbol{\theta}) + (1-\alpha) q(\boldsymbol{\theta}) - p(\boldsymbol{\theta})^\alpha q(\boldsymbol{\theta})^{1-\alpha}\right)\, d\boldsymbol{\theta}}{\alpha(1-\alpha)} \,.$$

(Amari, 1985).

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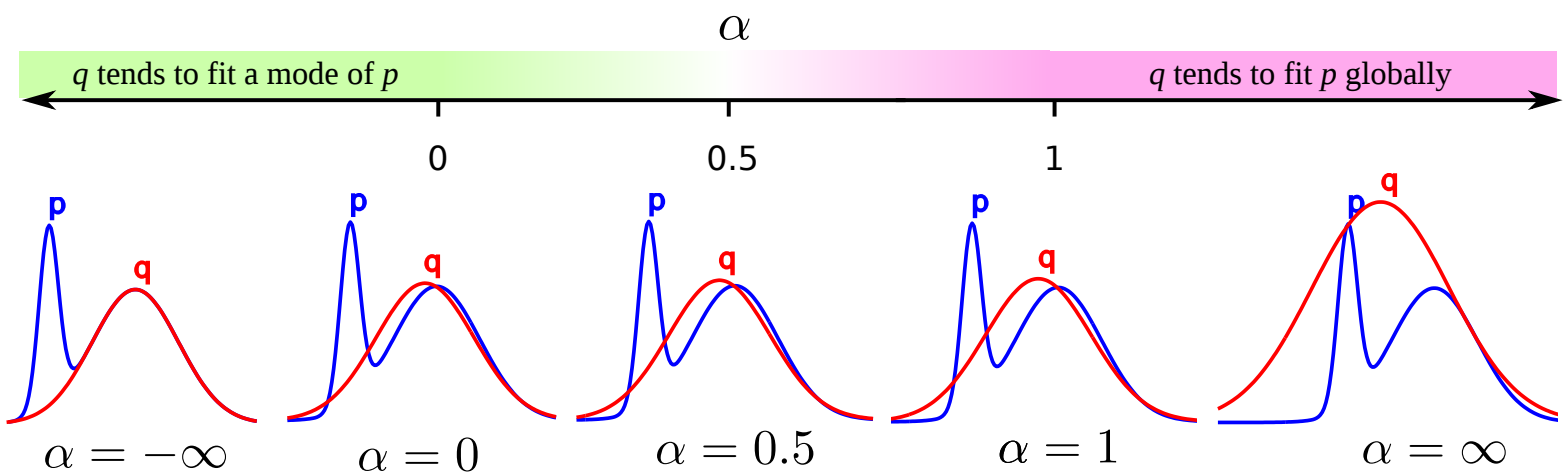

Figure source: (Minka, 2005).

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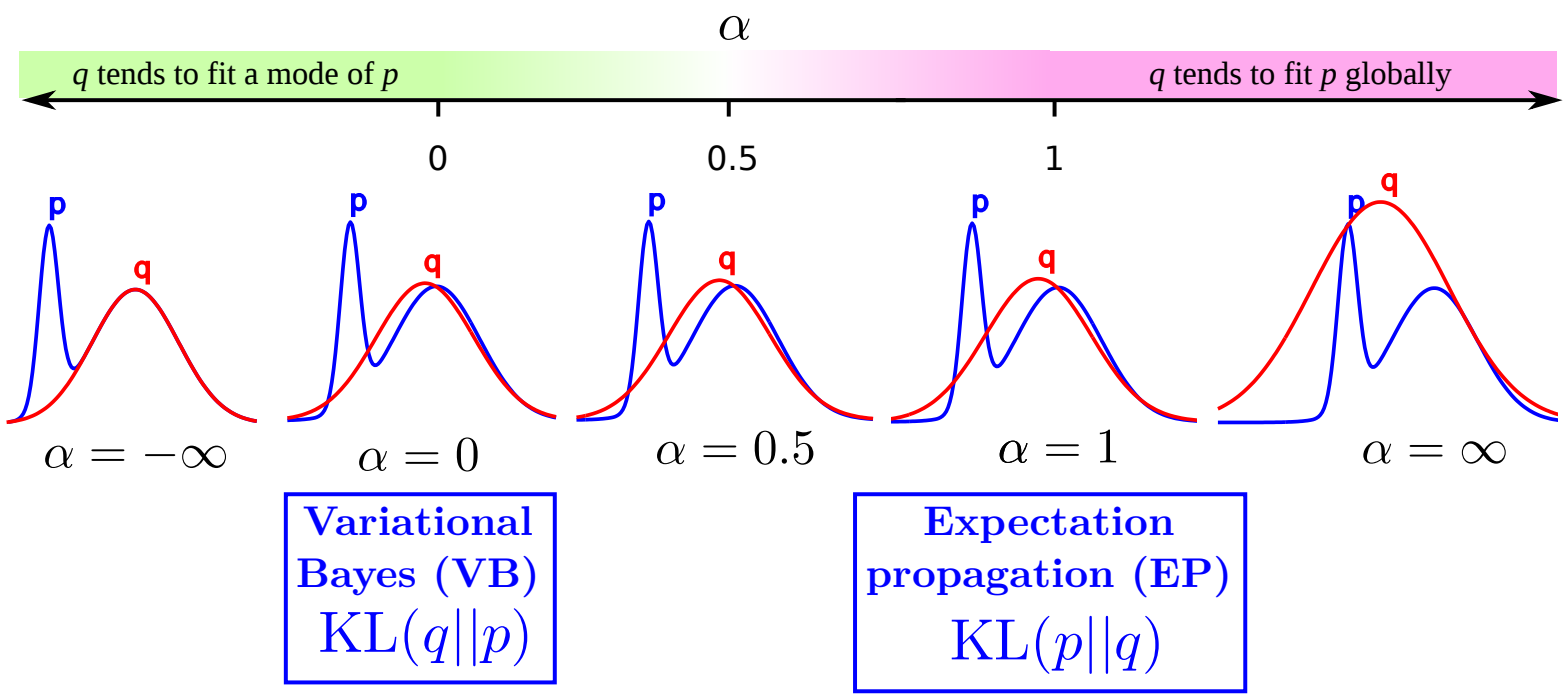

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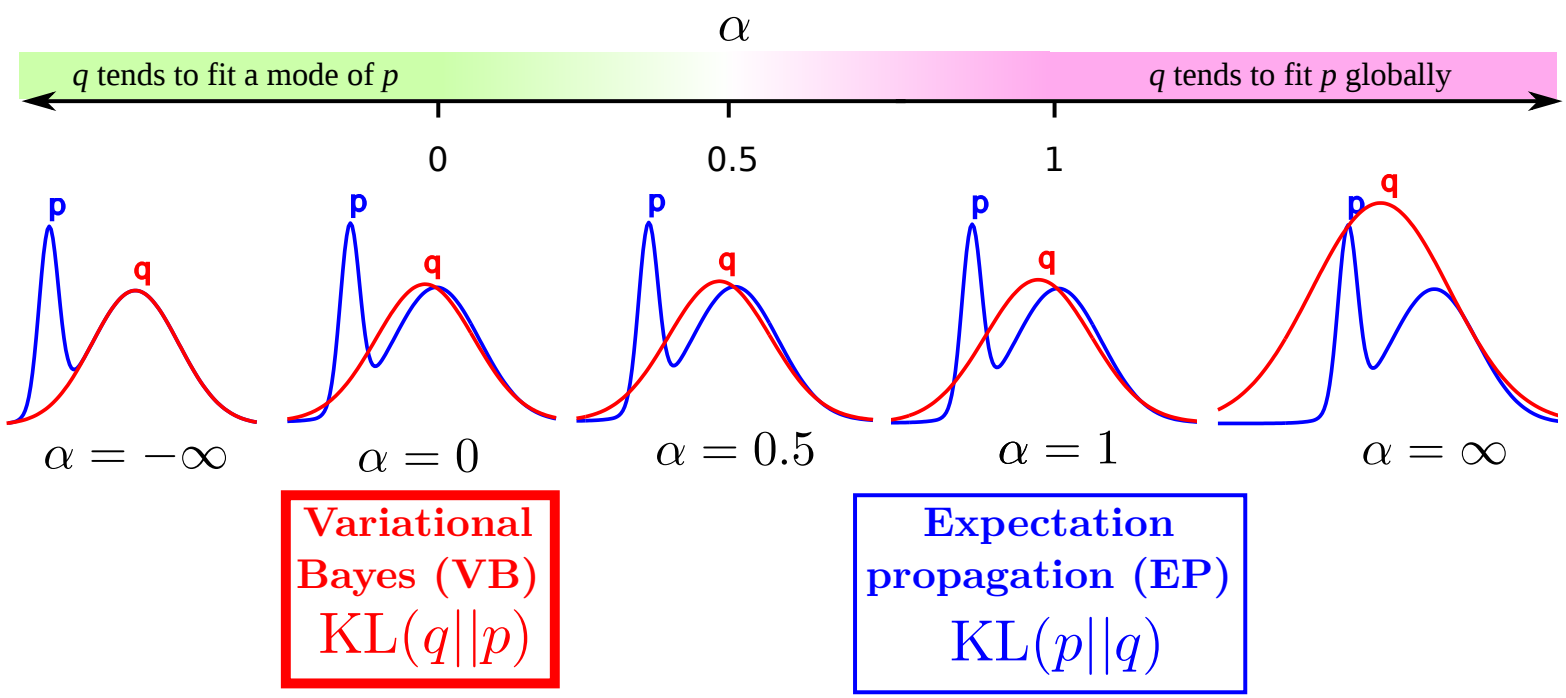

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Local α-divergence minimization (Power EP)

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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$\approx$

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The $\tilde{t}_j$ are tuned by minimizing local α-divergences

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

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It turns out that the α-divergence can be minimized in terms of the KL-divergence!

α-divergence minimization via KL minimization

Power EP steps to refine $\tilde{t}_i$:

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1. Compute cavity: $q^{\backslash \alpha i} \propto q/\tilde{t}_i^{\alpha}$.

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At convergence $\nabla_{\eta_q} D_{\alpha}[\hat{p}_n || q]$ equals zero!

PEP as an Optimization Problem

The PEP approximation to the **evidence** $p(\mathbf{y})$ is given by:

$$\log Z_{\text{PEP}} = g(\boldsymbol{\eta}_q) - g(\boldsymbol{\eta}_{\text{prior}}) + \sum_{i=1}^{N} \frac{1}{\alpha} \left(\log Z_i + g(\boldsymbol{\eta}_q) - g(\boldsymbol{\eta}_q^{\backslash \alpha i}) \right)$$

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Besides the PEP updates, the PEP solution for q is found by solving:

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Can be solved with a **double-loop** algorithm.

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Can be solved with a **double-loop** algorithm. **Too slow in practice!**

Approximate Power Expectation Propagation

$$p(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L|\mathbf{y}) \propto \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \quad p(y_1|f_1^L) \quad p(y_2|f_2^L) \quad p(y_3|f_3^L)$$

$$\approx \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_1(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}_2(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \propto q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$$

We tie the approximate factors!

$$\approx \tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \; \tilde{t}(\{\mathbf{u}^l\}_{l=1}^L) \propto q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$$

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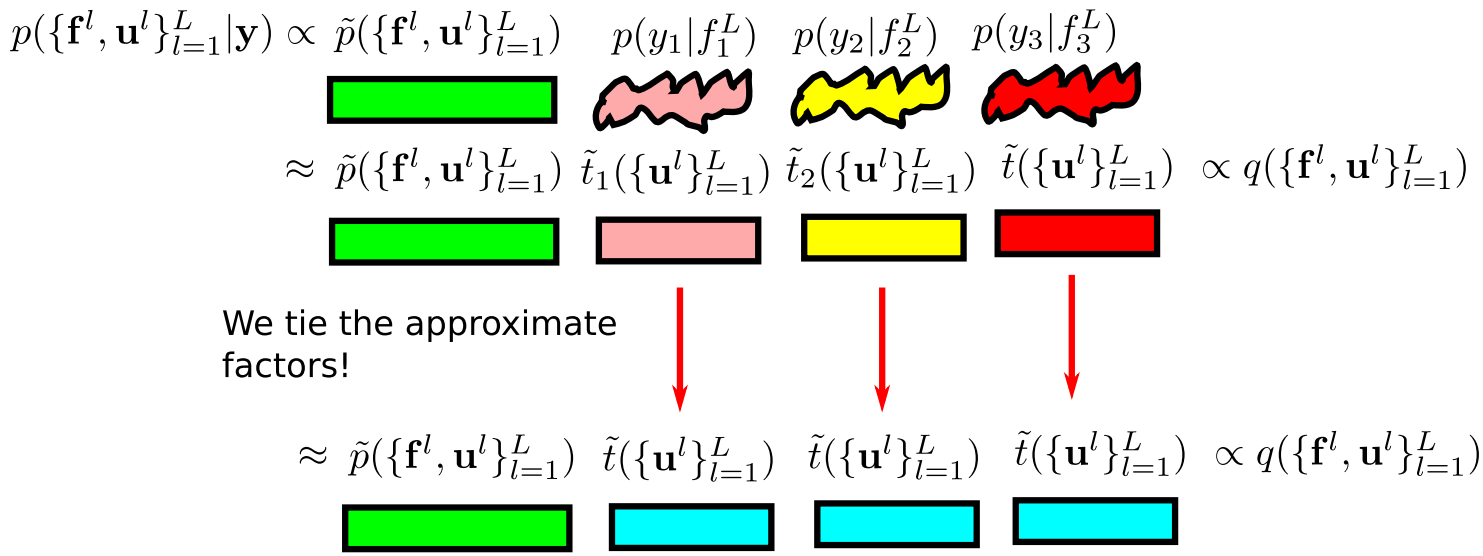

