Part III: Deep Gaussian Processes

Daniel Hernández–Lobato
Computer Science Department
Universidad Autónoma de Madrid

http://dhnzl.org, daniel.hernandez@uam.es

Summary so Far about GPs

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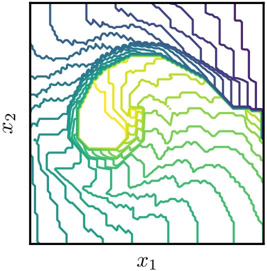
Deep GPs constitute a nice alternative to address these issues!

Motivation for Deep Gaussian Processes

Target function



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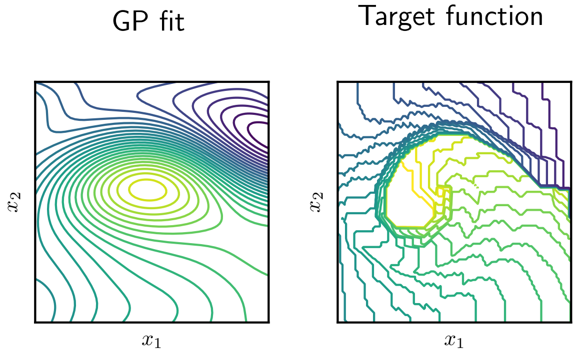

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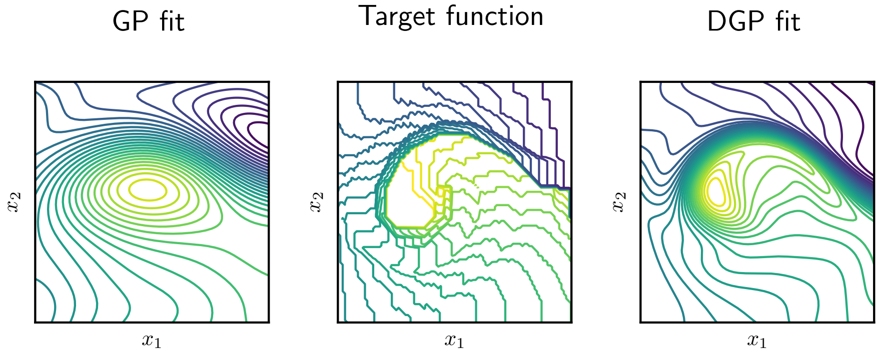
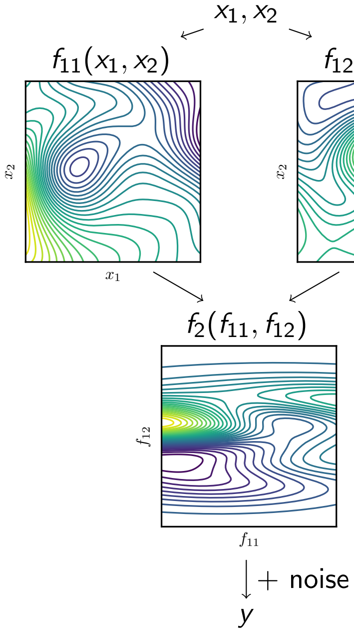


How do deep GPs work?



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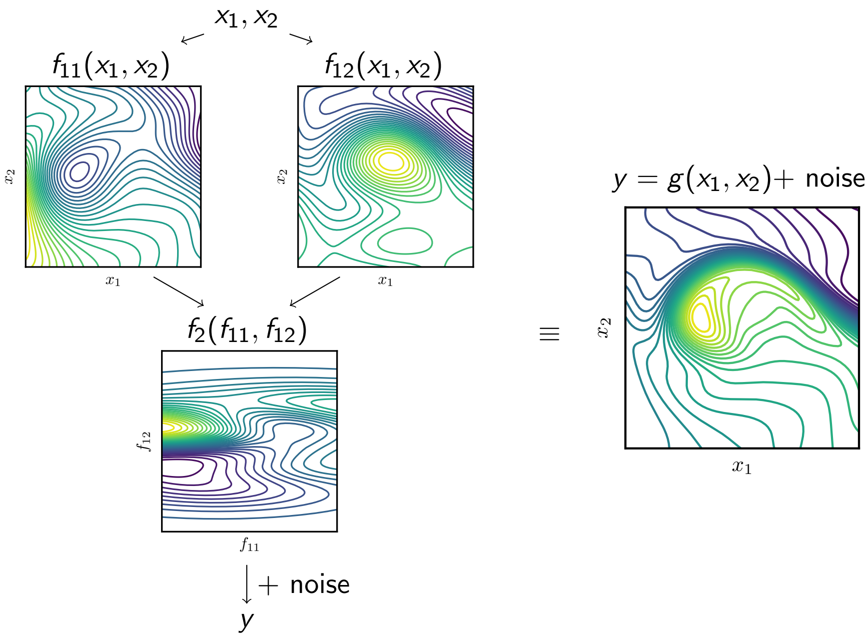

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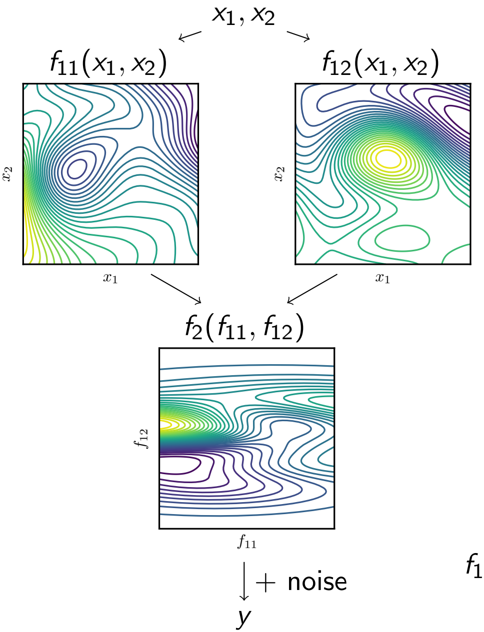
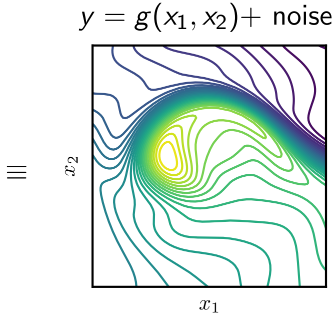
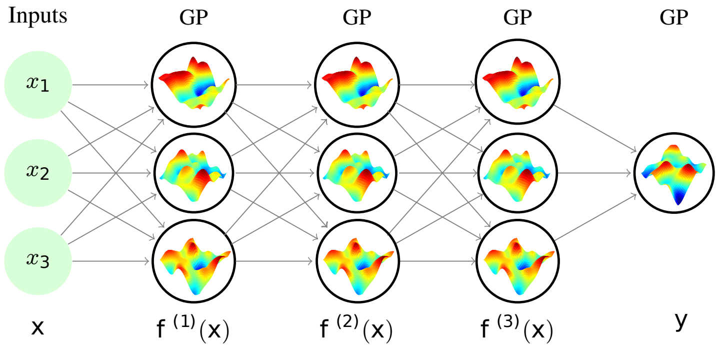




$f_{11}, f_{12}, f_2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$

Deep GPs as Deep Neural Networks



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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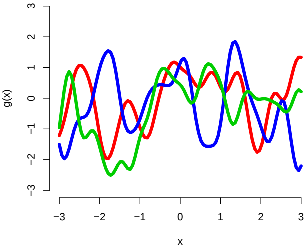

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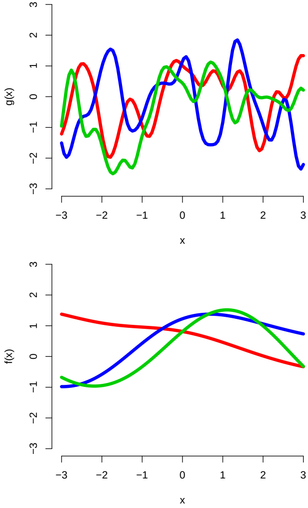

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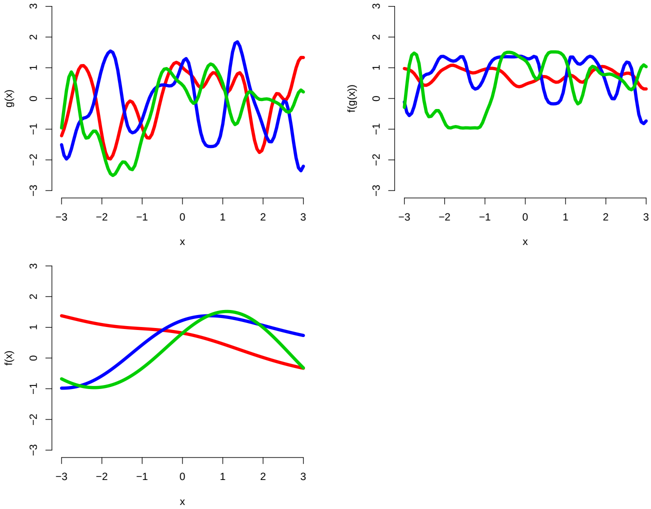

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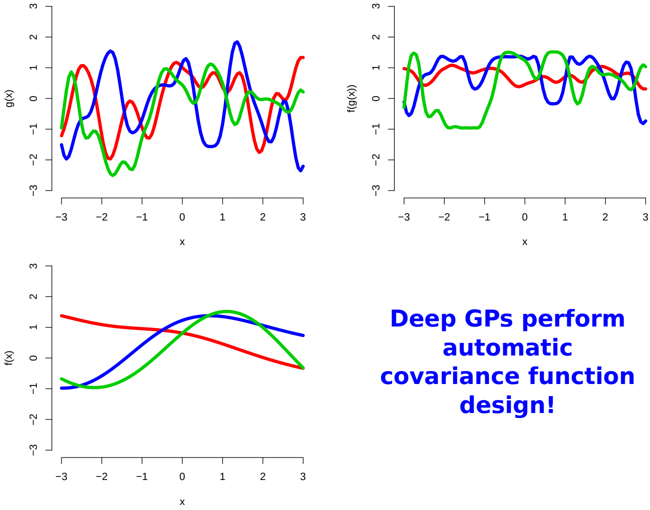
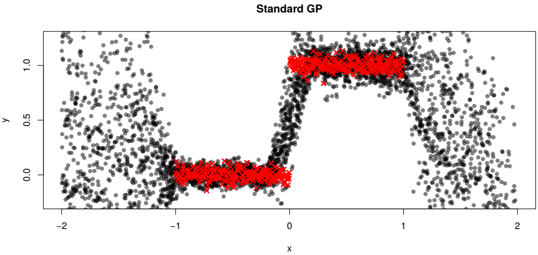


Deep GPs perform automatic covariance function design!