- $\max_q \min_{\tilde{f}_1,\ldots,\tilde{f}_N}$ problem $\rightarrow$ $\max_q$ problem, **no double-loop needed!**

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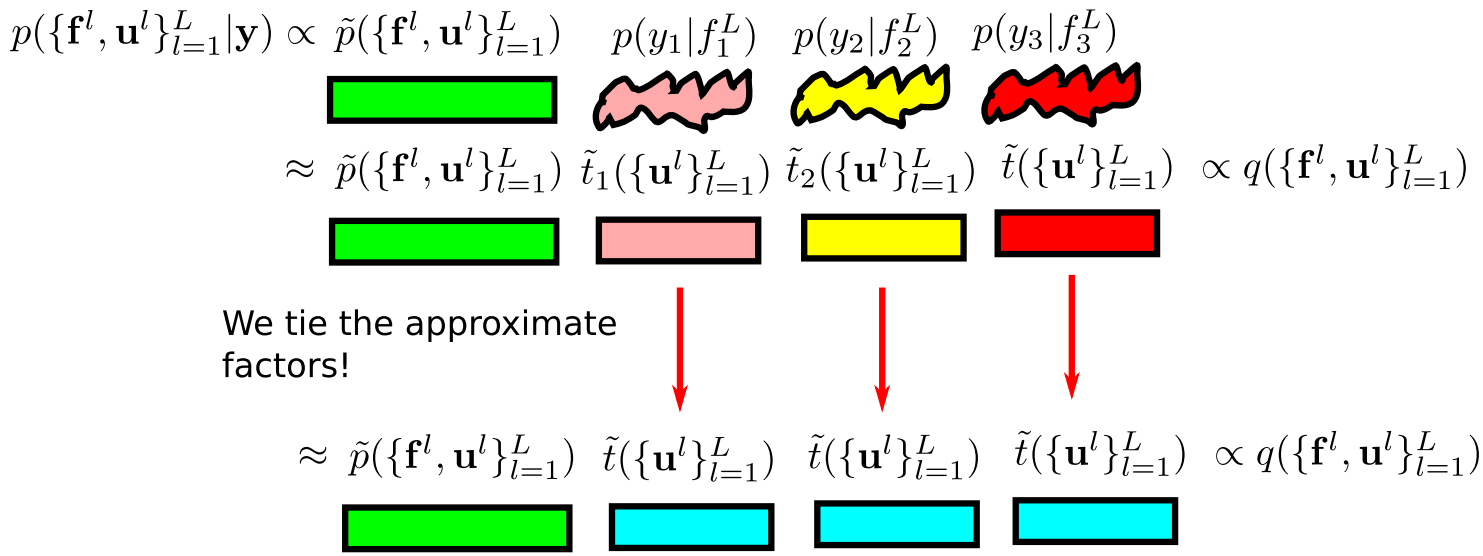

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The final objective is:

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which is suitable for standard optimization and mini-batch training.
(Villacampa, 2022)(Li, 2017)

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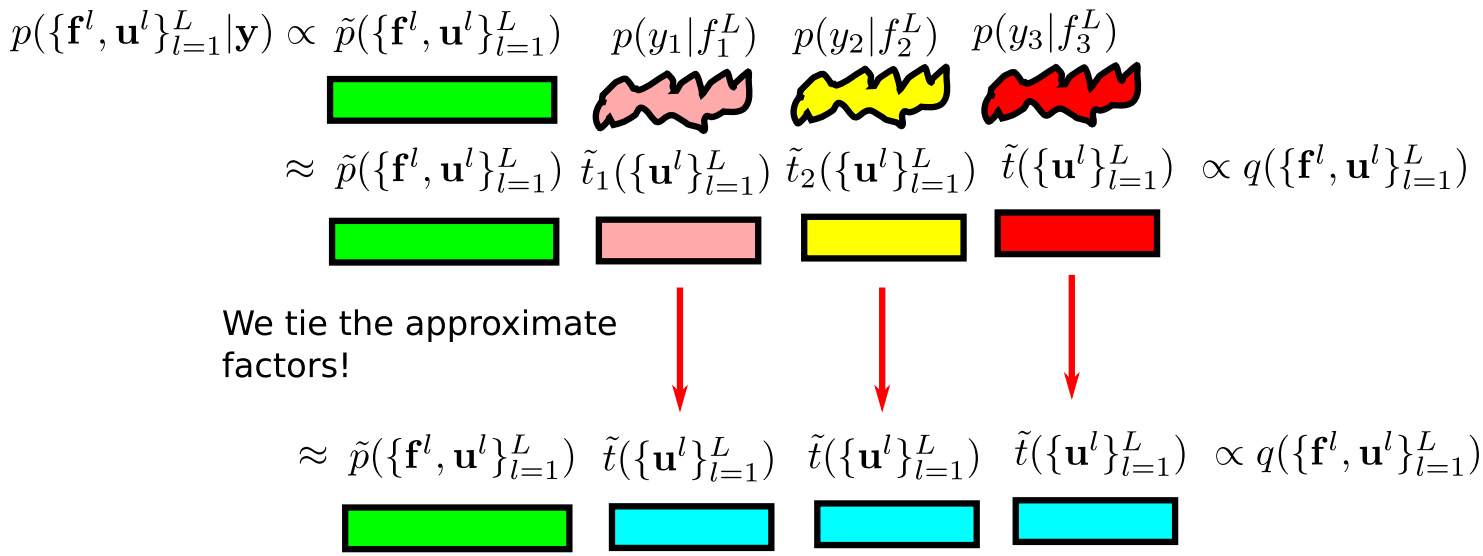

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(Villacampa, 2022)(Li, 2017)

Approximating $\log Z_i$

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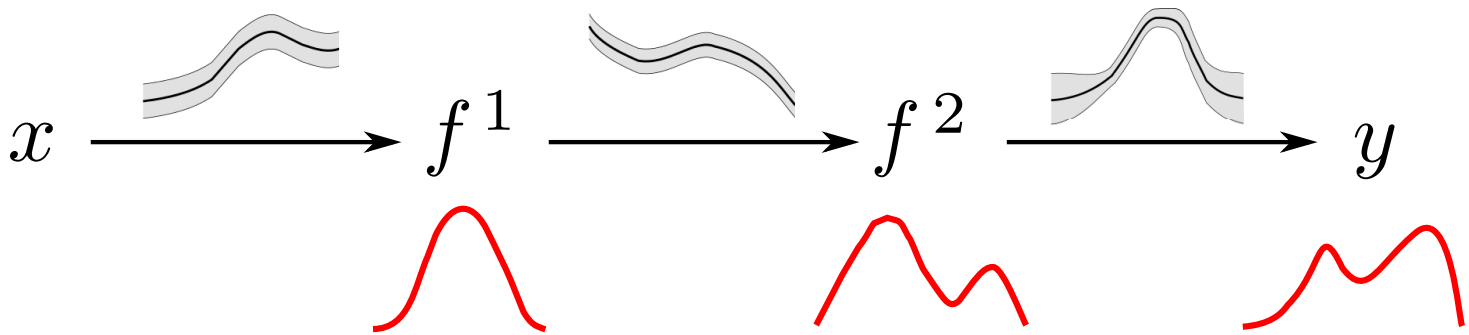

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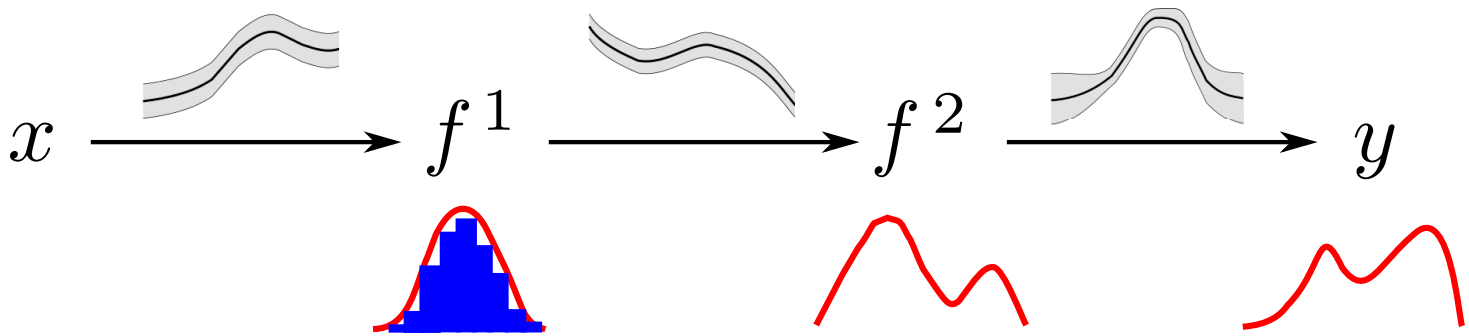

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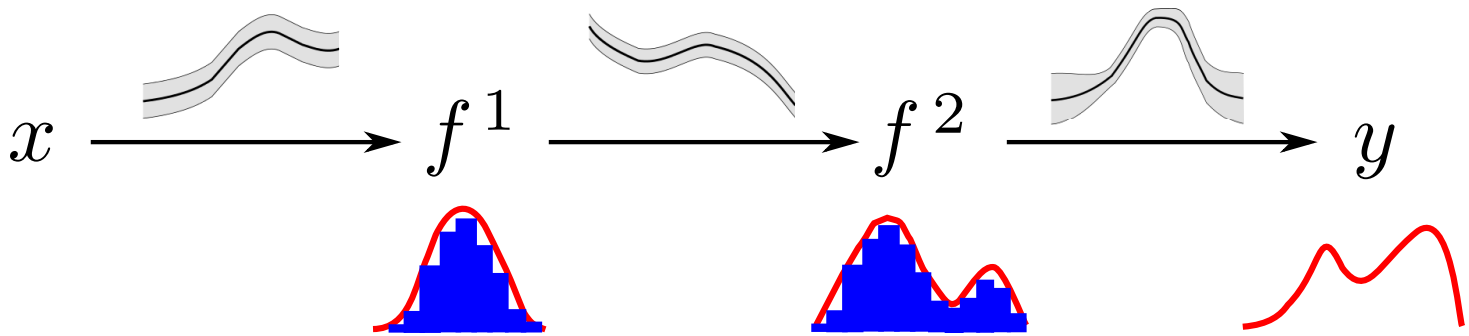

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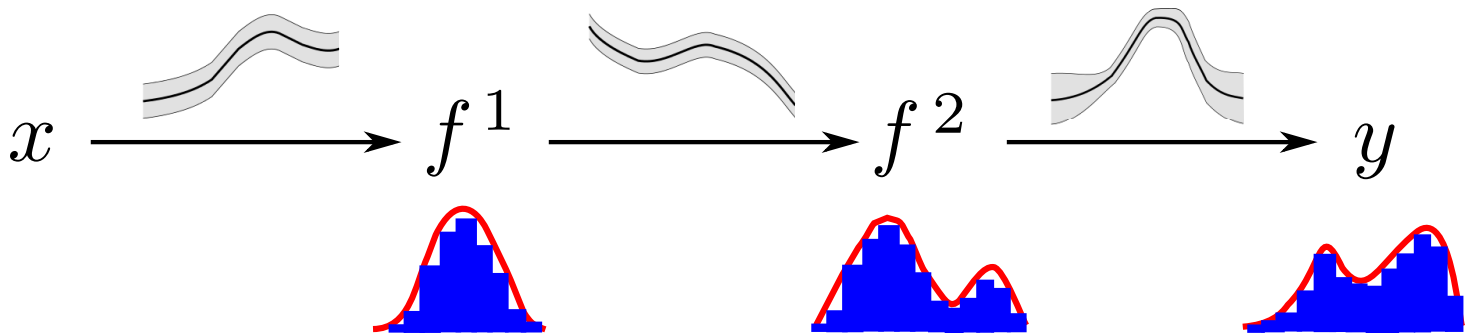

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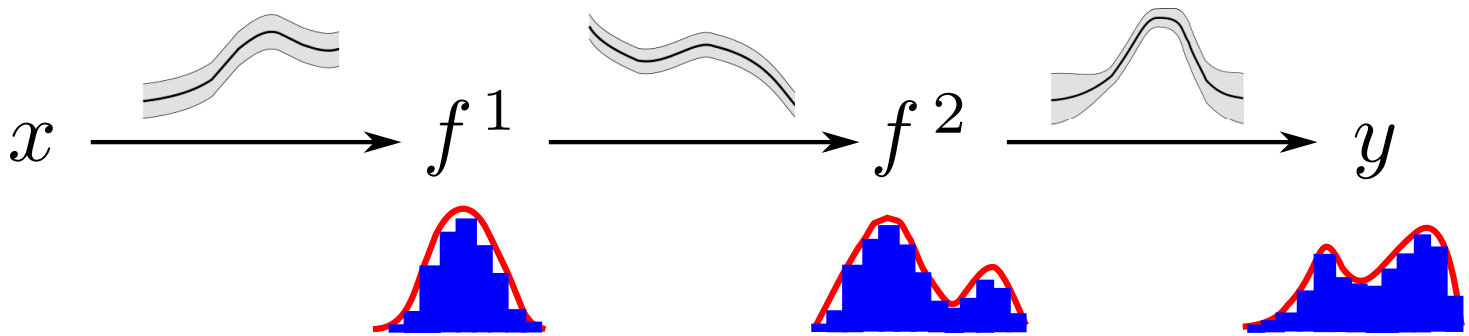

Expected to be more accurate than the Gaussian projection method used by AEP!

Further Approximations

Consider $\alpha \approx 0$ or $N \to \infty$ (*i.e.*, the cavity becomes q):

$$\log Z_{\text{PEP}} \approx g(\boldsymbol{\eta}_q) - g(\boldsymbol{\eta}_{\text{prior}}) + \sum_{i=1}^{N} \frac{1}{\alpha} \big(\log \tilde{Z}_i + g(\boldsymbol{\eta}_q) - g(\boldsymbol{\eta}_{q_\alpha^{\text{cav}}}) \big)$$

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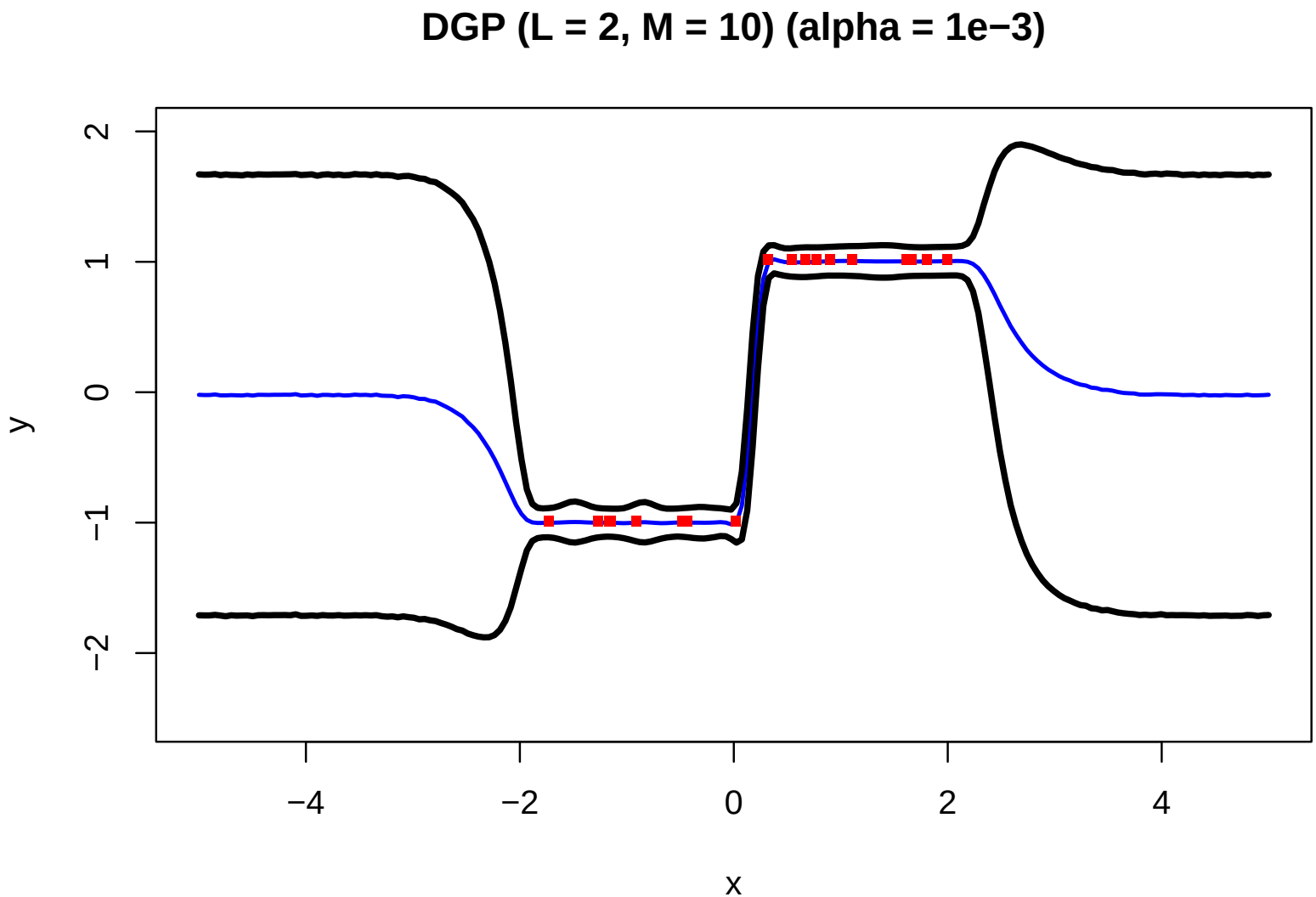
Which for $\alpha \to 0$ gives the DVSVI objective and for $\alpha = 1$ is expected to give similar results to AEP (better estimating $\log Z_i$)!

α-Divergence Minimization: Illustrative Example



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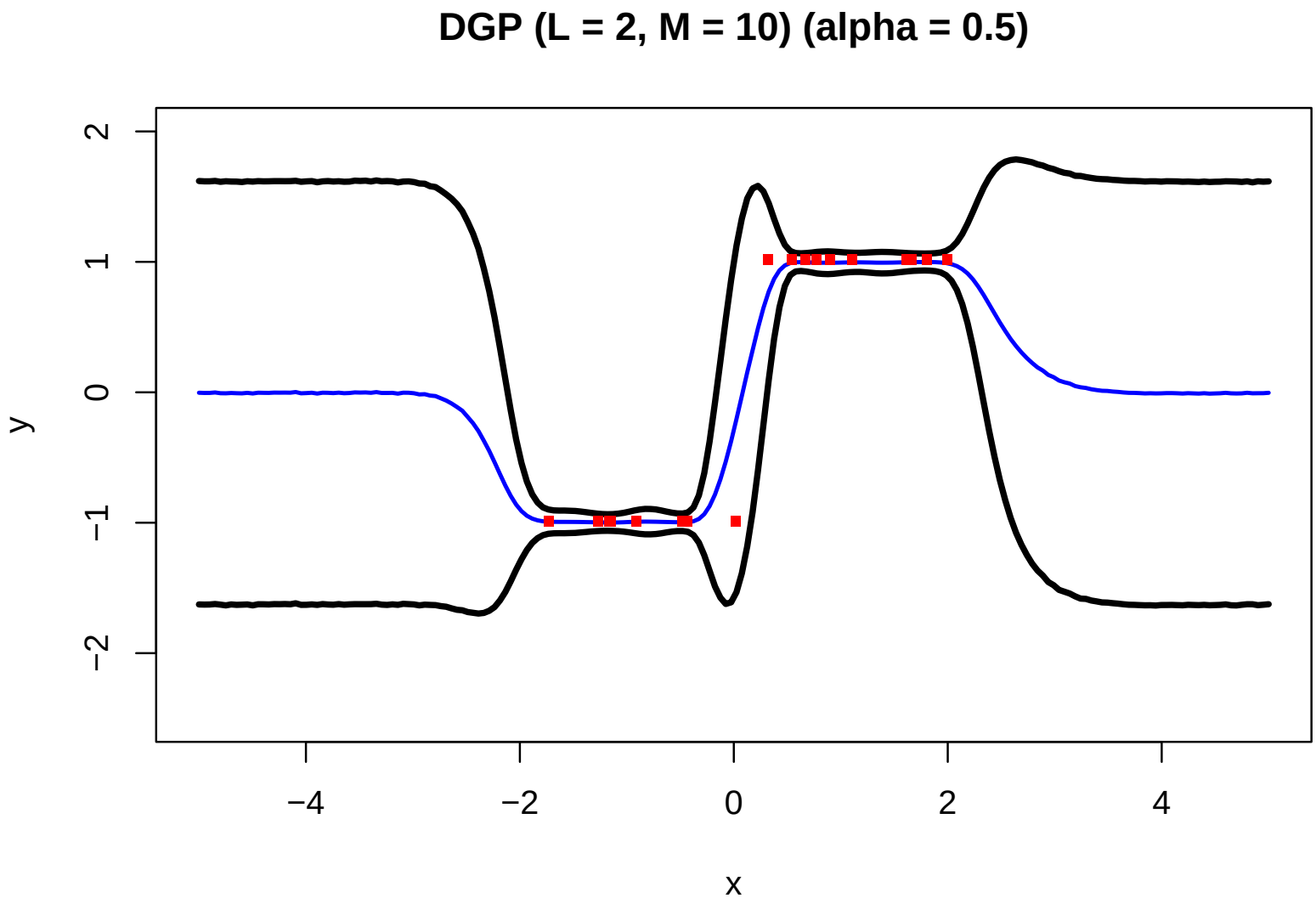

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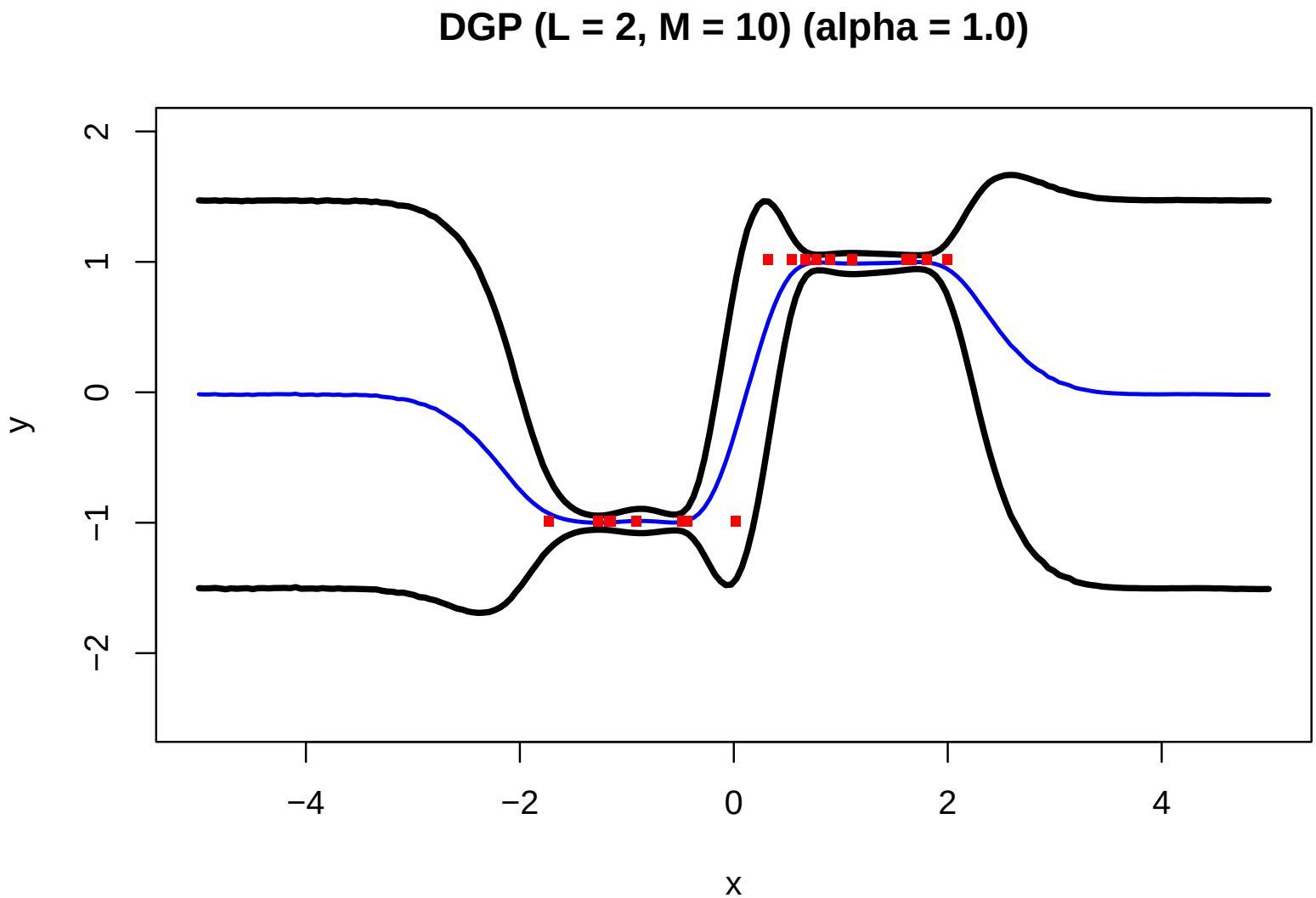