Deep GP Predictive Distribution



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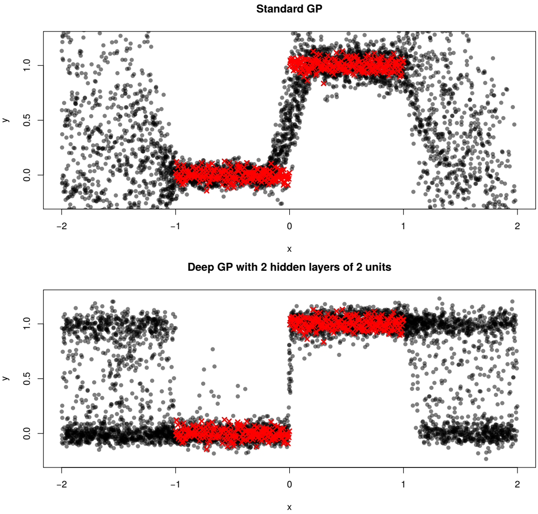

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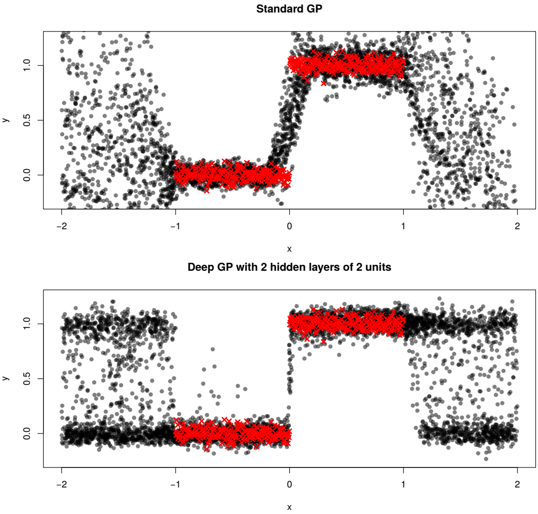

In a deep GP the predictive distribution needs not be Gaussian!

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Drawbacks:

- 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

$$
\begin{aligned}
m^\star &= \mathbf{\Sigma}_{f^\star,\mathbf{u}}\mathbf{\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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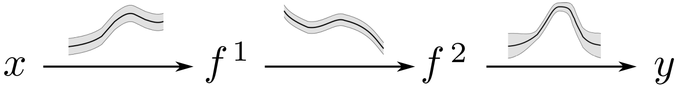
Ideally we would like to make inference about $\{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^{L}$!

Challenges of Approximate Inference for DGPs



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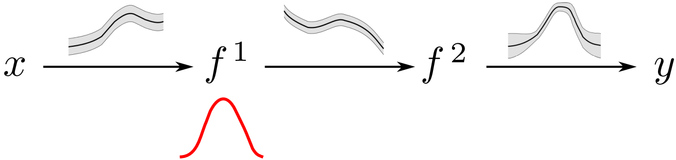

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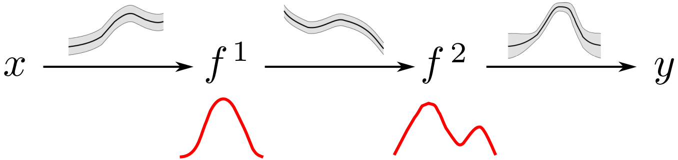

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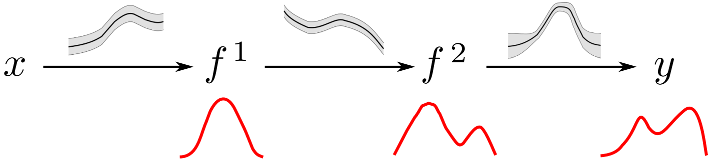

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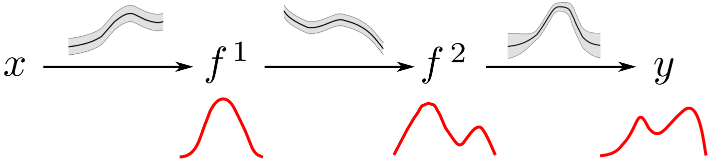

The predictive distribution after the first layer is non Gaussian!

Methods for Training DGPs

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- 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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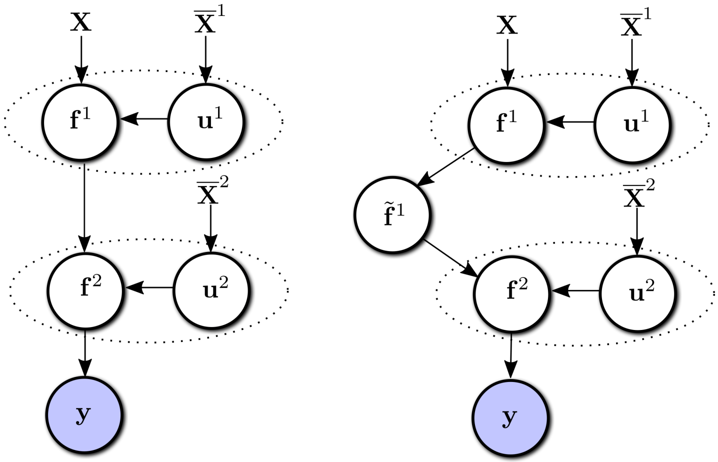
The joint distribution is now:

$$p(\mathbf{y}, \{\mathbf{u}^l, \mathbf{f}^l\}_{l=1}^{L}, \{\tilde{\mathbf{f}}^l\}_{l=1}^{L-1}) = \overbrace{\prod_{i=1}^{N} p(y_i|f_i^L)}^{\text{Likelihood}} \times$$

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

Original Graphical Model and Extended



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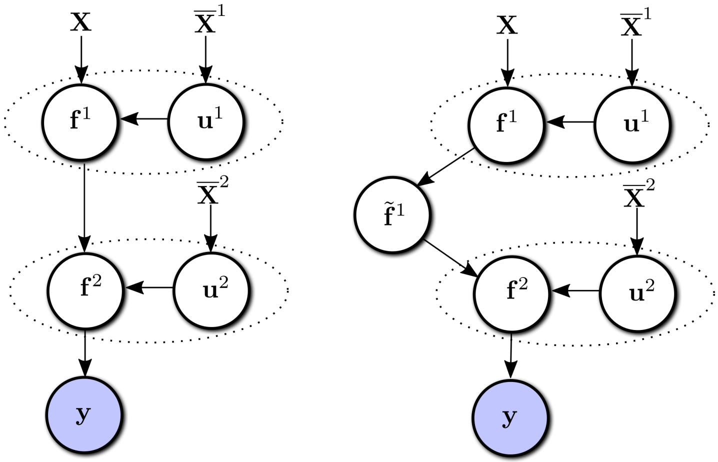

Both models are equivalent, but this setting simplifies inference!

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The posterior approximation q considered assumes independence among layers!

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Posterior approximation:

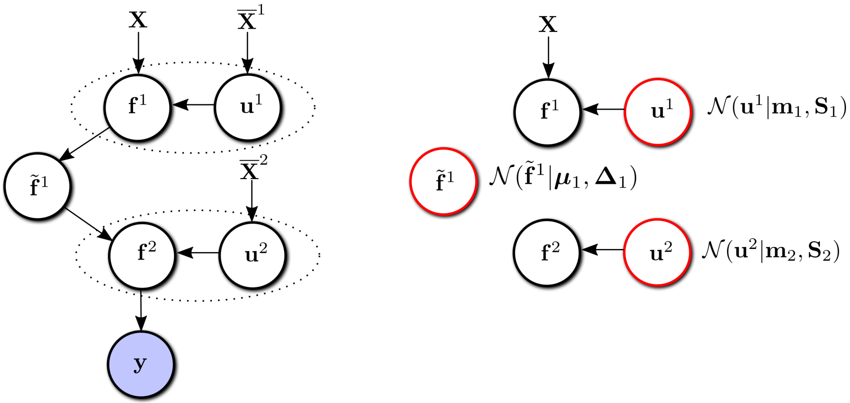
$$q(\{\mathbf{u}^l, \mathbf{f}^l, \tilde{\mathbf{f}}^l\}_{l=1}^{L}) = q(\mathbf{u}^L) p(\mathbf{f}^L | \mathbf{u}^L, \overline{\mathbf{X}}^l) \prod_{l=1}^{L-1} q(\mathbf{u}^l) q(\tilde{\mathbf{f}}^l) p(\mathbf{f}^l | \mathbf{u}^l, \overline{\mathbf{X}}^l)\,,$$

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 $\log p(\mathbf{y})$:

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

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

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(Damianou, 2013)

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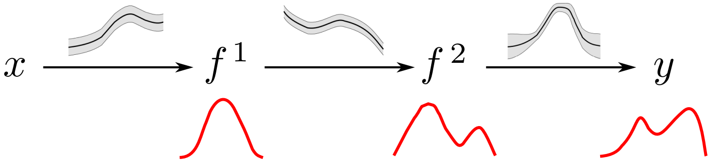
$$+ \sum_{l=1}^{L} \mathrm{KL}(q(\mathbf{u}^l) | p(\mathbf{u}^l)) .$$

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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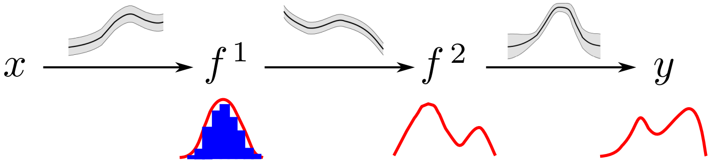

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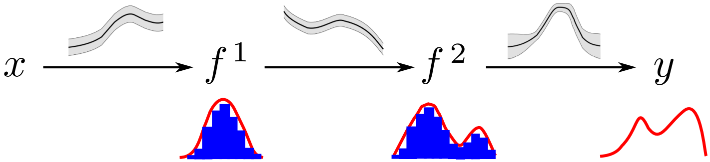

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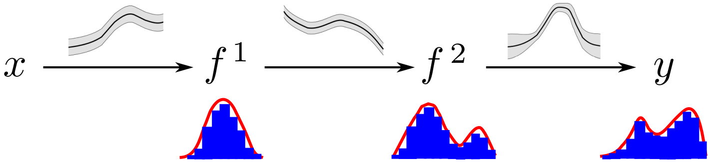

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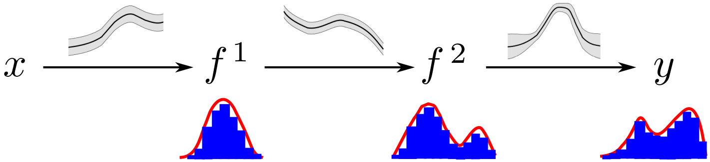
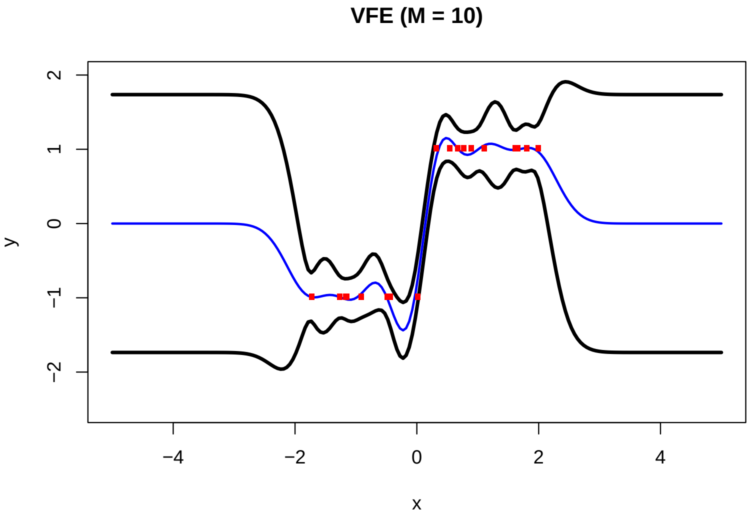


For a particular fixed input, the predictive distribution of each layer is Gaussian!