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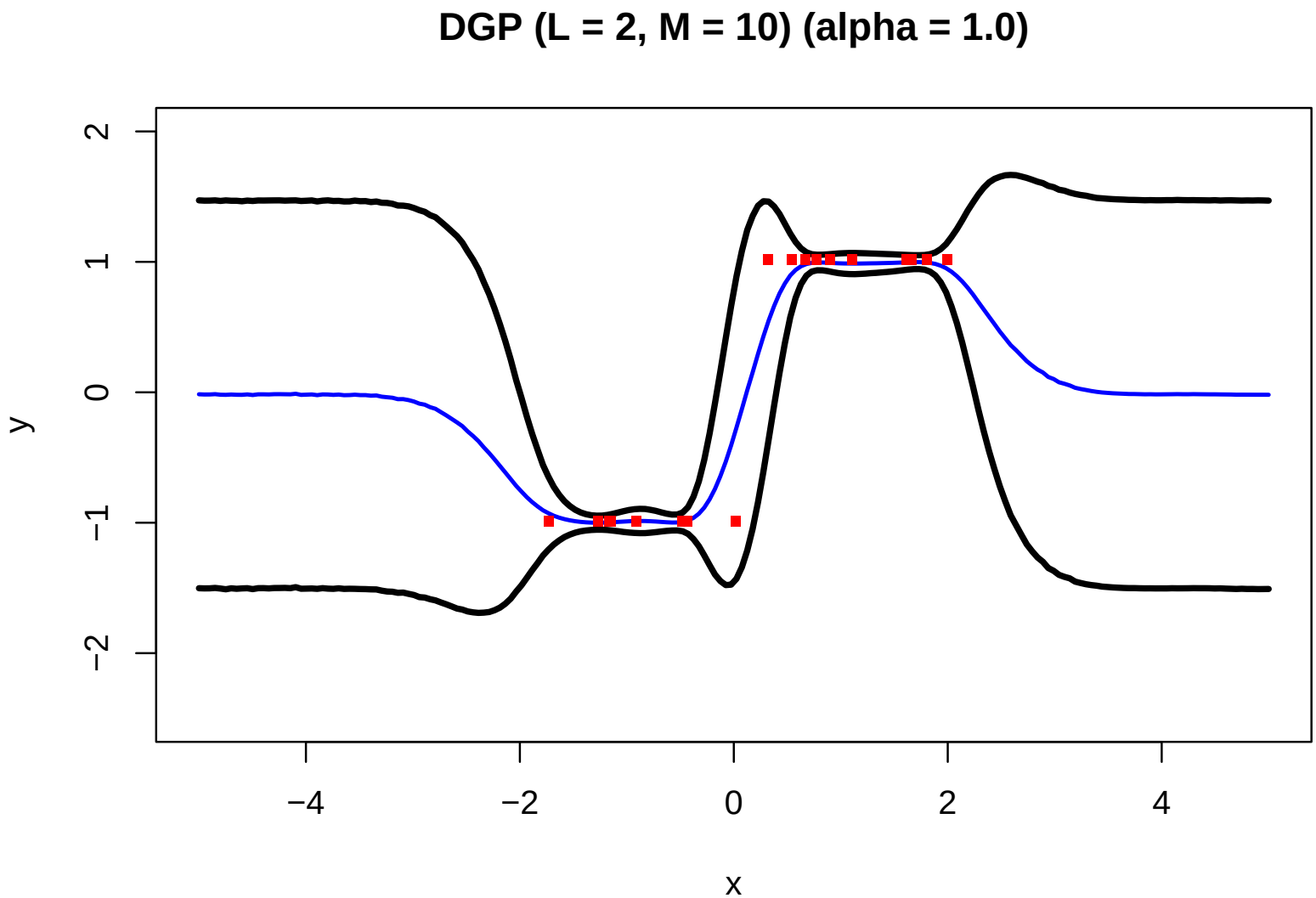
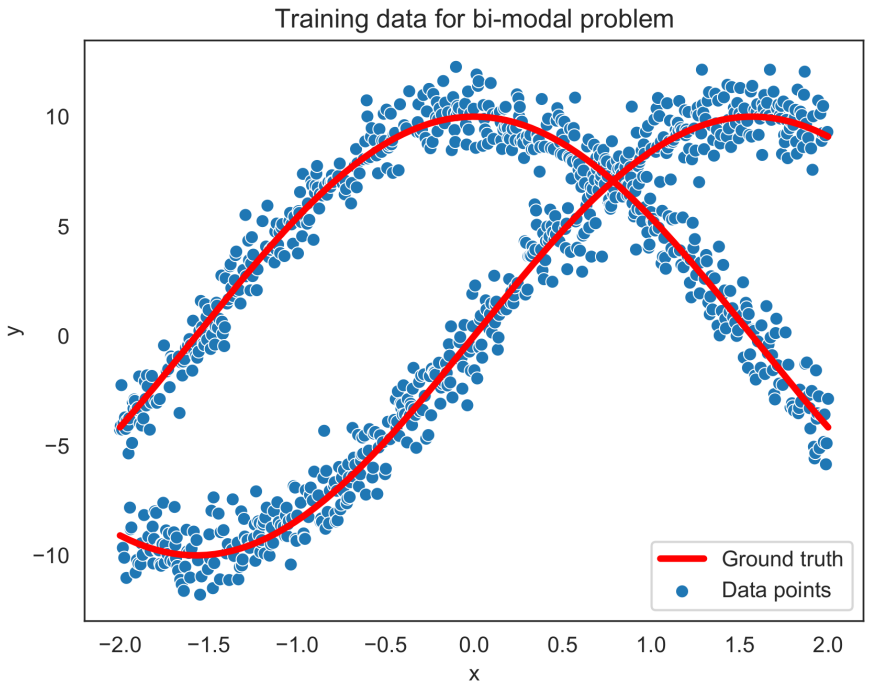
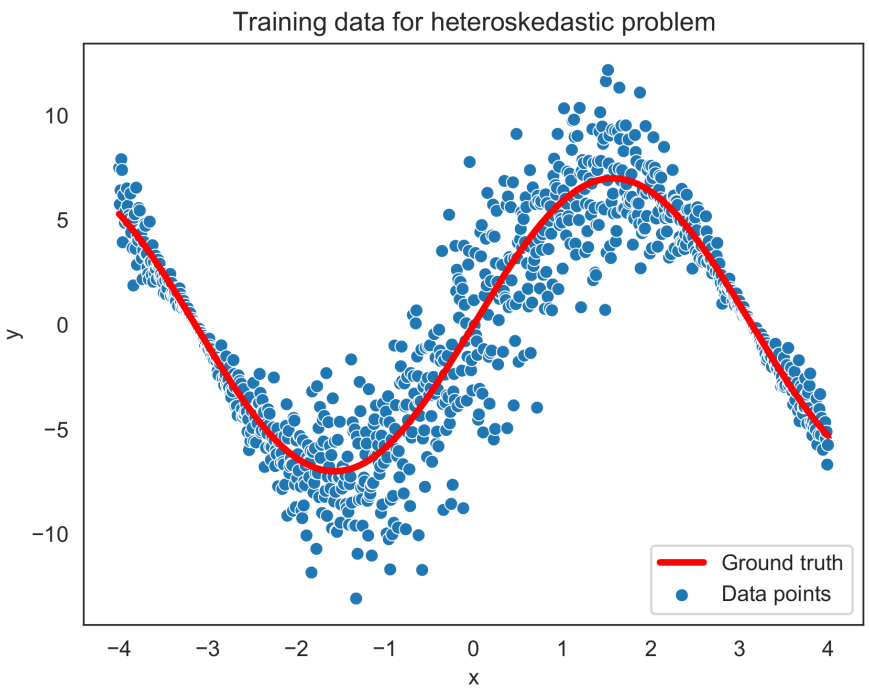


The value of α has an impact on the final predictive distribution!

α-Divergence Minimization: Toy Problems





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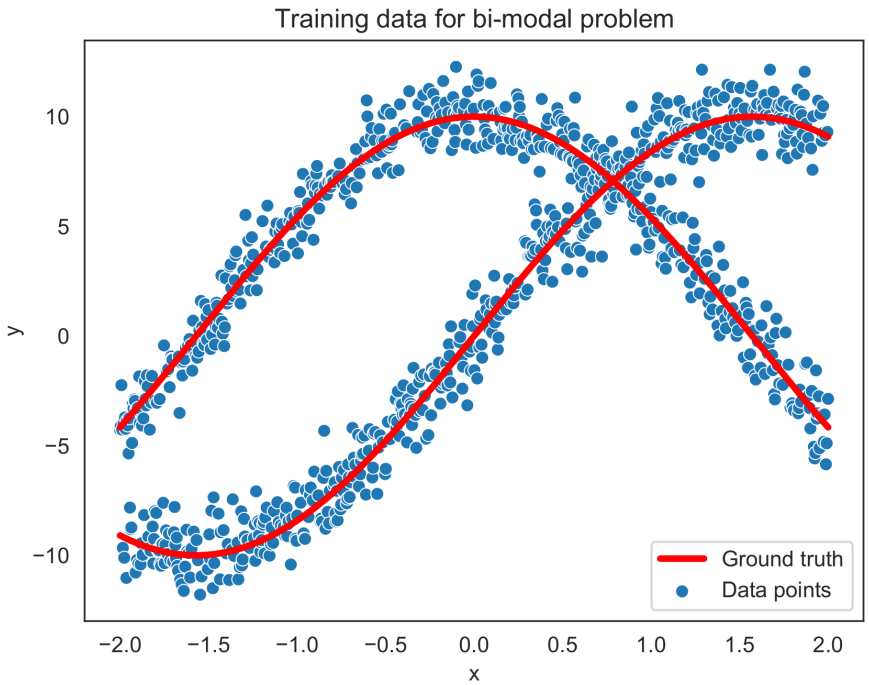

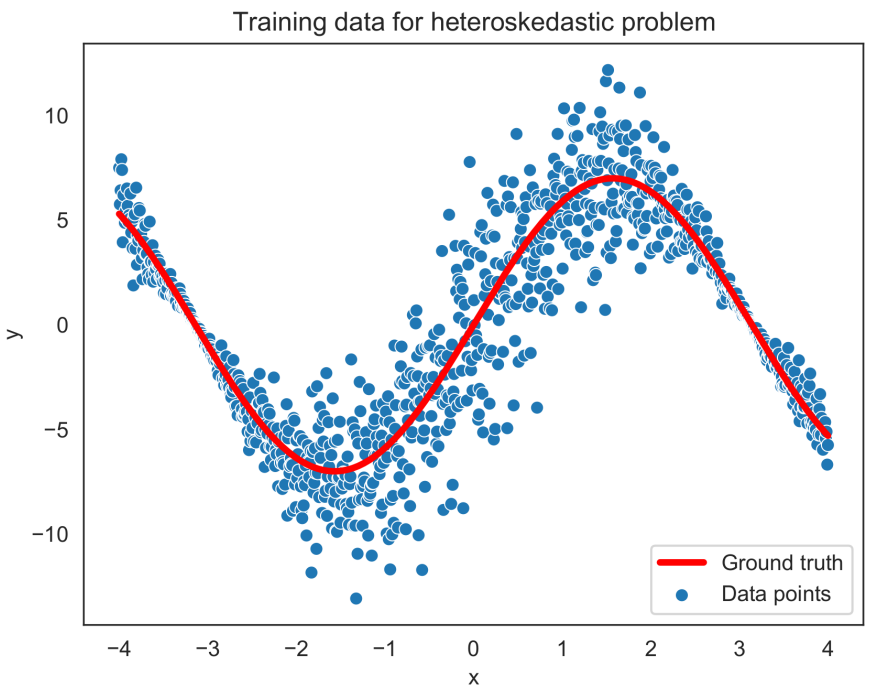

The first problem has a bimodal predictive distribution. The second, has heteroscedastic noise!

(Depeweng, 2016)

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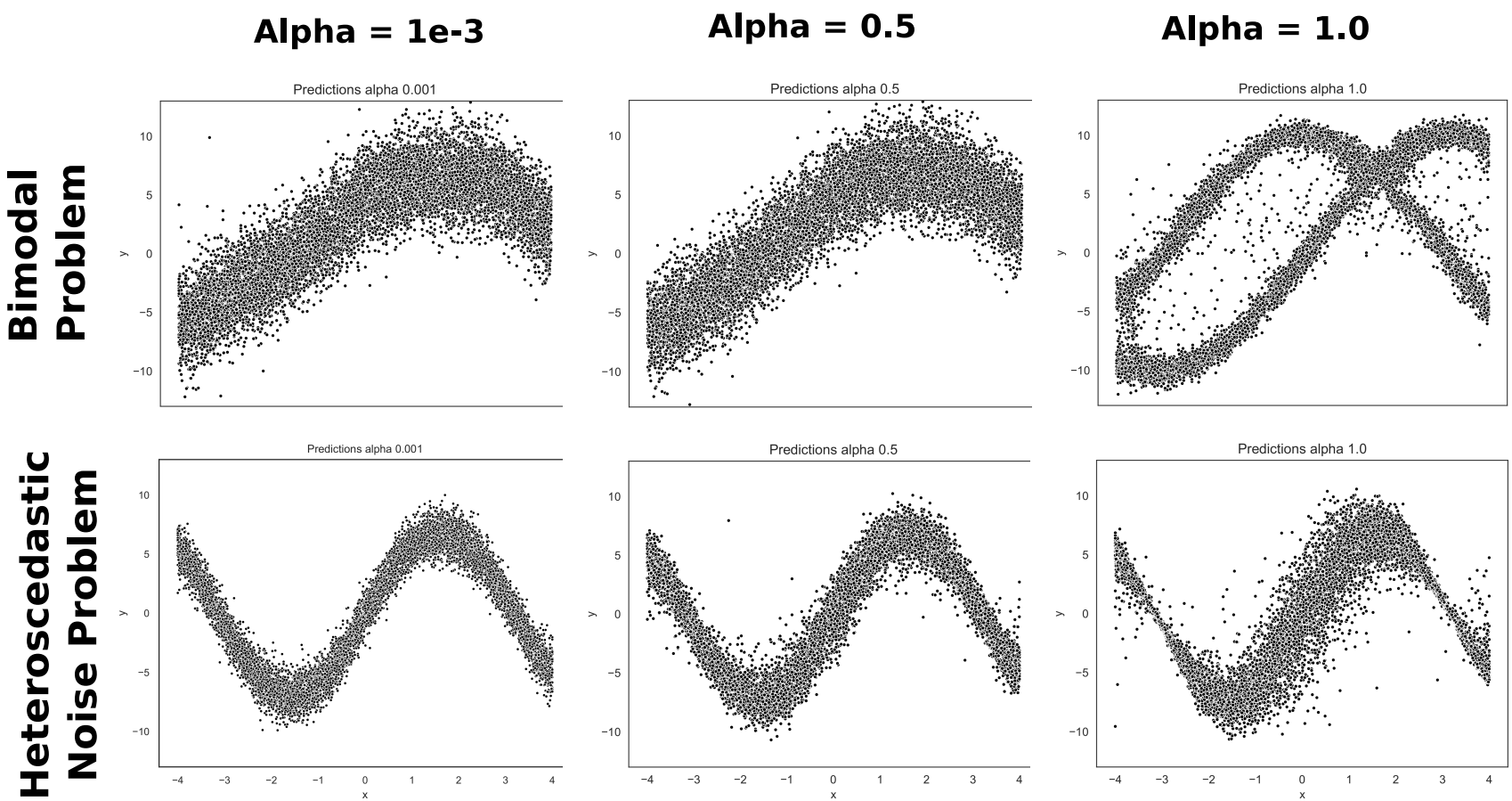

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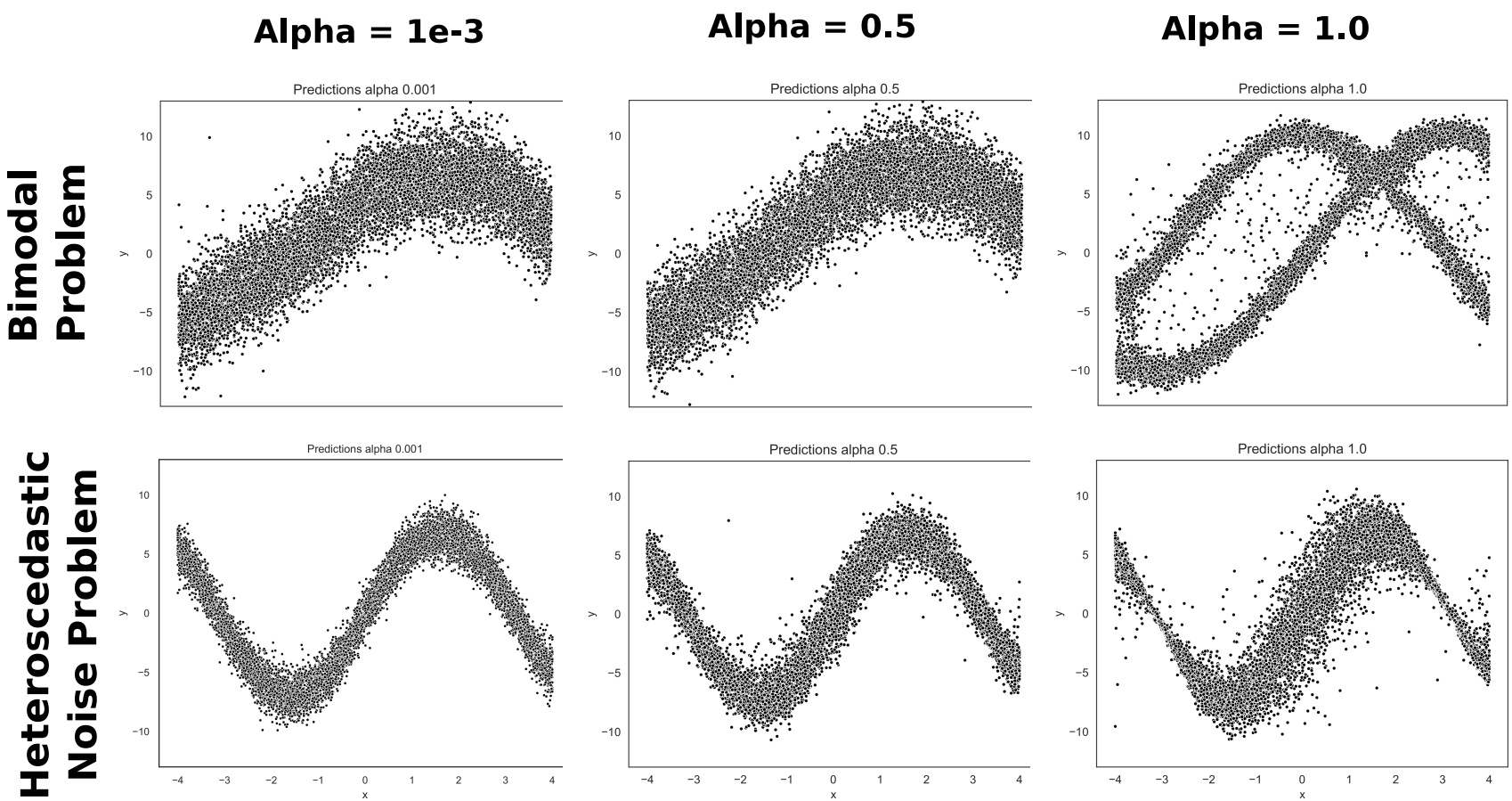
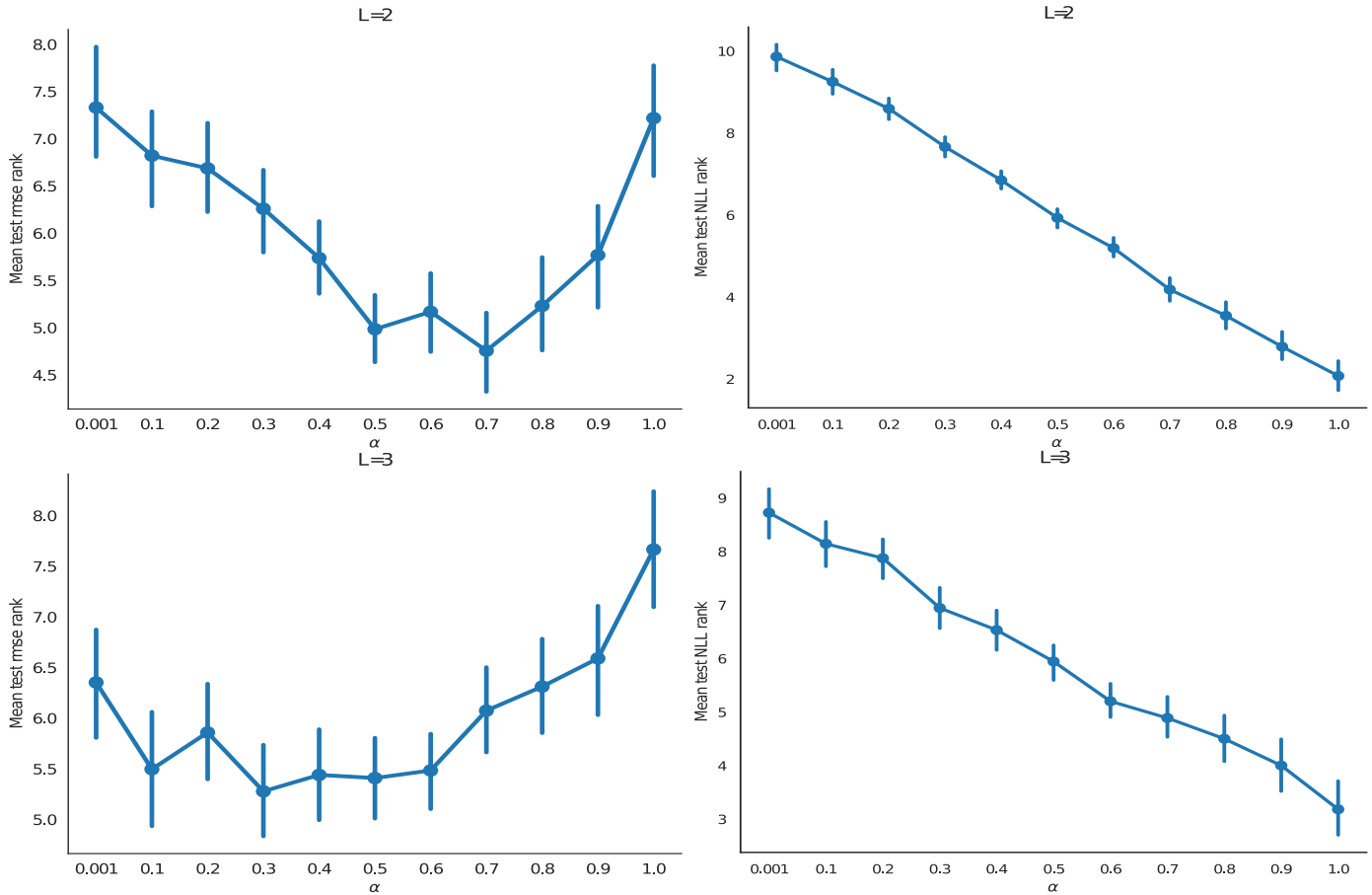


The value $\alpha = 1.0$ provides more sensible predictive distributions!

(Villacampa, 2022)

α-Divergence Minimization: Average Ranks



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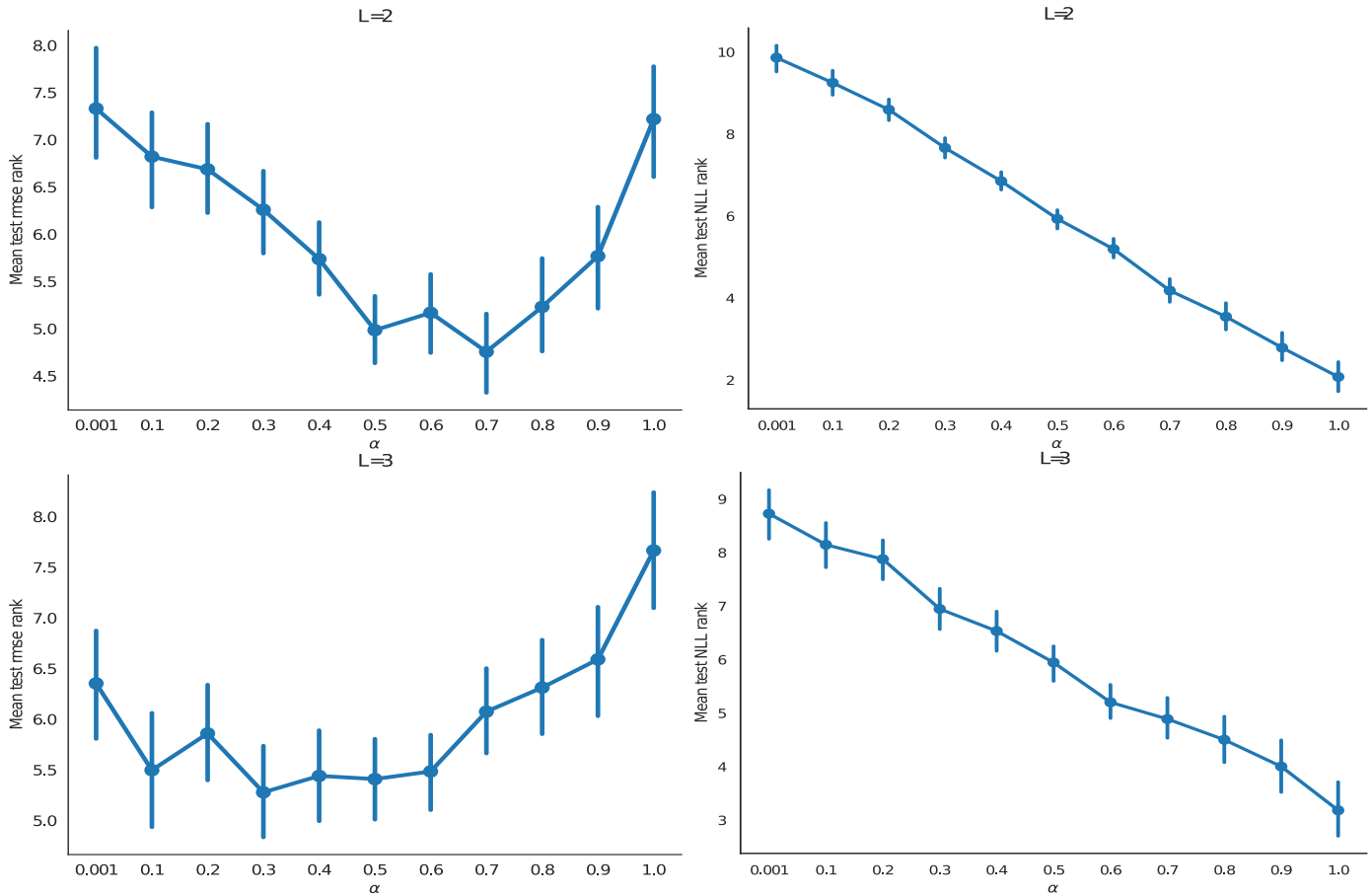