DGPs Tractable Bound: Illustrative Example



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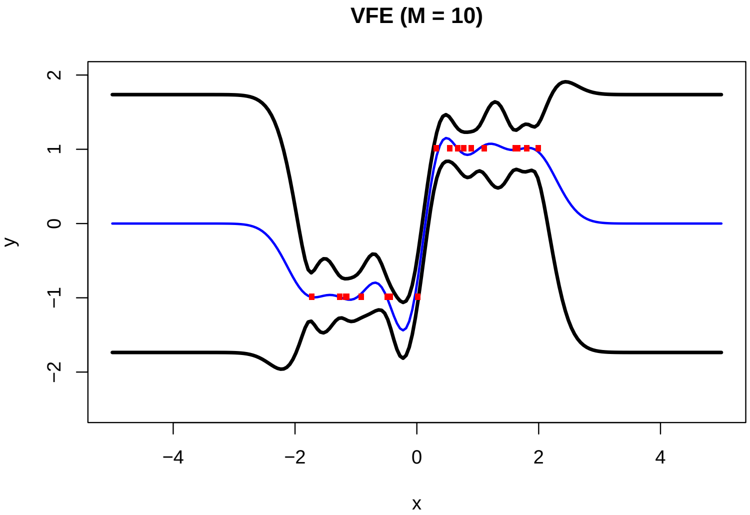

The VFE sparse GP reduces the length-scale to explain the data!

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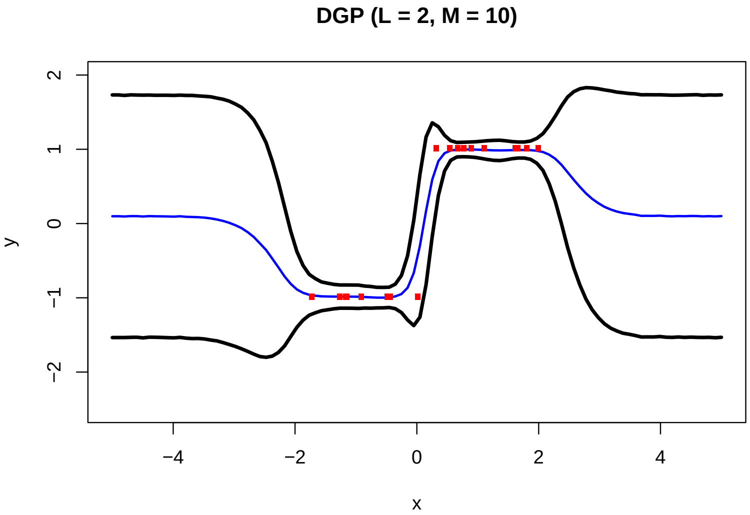

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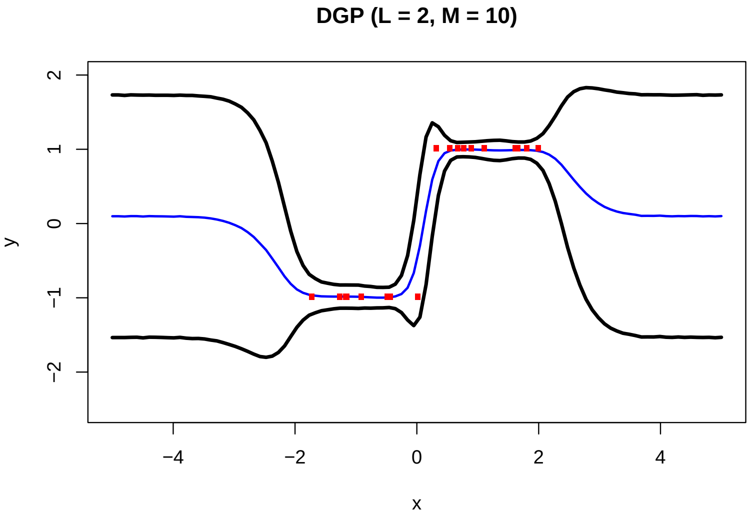
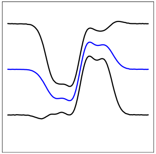


The DGP provides a more sensible predictive distribution!

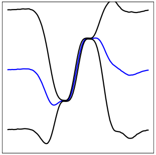
DGPs Tractable Bound: Illustrative Example

$$x$$
$$\downarrow$$
$$f^1(x)$$



$$\Big\downarrow + \text{noise}$$

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



$$\Big\downarrow + \text{noise}$$

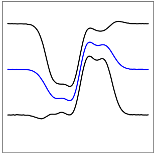
$$y$$

DGPs Tractable Bound: Illustrative Example

x

$\downarrow$

$f^1(x)$



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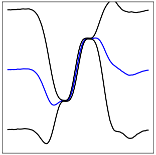
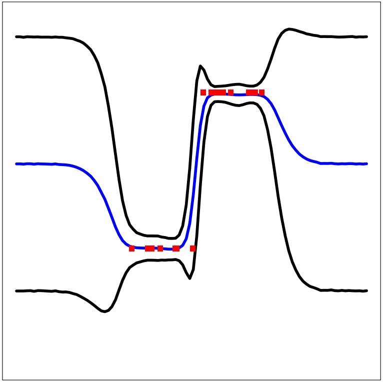


$\downarrow$ + noise

y

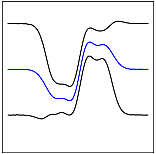
$\equiv$

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



DGPs Tractable Bound: Illustrative Example

$$x \downarrow f^1(x)$$



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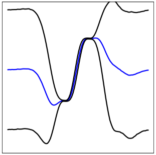

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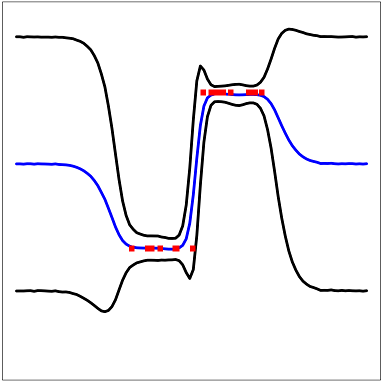

$$f^1, f^2 \sim \mathcal{GP}(0, C(\cdot,\cdot))$$

Limitations of DGPs via Tractable VI Bound

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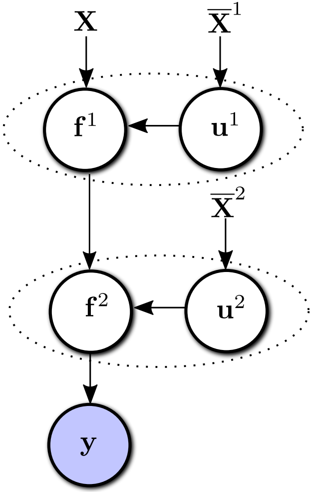
- Uses the FITC approximation for tractable scaling and allows for mini-batch training. Thus, the model is changed.
- Relies on a modified version of EP to estimate the approximate distribution q using standard optimization techniques.
- The intractable predictive distribution at each layer is approximated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

(Bui et al., 2016)

Alternative Graphical Model



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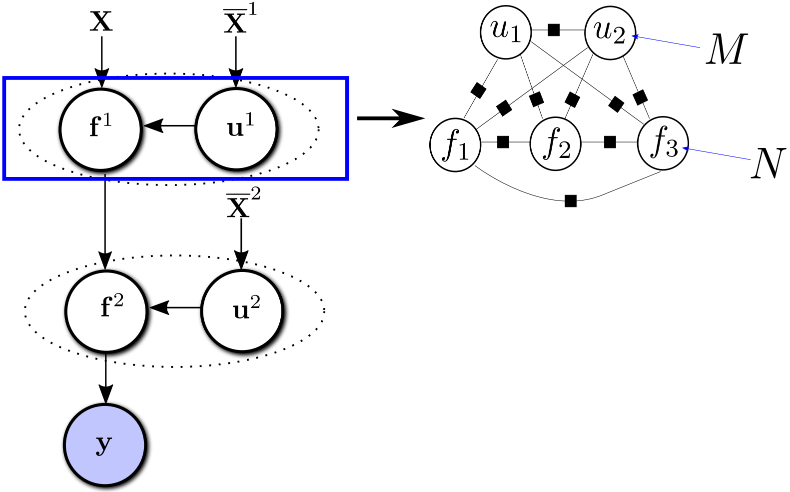

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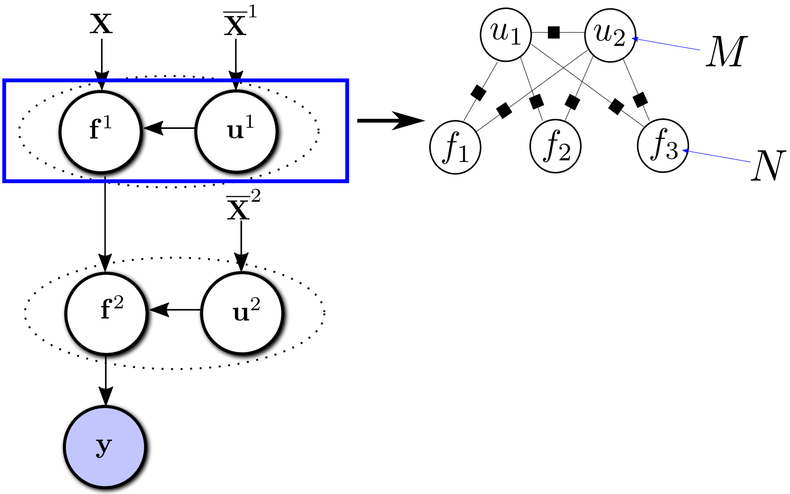

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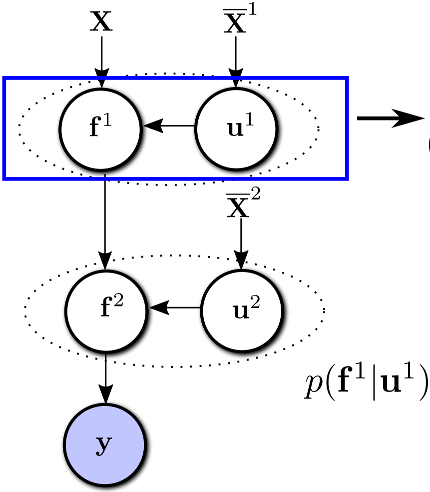

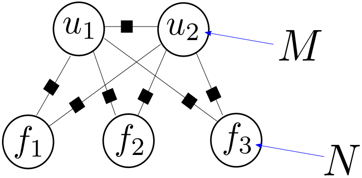

$$p(\mathbf{f}^1|\mathbf{u}^1) \approx \prod_{i=1}^{N} p(f^1(\mathbf{x}_i)|\mathbf{u}^1)$$

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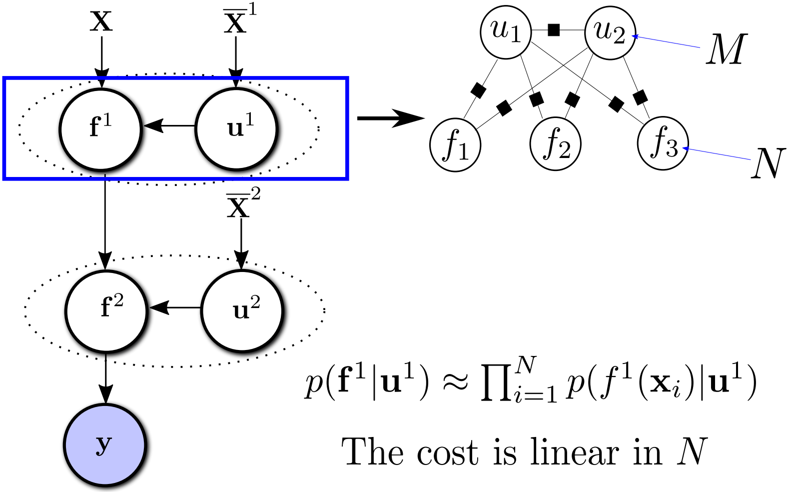

$$p(\mathbf{f}^1|\mathbf{u}^1) \approx \prod_{i=1}^{N} p(f^1(\mathbf{x}_i)|\mathbf{u}^1)$$

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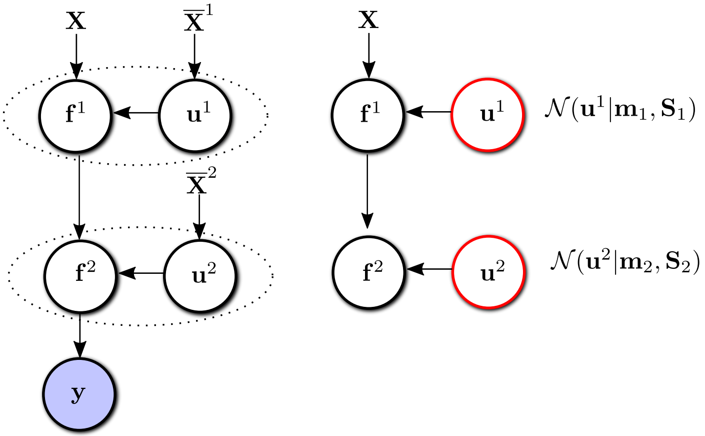
The FITC approximation enforces $\tilde{p}(\mathbf{f}^l | \mathbf{u}^l, \overline{\mathbf{X}}^l)$ to factorize across the N data instances!

Graphical Model and Approximate Distribution



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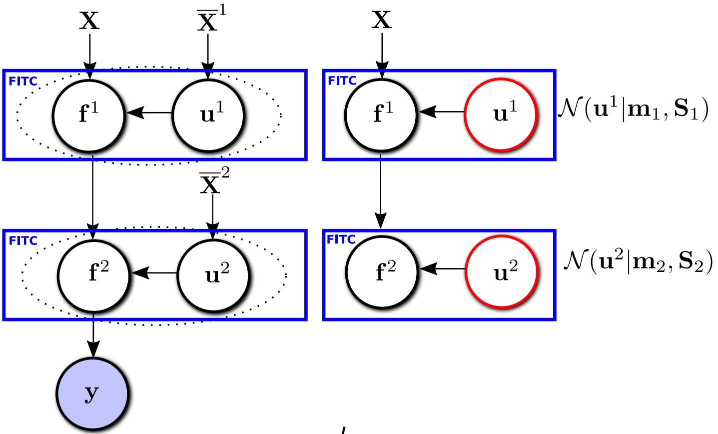

$$q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) = \prod_{l=1}^L \tilde{p}(\mathbf{f}^{l-1}|\mathbf{u}^l)\, q(\mathbf{u}^l)$$

- Fixed and factorizing across data
- Tunable Gaussian

Graphical Illustration of EP for DGPs

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

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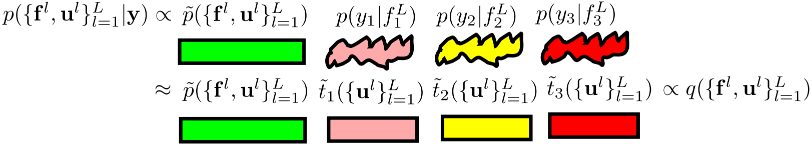

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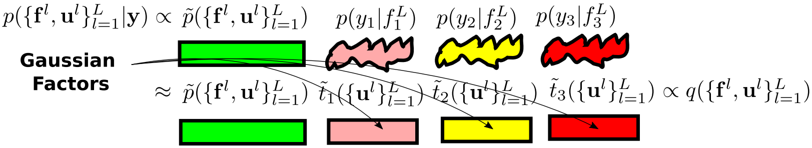

The $\tilde{t}_i$ are tuned by minimizing the KL-divergence $\mathrm{KL}[\hat{p}_i||q] \quad \forall i$,

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

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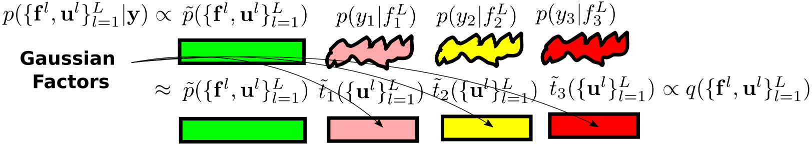

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Since $\tilde{p}(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L)$ is fixed, we only have to match the moments of $\hat{p}_j$ and q over $\{\mathbf{u}^l\}_{l=1}^L$!

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

$$\max_{q} \min_{\tilde{t}_1,\ldots,\tilde{t}_N} \log Z_{\text{EP}} \quad \text{subject to} \quad q \propto \tilde{p} \prod_{i=1}^{N} \tilde{t}_i \,.$$

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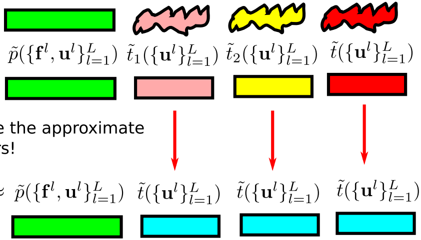
Can be solved with a **double-loop** algorithm. **Too slow in practice!**

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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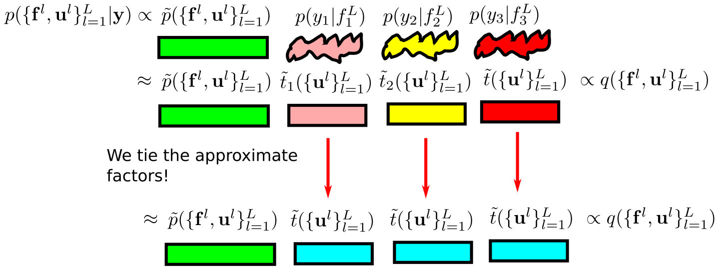

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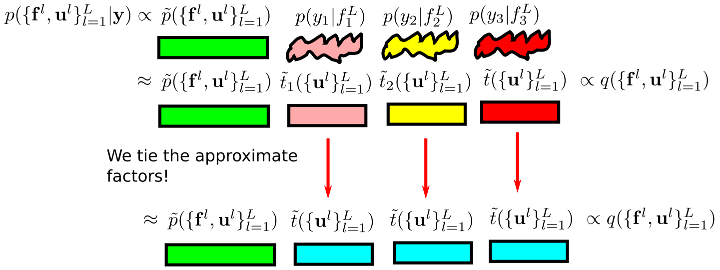

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which is suitable for standard optimization and mini-batch training.

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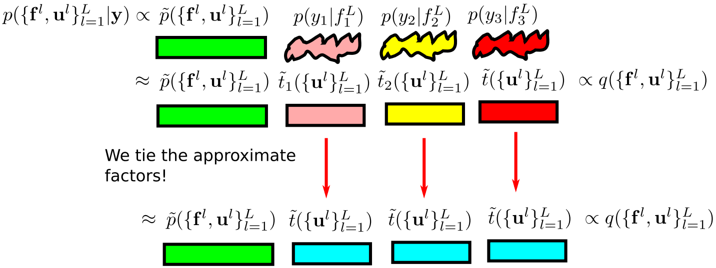

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Approximating $\log Z_i$

Note that $\log Z_i = \log \int p(y_i|f_i^L) q^{\setminus i}(f_i^L) df_i^L$ is the log predictive likelihood of instance i when removed from the training set.