The value $\alpha = 1.0$ provides better results in terms of the NLL and intermediate values of α give better RMSE!

(Villacampa, 2022)

Run the last cells of the notebook to fit a DGP by minimizing alpha-divergences and complete task 2!

Deep GPs Application: Multifidelity Modeling

In many settings there is a difficulty of generating observed data!

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Example:

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- Computer simulation of the robot (cheap but inaccurate).

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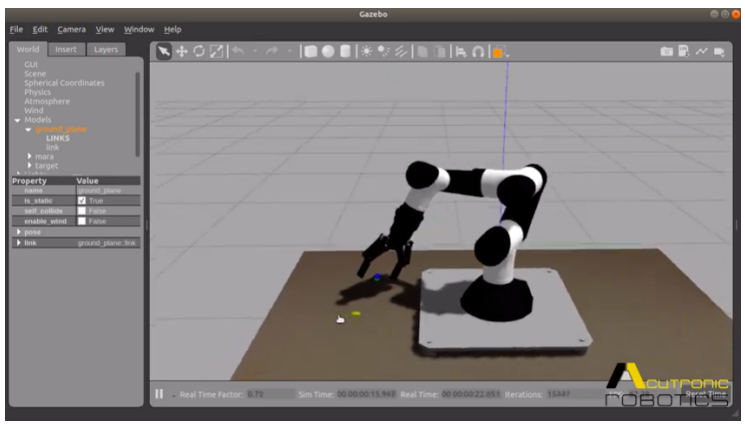

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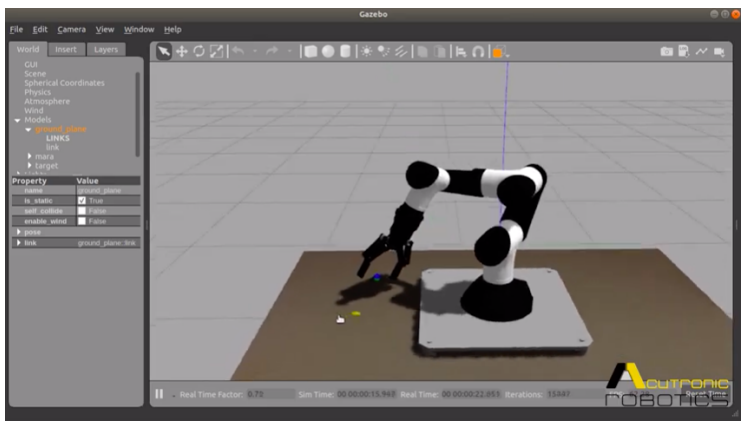

Other examples include a big and a small neural network, etc.

Deep GPs for Multifidelity Modeling

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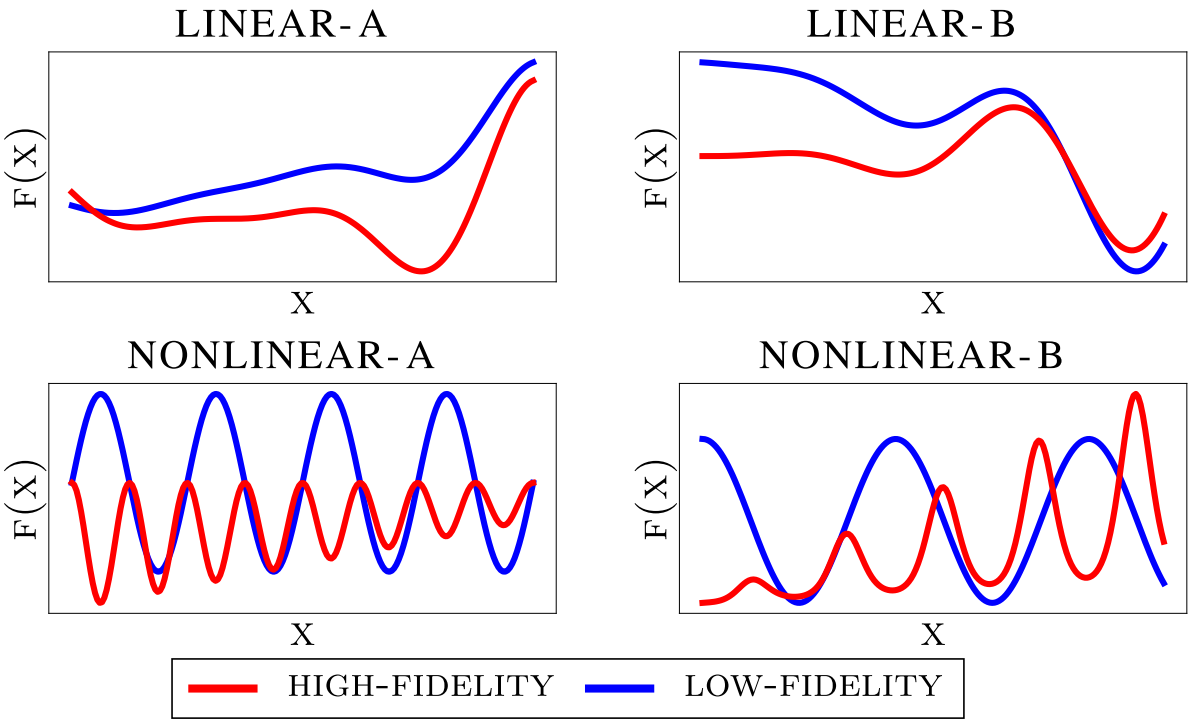

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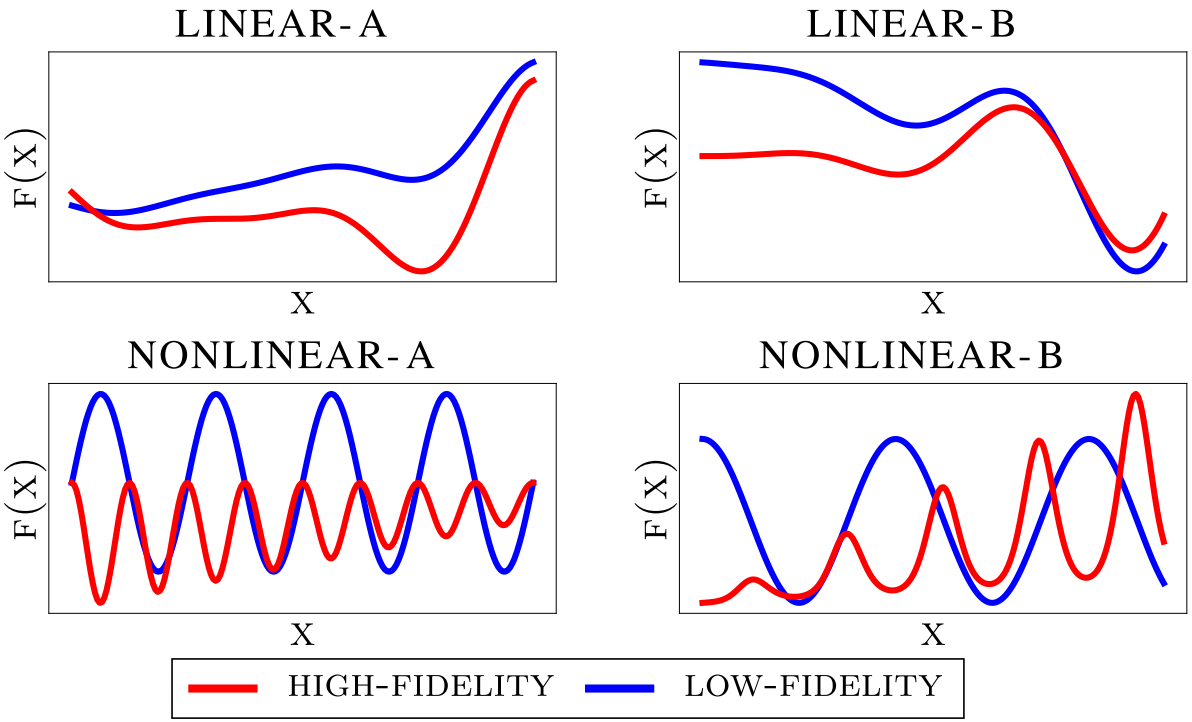

There are potential non-linear correlations between high and low fidelity target values!

(Kutajar et al., 2019)

MFDGPs: Architecture Employed

A DGP may capture dependencies between fidelity levels!

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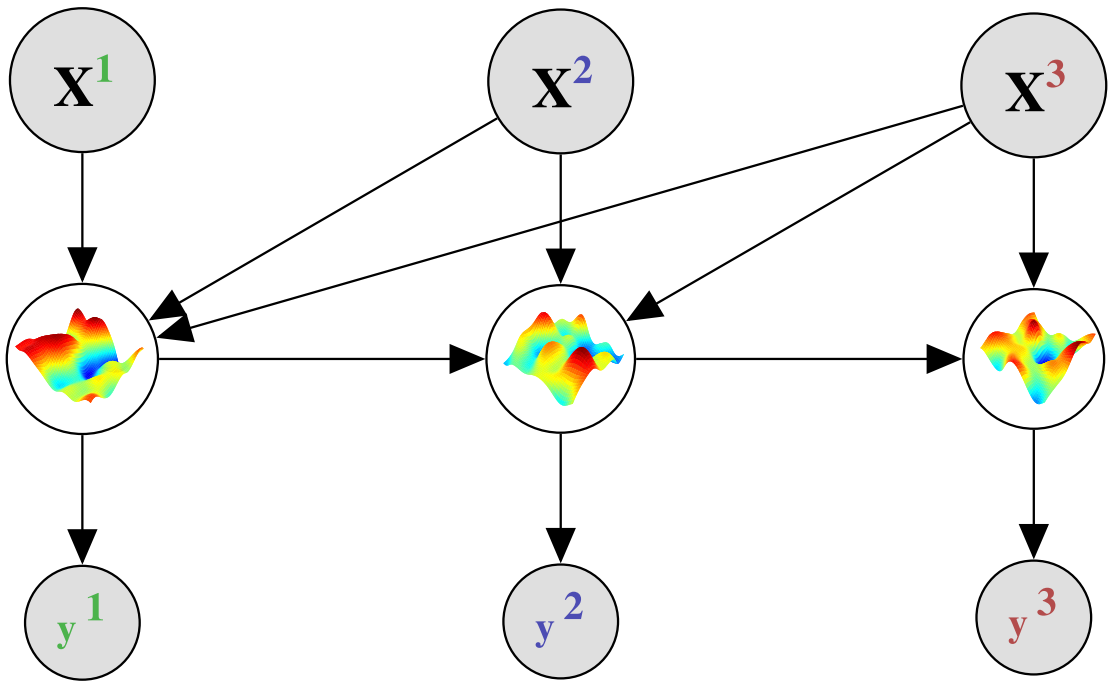