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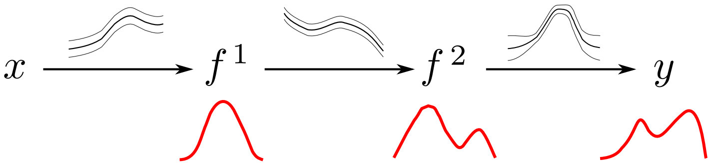
We can use an iterative Gaussian approximation:



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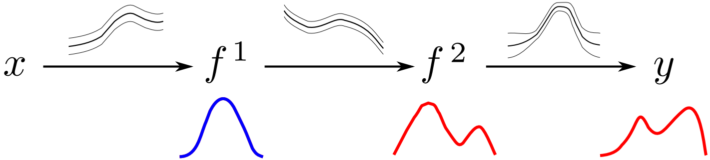

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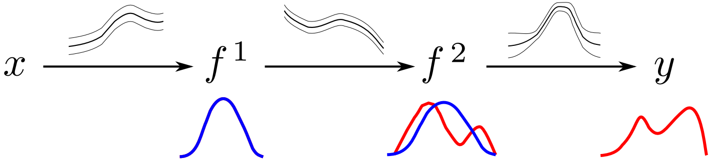

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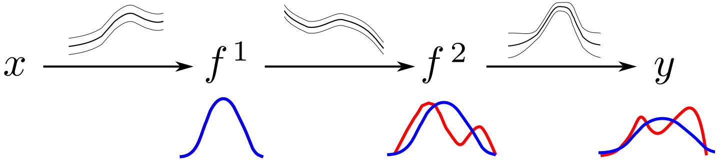

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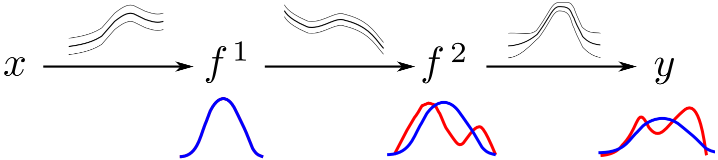
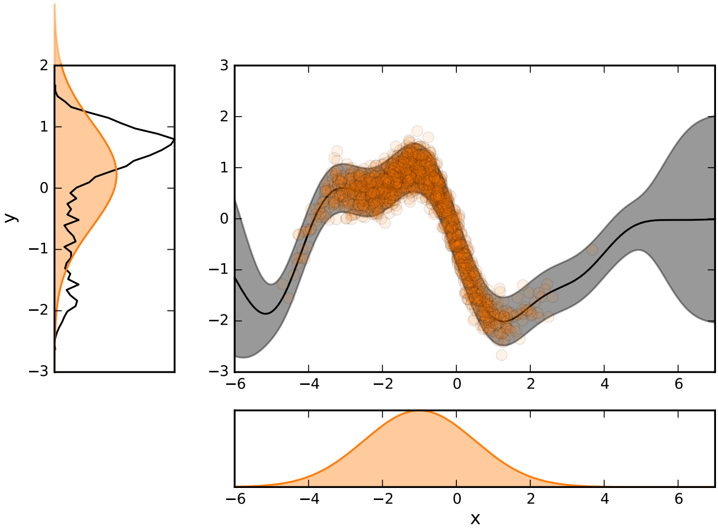
Note that $\log Z_i = \log \int p(y_i|f_i^L)q^{\setminus i}(f_i^L)df_i^L$ is the log predictive likelihood of instance i when removed from the training set.

We can use an iterative Gaussian approximation:

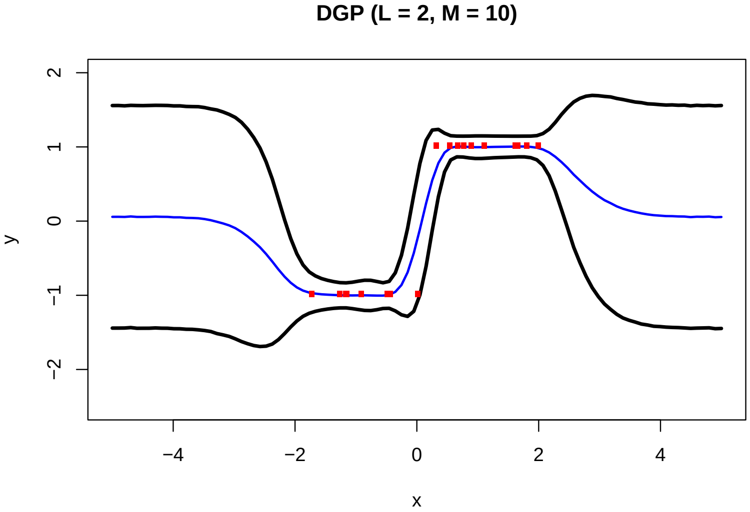


Doable for certain covariance functions, e.g., the squared exponential!

Gaussian Projection Example



Approx. EP for DGPs: Illustrative Example



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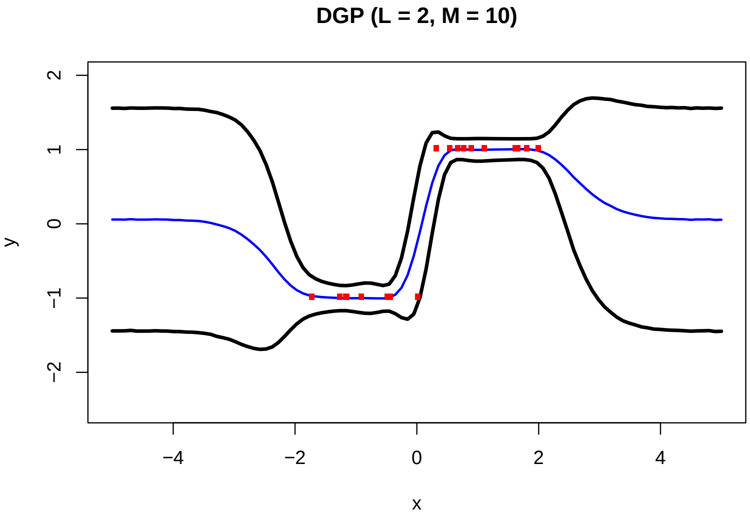


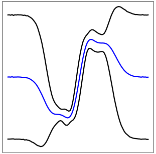
The AEP method provides a similar predictive distribution to the previous method!

Approx. EP for DGPs: Illustrative Example

x

$\downarrow$

$f^1(x)$



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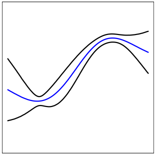
$f^2(f_1)$



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$y + \text{noise}$

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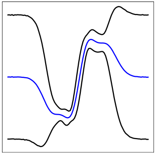

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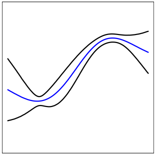
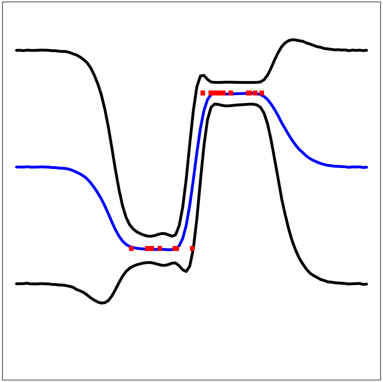


$\downarrow$

$y +$ noise

$\equiv$

$y = f^2(f^1(x)) +$ noise



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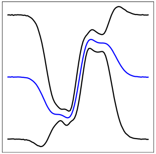

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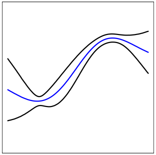

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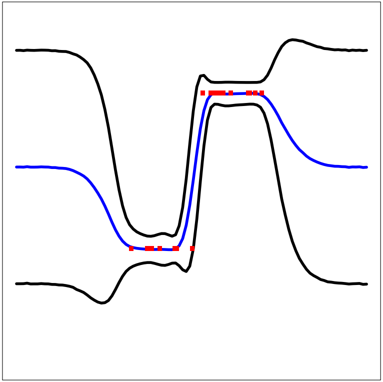

$f^1, f^2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$

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- The approximate predictive distribution of q at each layer is a Gaussian projection, which can be a crude approximation.

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- It modifies the deep GP prior and hence the model, by introducing the FITC approximation.

Doubly Stochastic Variational Inference for DGPs

Features:

- Considers dependencies between inputs and outputs at each layer.

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- Each layer predictive distribution is approximated by Monte Carlo.

(Salimbeni, 2017)

Black-box Variational Inference

VI works when we can compute $\mathbb{E}_q[\log p(\mathbf{f}, \mathbf{y})]$ in closed form!

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Black-box VI can be used with arbitrarily complicated models:

$$
\begin{aligned}
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&= \mathbb{E}_q \left[\log p(\mathbf{f}, \mathbf{y}) \frac{\partial}{\partial \theta} \log q_\theta(\mathbf{f}) \right] + \frac{\partial H_q}{\partial \theta} \\
&\approx \frac{1}{S} \sum_{s=1}^{S} \log p(\mathbf{f}_s, \mathbf{y}) \frac{\partial}{\partial \theta} \log q_\theta(\mathbf{f}_s) + \frac{\partial H_q}{\partial \theta}
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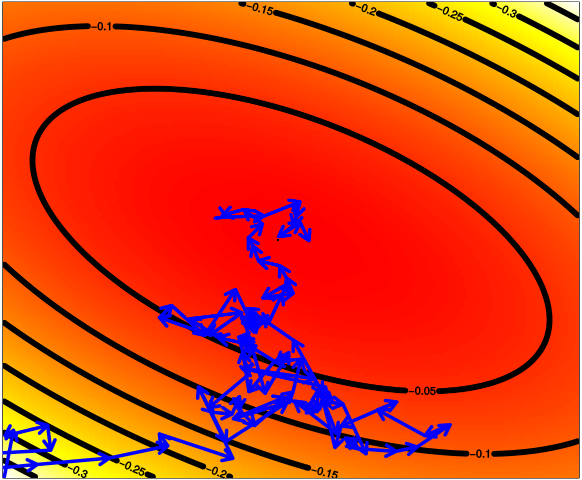
\end{aligned}$$

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

Stochastic Optimization



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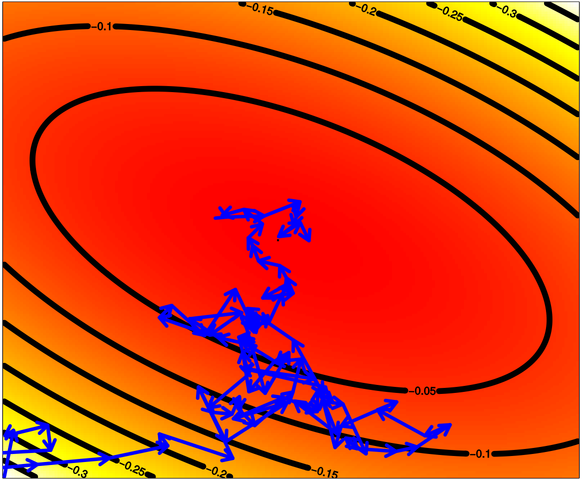

To converge to a local neighborhood of the optimum stochastic methods only require an unbiased estimate of the gradient!

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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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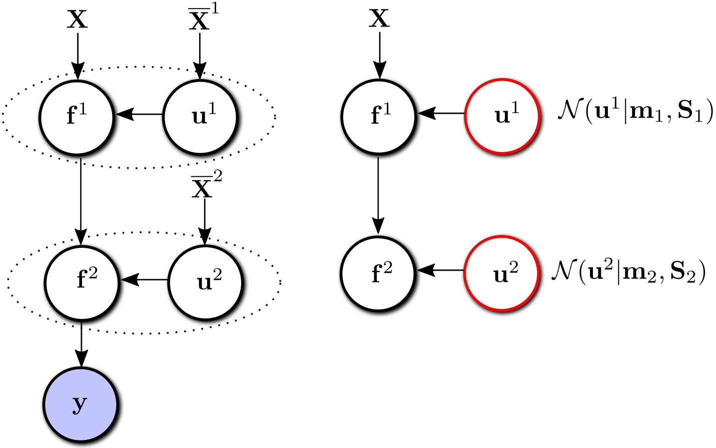
No change in the model is made at all!

Graphical Model and Posterior Approximation



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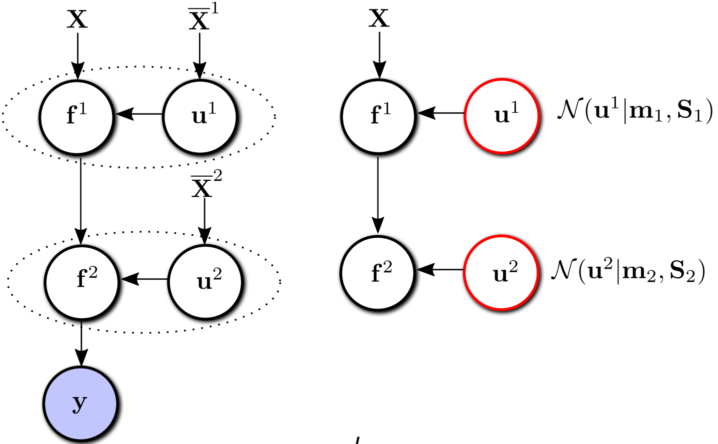

$$q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^L) = \prod_{l=1}^{L} p(\mathbf{f}^l|\mathbf{u}^l)\, q(\mathbf{u}^l)$$

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

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

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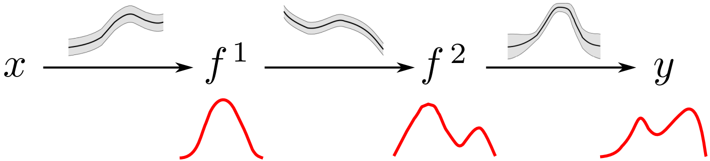
- The expectations can be approximated by Monte Carlo.
- Suitable for mini-batch training by subsampling the data.

(Salimbeni, 2017)

Predictive Distribution via Monte Carlo Sampling



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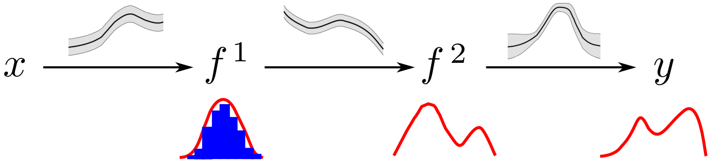

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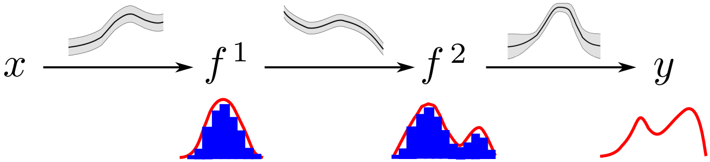

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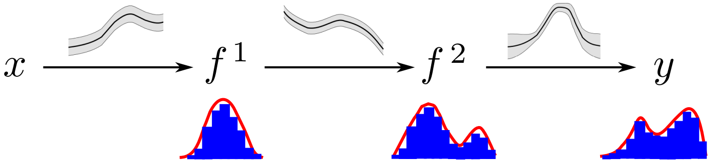

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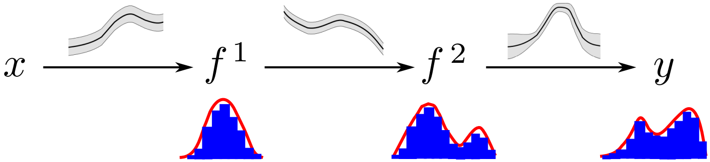
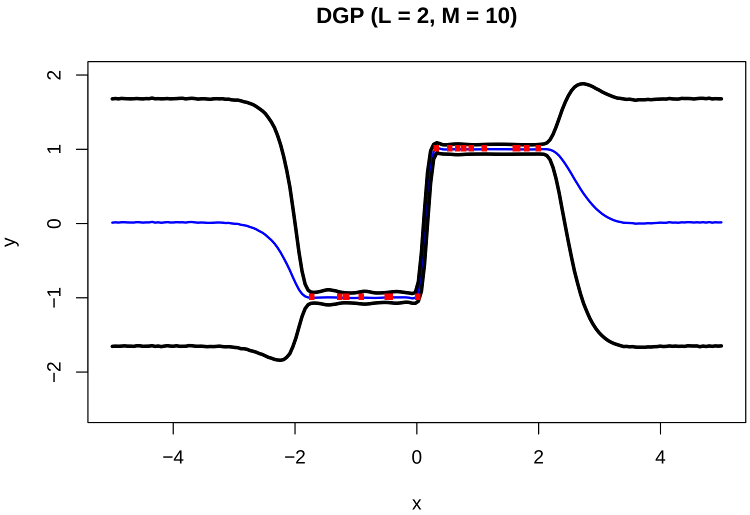


Used not only for testing, but also during training, unlike the previous methods!

DSVI for DGPs: Illustrative Example



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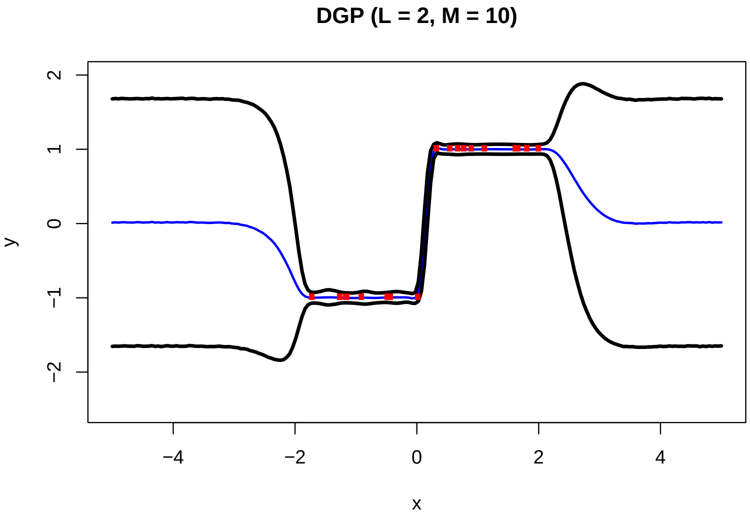


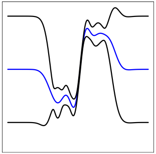
DSVI provides better results than the previous methods!

DSVI for DGPs: Illustrative Example

x

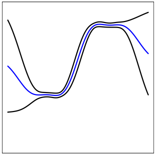
$\downarrow$

$f^1(x)$



$\downarrow$

$f^2(f_1)$



$\downarrow$

$y + \text{noise}$

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$$\downarrow$$
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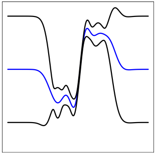

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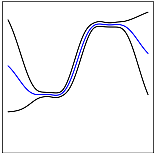
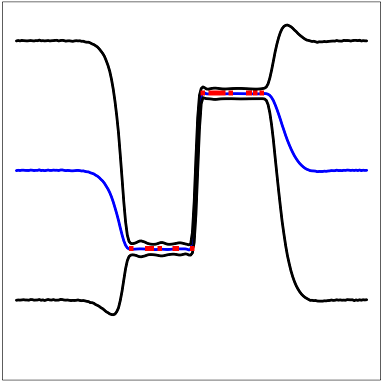


$$\downarrow$$
$$y + \text{noise}$$

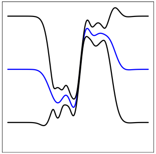
$$\equiv$$

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



DSVI for DGPs: Illustrative Example

$$x \downarrow f^1(x)$$



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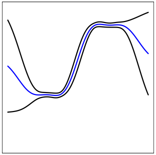

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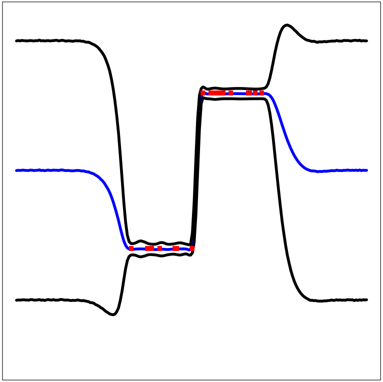
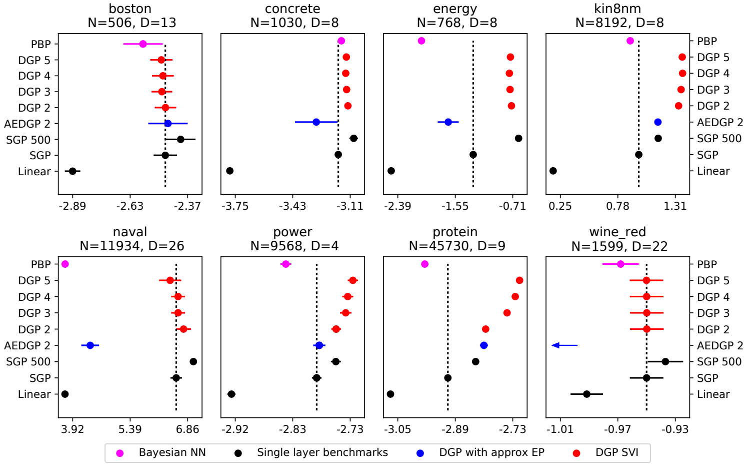


$$f^1, f^2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$$

DGPs via DSVI: LL Experimental Results



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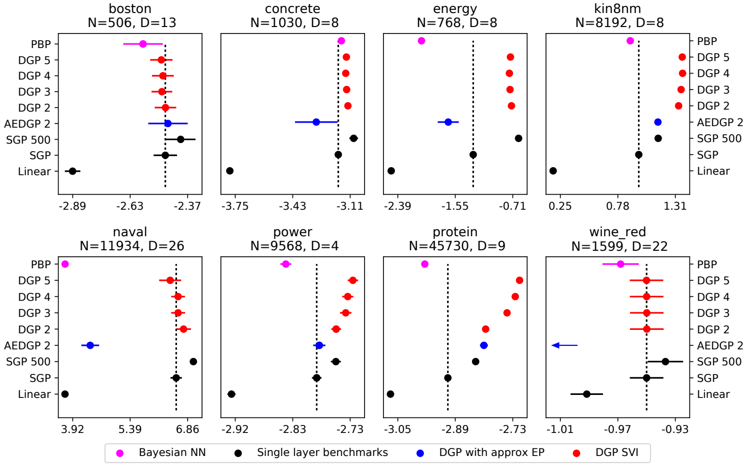

DGPs perform similar or better than the sparse GP and adding more layers does not seem to overfit!