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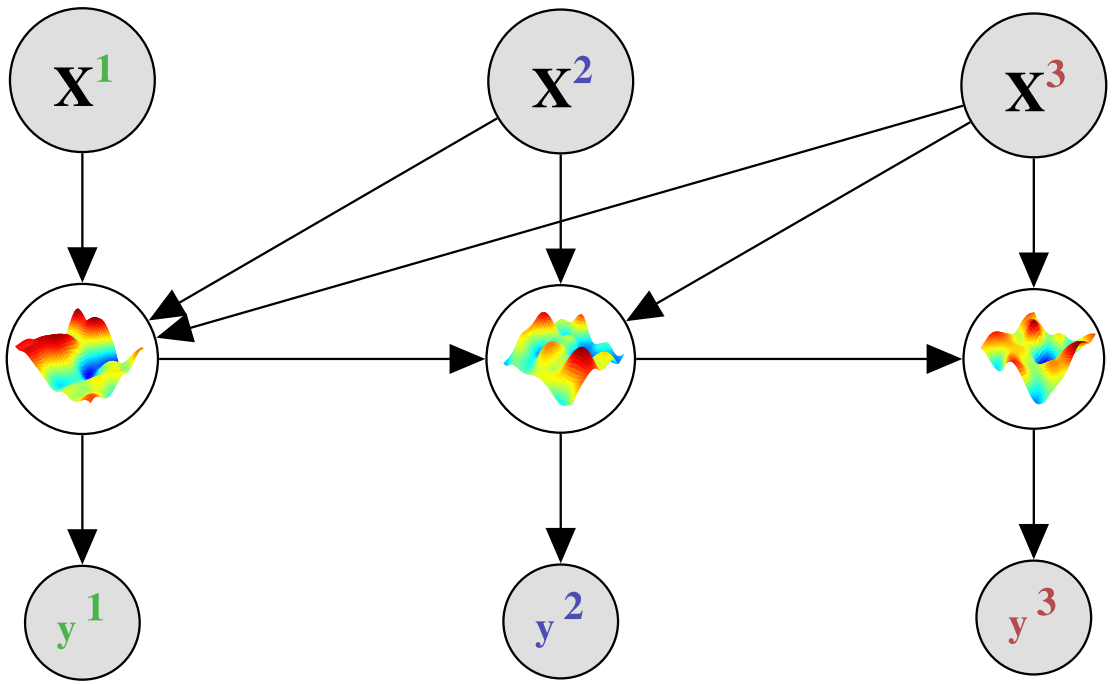

Each higher fidelity levels depends on the inputs but also on the lower fidelity level!

(Kutajar et al., 2019)

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To capture dependencies between fidelity levels we need a specific covariance function!

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- RBF: Captures un-explained components

MFDGPs: Training via DSVI

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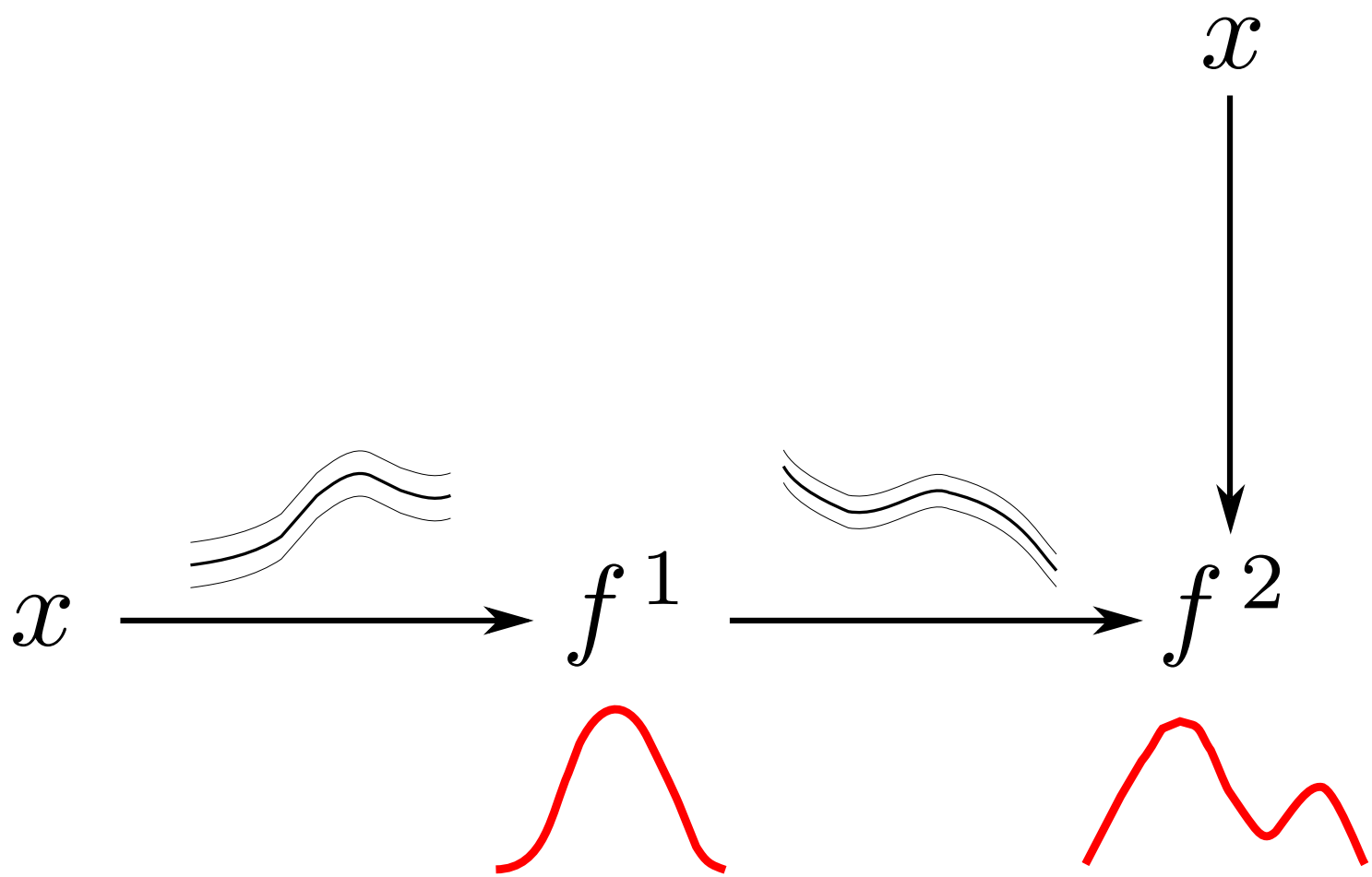
- The expectations can be approximated by Monte Carlo.
- Suitable for mini-batch training by subsampling the data.
- Difficult to optimize: Requires a two-phase training approach!

(Kutajar et al., 2019)

Predictive Distribution via Monte Carlo Sampling



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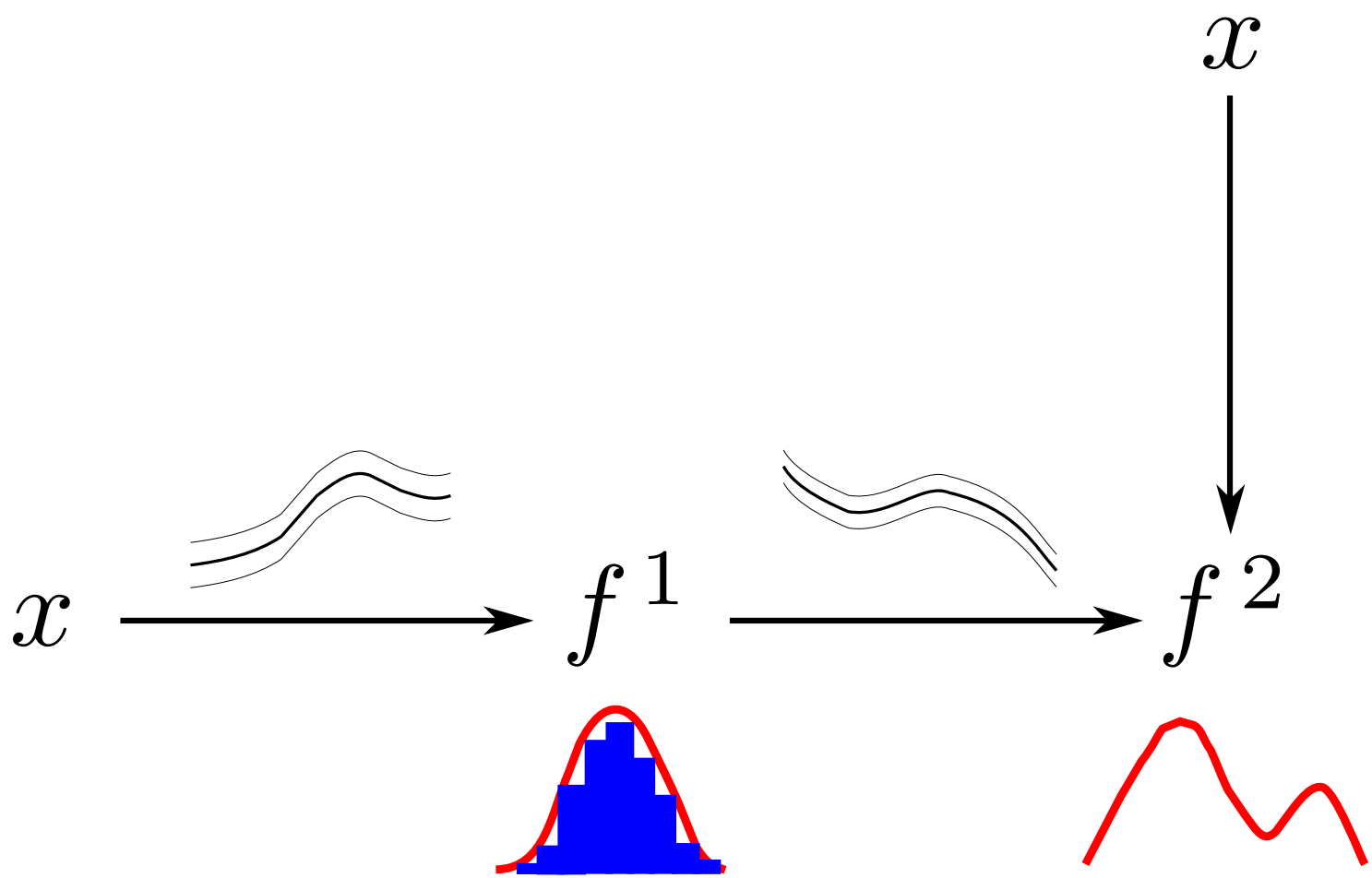

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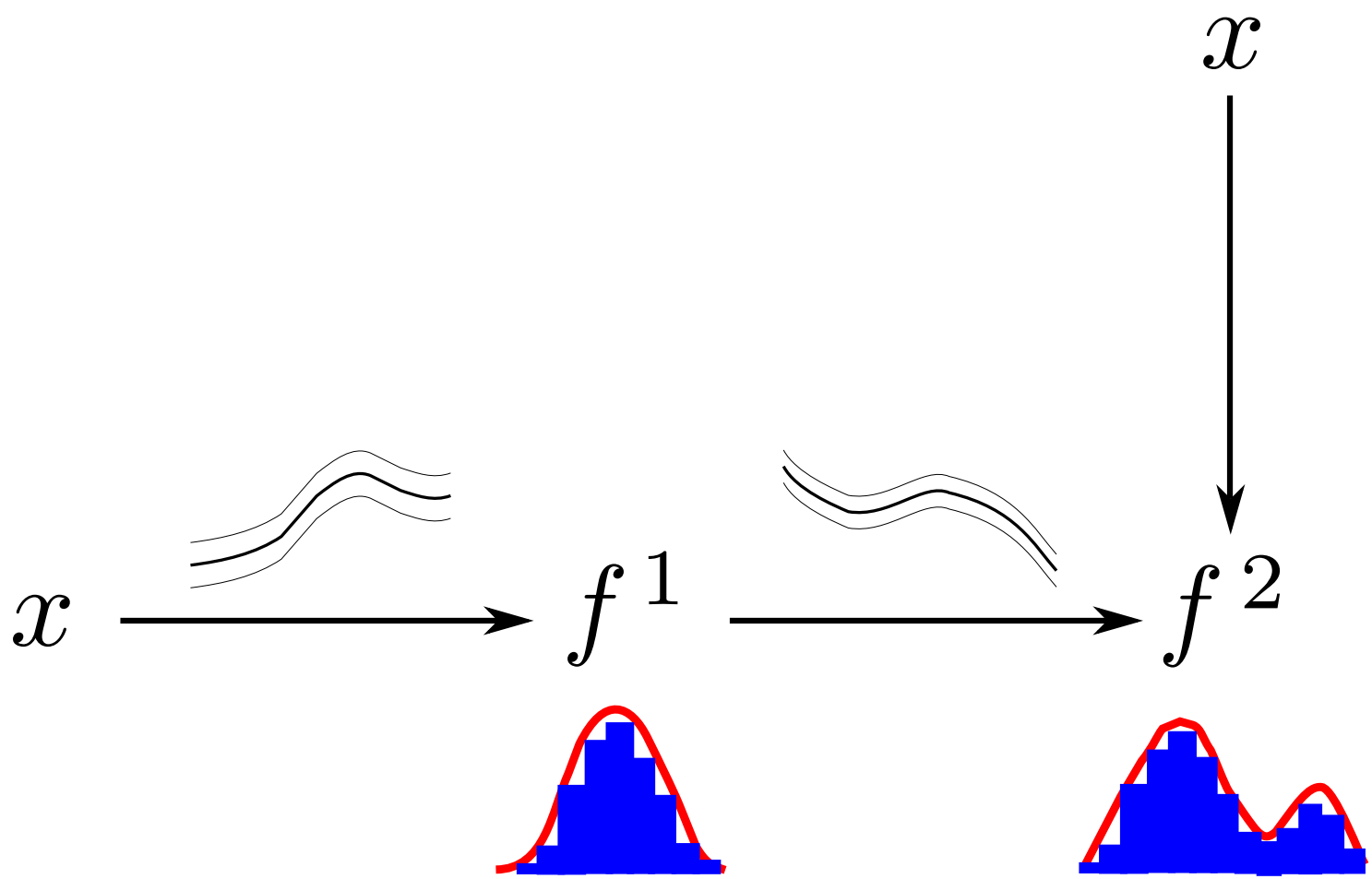