(Salimbeni, 2017)

Limitations of DSVI for DGPs

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

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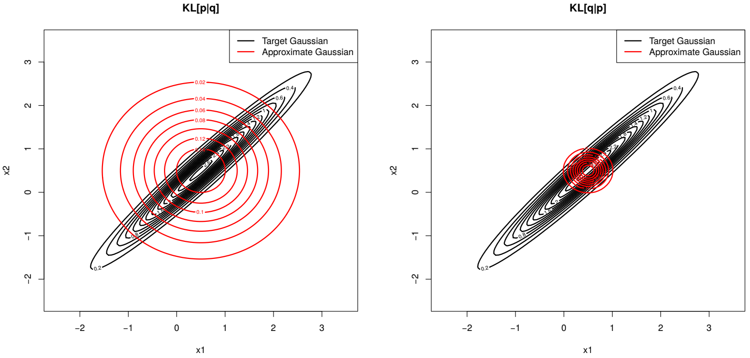

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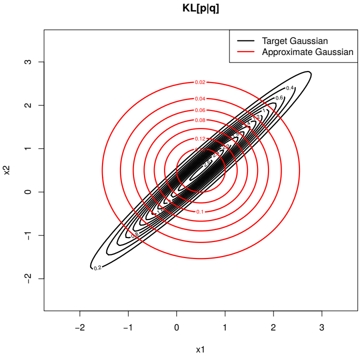

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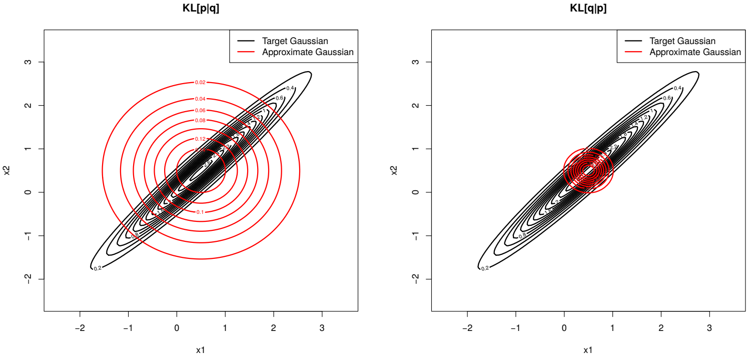

KL$[q|p]$ may result in too compact approximations while KL$[p|q]$ may put mass in regions with no posterior density. Can we have something in between?

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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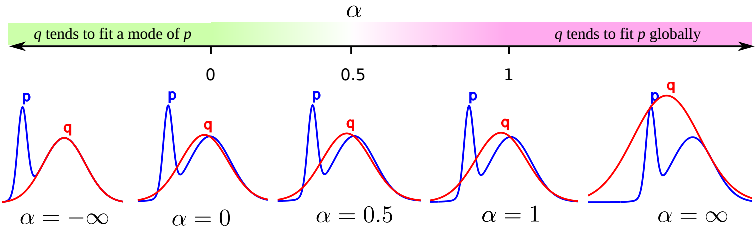

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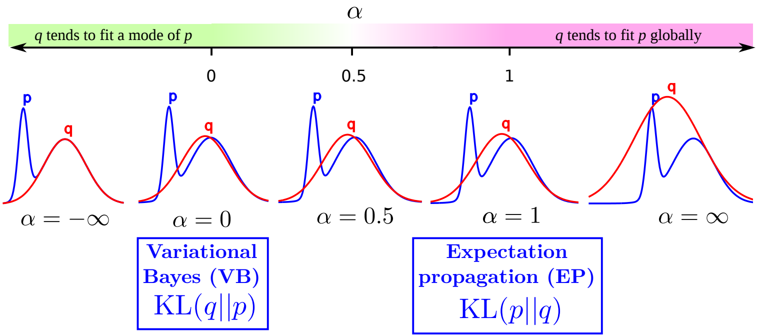

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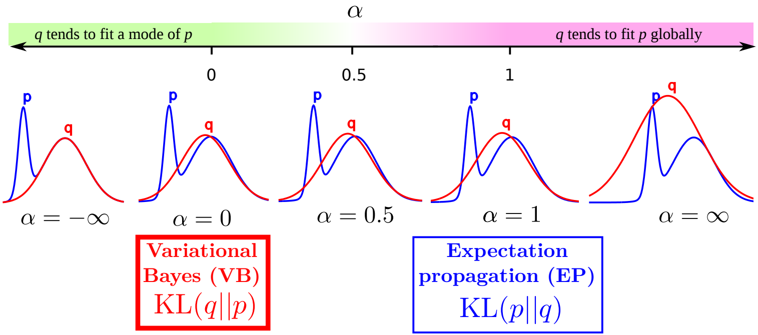

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Local α-divergence minimization (Power EP)

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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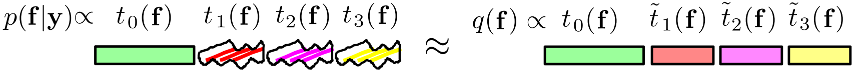

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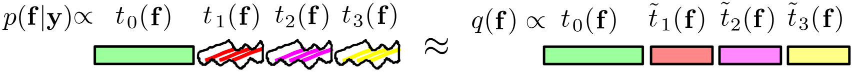

The $\tilde{t}_j$ are tuned by minimizing local α-divergences

$$
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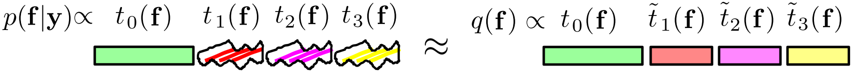

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It turns out that the α-divergence can be minimized in terms of the KL-divergence!

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

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

PEP as an Optimization Problem

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

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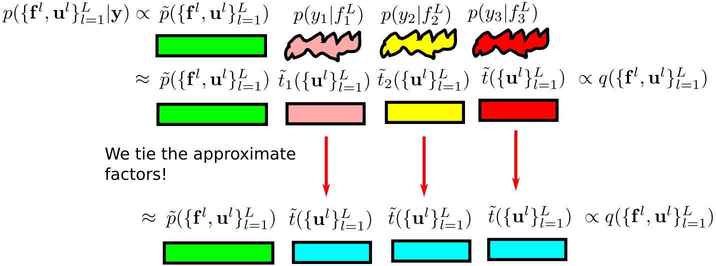
Approximate Power Expectation Propagation



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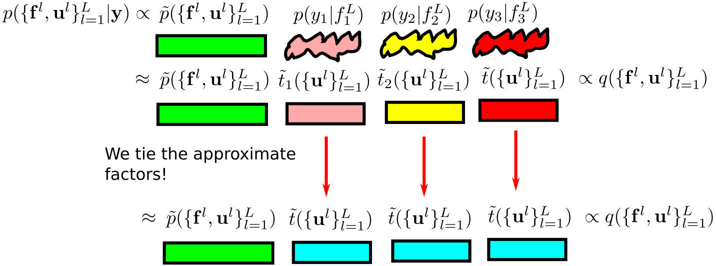

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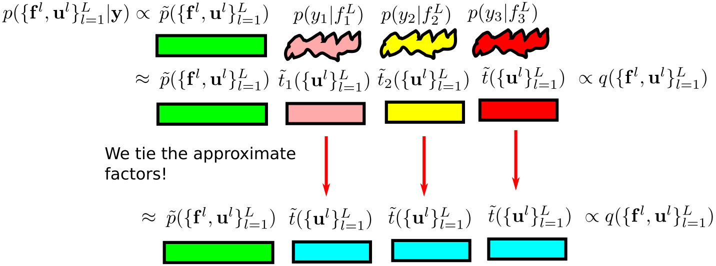

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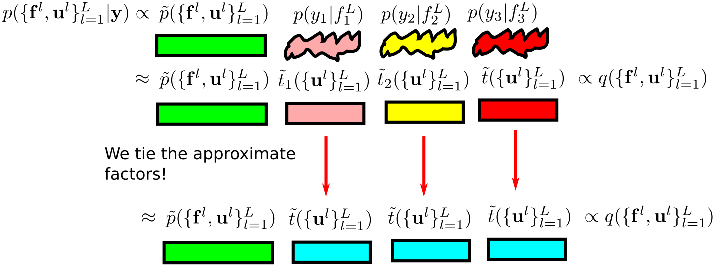

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Note that $\log Z_i = \log \int p(y_i|f_i^L)^\alpha q^{\setminus \alpha i}(f_i^L) df_i^L$ is the log predictive likelihood of instance i when removed from the training set.

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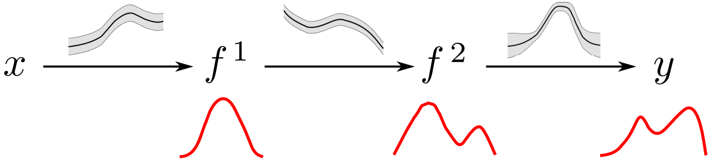

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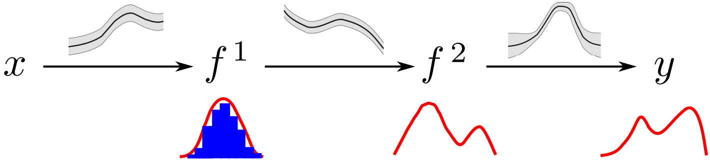

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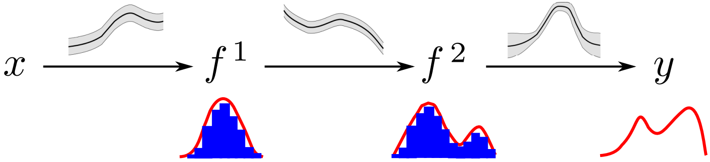

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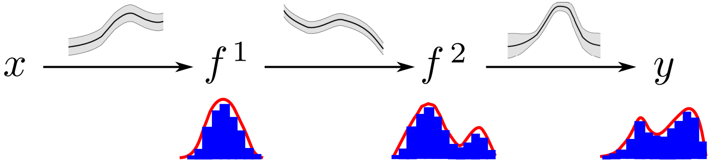

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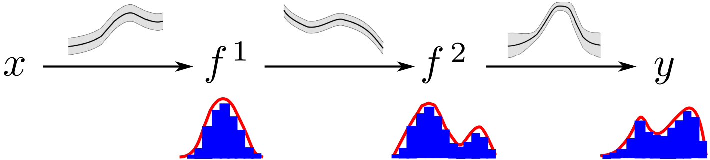

Expected to be more accurate than the Gaussian projection method used by AEP!

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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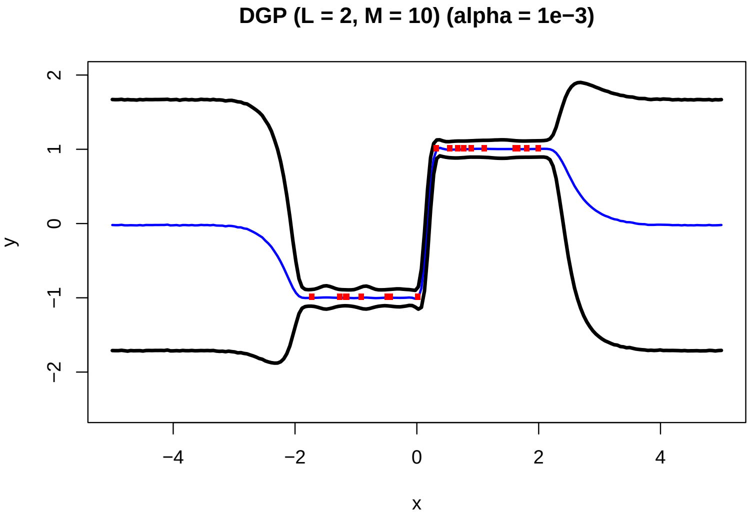
$$\log Z_{\mathrm{PEP}} \approx \sum_{i=1}^{N} \frac{1}{\alpha} \log \tilde{Z}_i - \mathrm{KL}[q|\mathrm{prior}]\,,$$

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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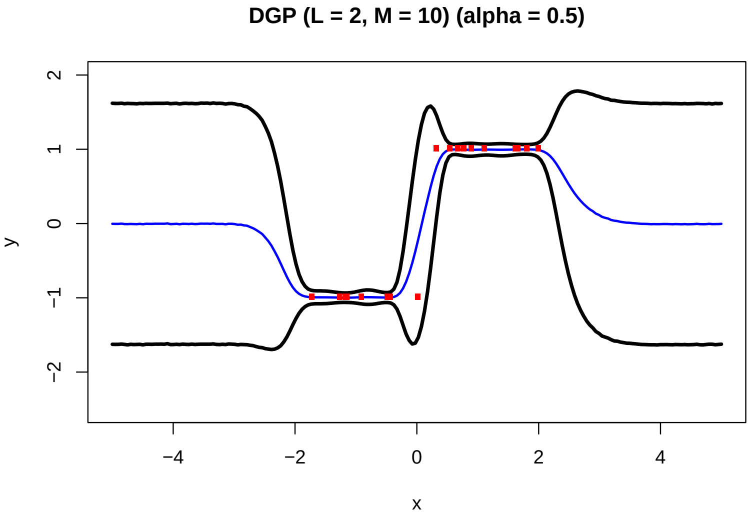

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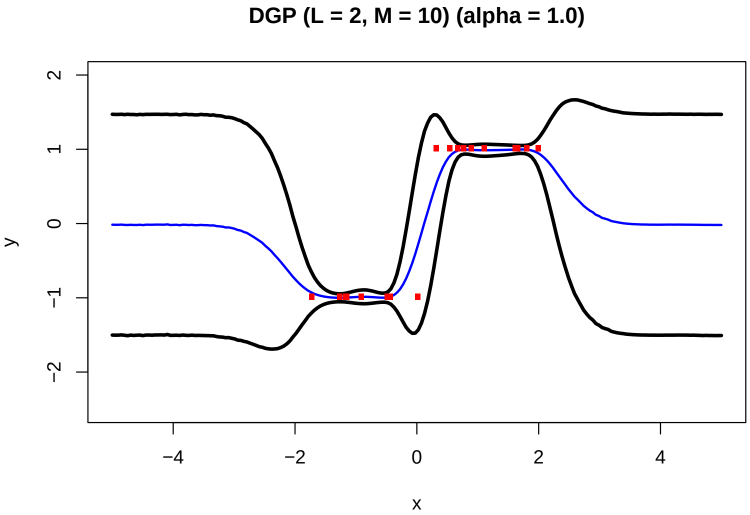

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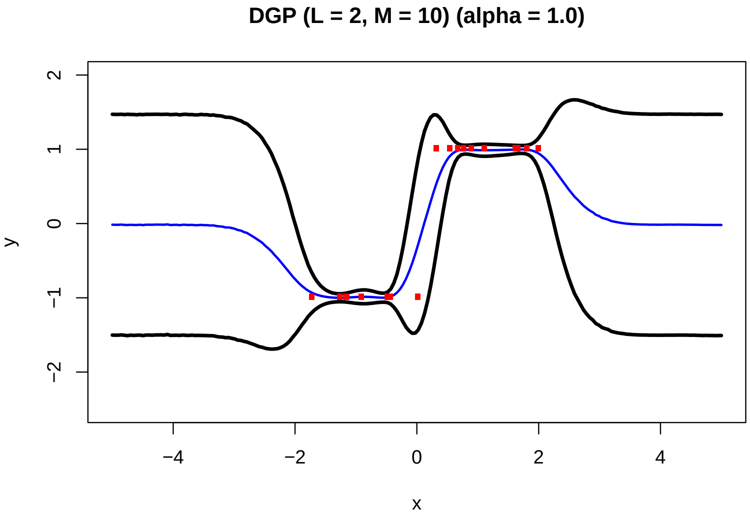
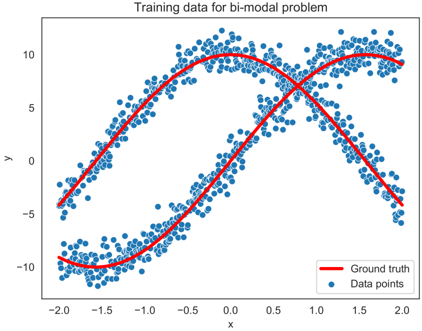
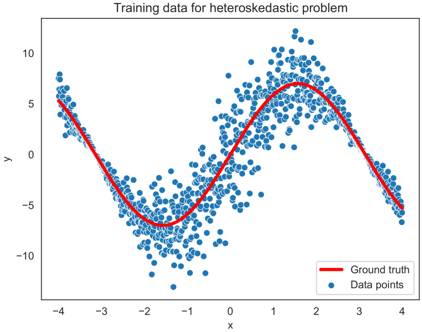


The value of α has an impact on the final predictive distribution!

α-Divergence Minimization: Toy Problems





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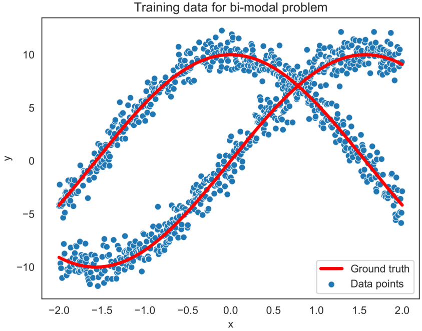

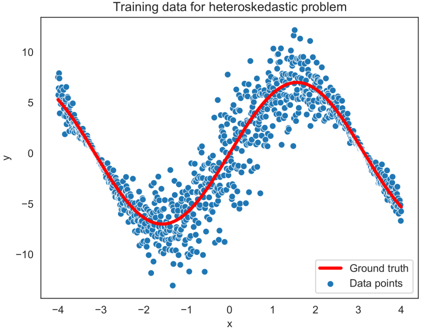

The first problem has heteroscedastic noise. The second, a bimodal predictive distribution!

(Depeweng, 2016)

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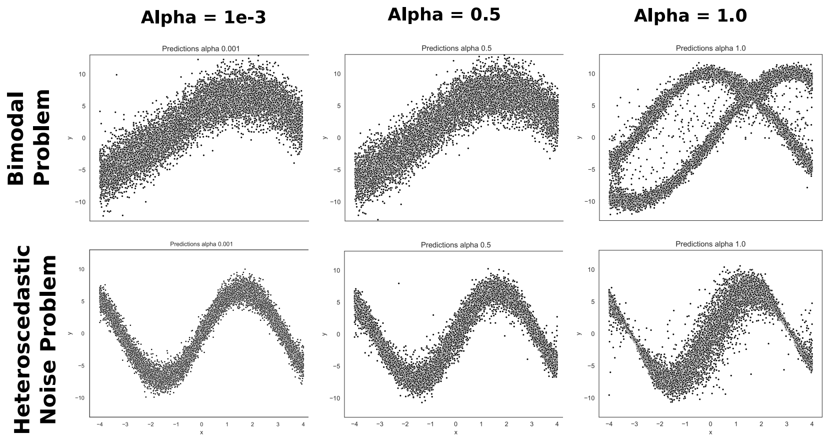

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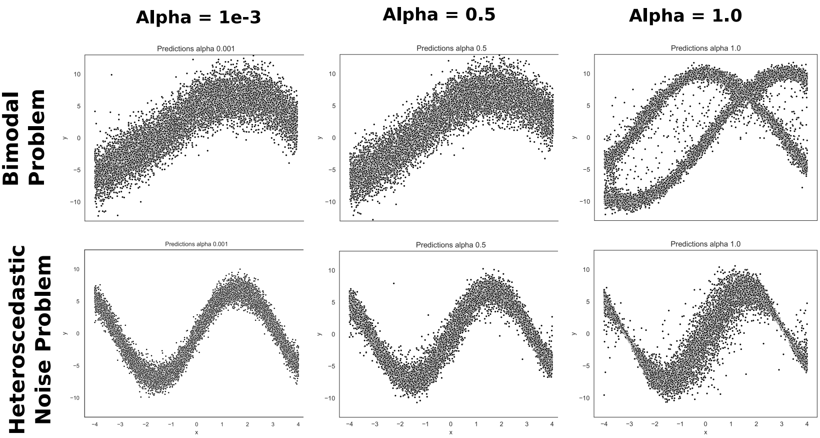
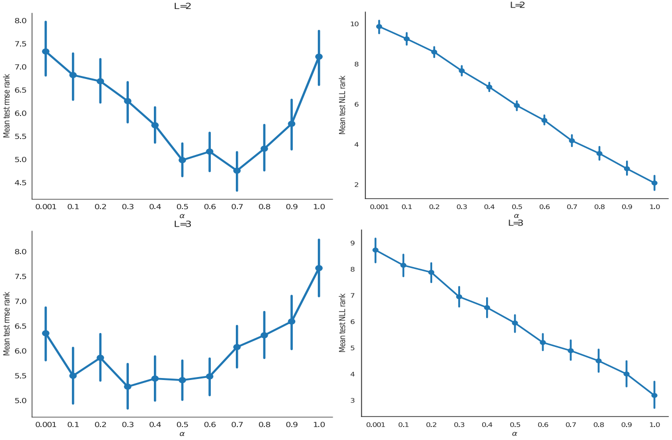


The value $\alpha = 1.0$ provides more sensible predictive distributions!

(Villacampa, 2022)

α-Divergence Minimization: Average Ranks



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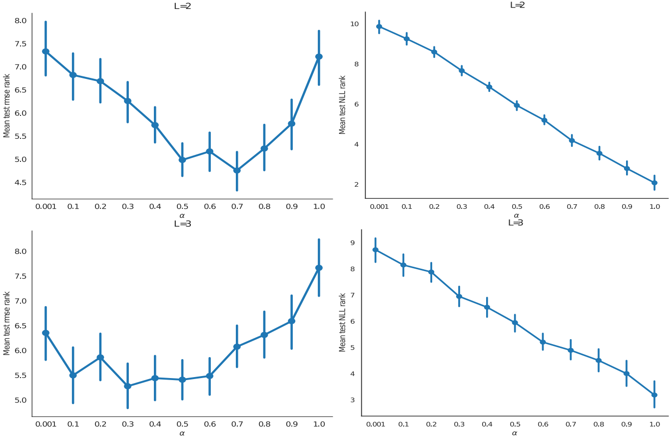

The value $\alpha = 1.0$ provides better results in terms of the NLL and intermediate values of α give better RMSE!

(Villacampa, 2022)

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- α-divergence minimization generalizes the other methods.

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