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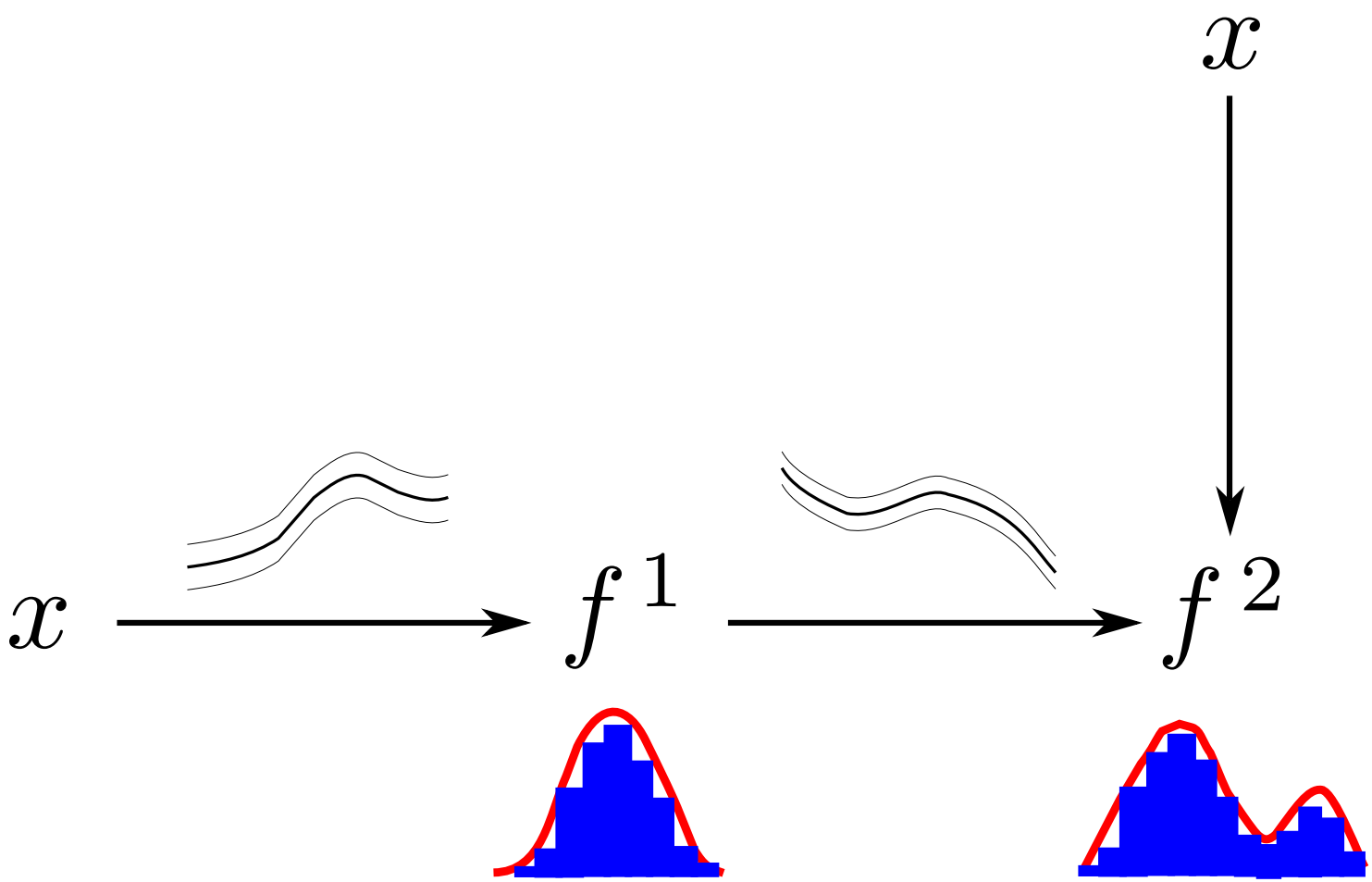
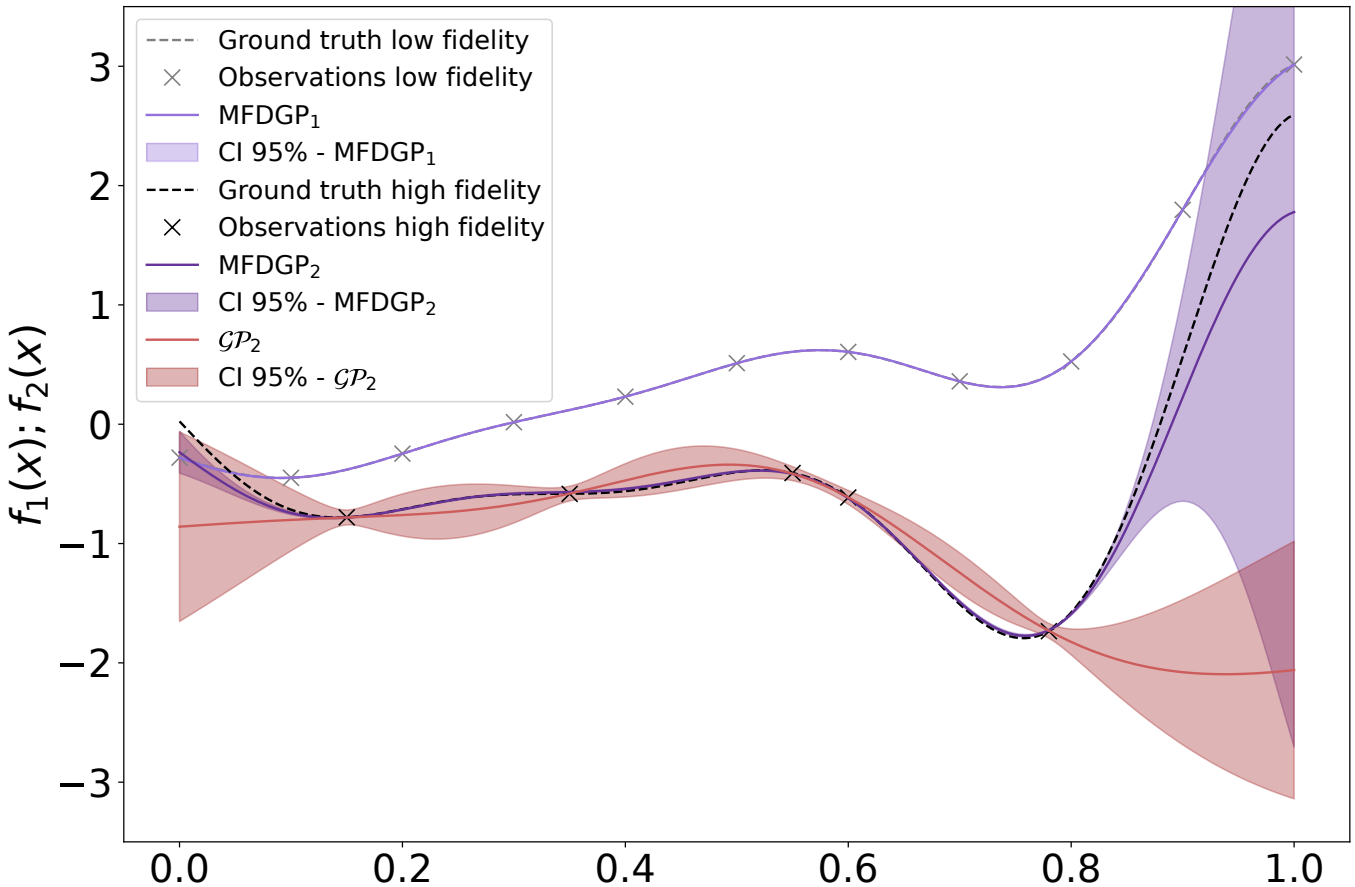


Used for testing and training (1 sample is enough)!

Comparison of a MFDGP and a standard GP



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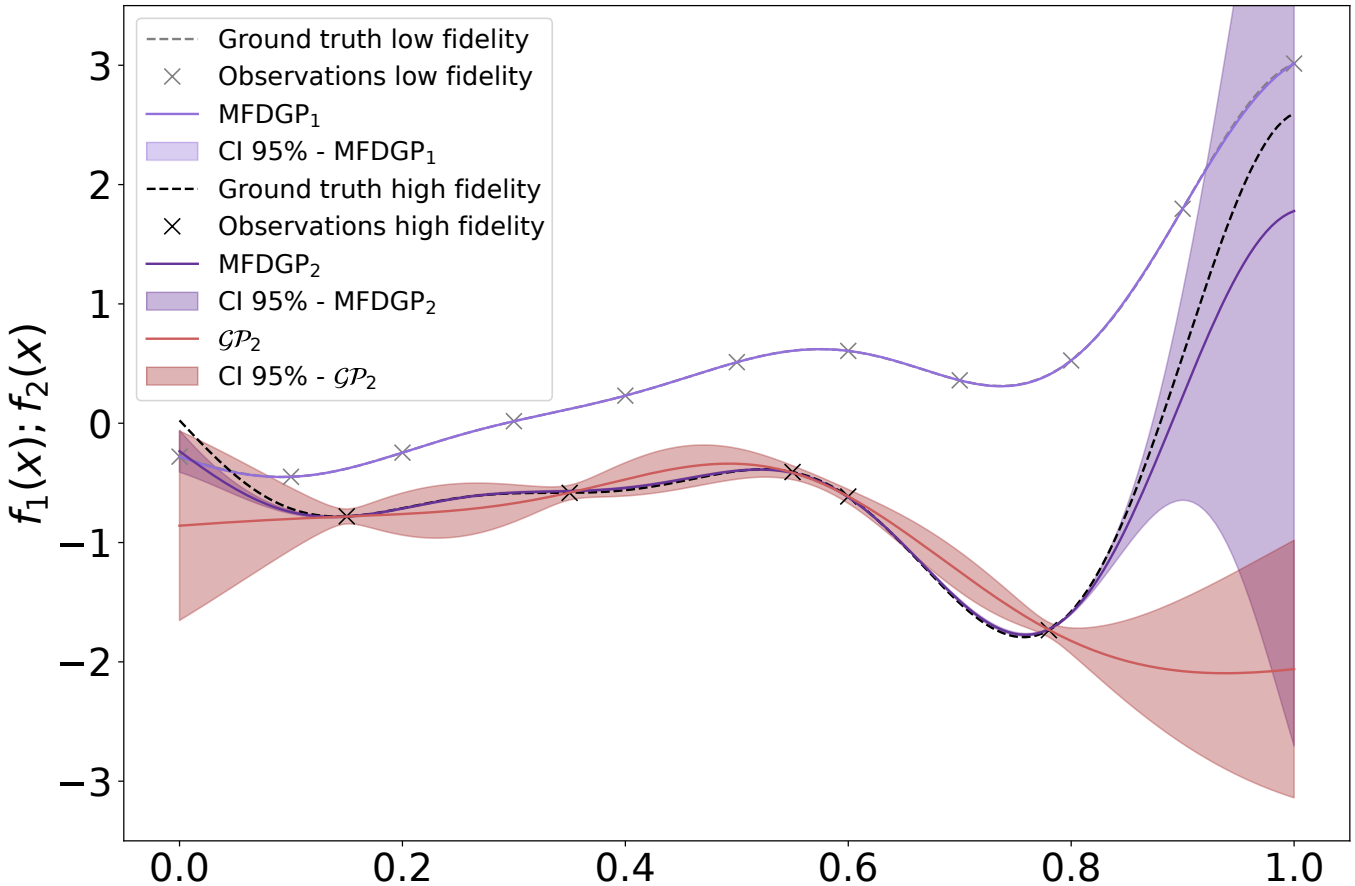

MFDGP takes advantage of low fidelity data and does a better job at predicting the higher fidelity!

Run the notebook illustrating the use of MFDGP and complete task 1!

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- DGPs are flexible models and can exploit multi-fidelity data.

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