Approximate Inference in Multi-class and Deep Gaussian Processes by Minimizing Alpha Divergences

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Joint work with
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Outline

- Introduction to Multi-class GPs
  1. Multi-class GPs using Variational Inference
  2. Multi-class GPs using Expectation Propagation
  3. Multi-class GPs using Alpha Divergence Minimization

- Introduction to Deep-GPs
  1. Deep-GPs using Variational Inference
  2. Deep-GPs using Approximate Expectation Propagation
  3. Deep-GPs using Alpha Divergence Minimization

Introduction to Multi-class Classification with GPs

Given $\mathbf{x}_i$ we want to make **predictions** about $y_i \in \{1, \ldots, C\}$, $C > 2$.

One can **assume** that (Kim & Ghahramani, 2006):

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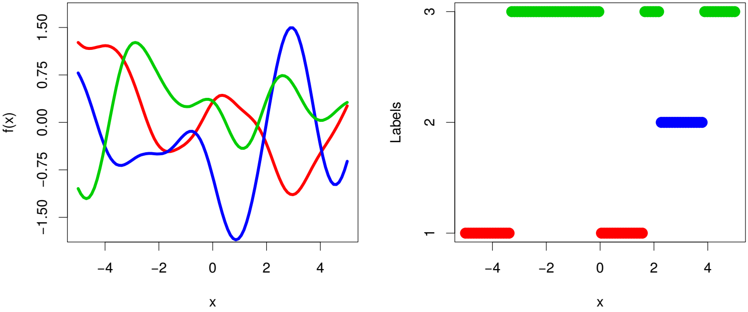

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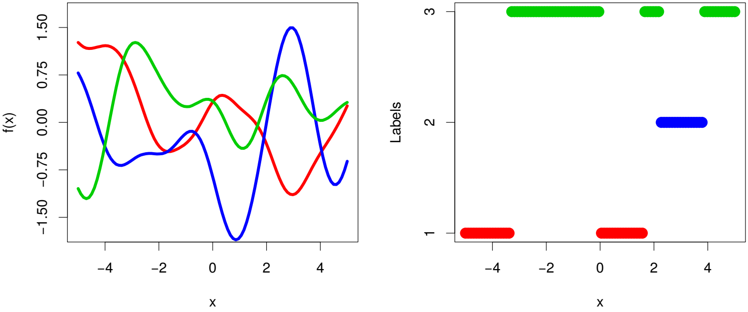

Find $p(\mathbf{f}|\mathbf{y}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f})/p(\mathbf{y})$ **under** $p(\mathbf{f}^k) \sim \mathcal{GP}(0, k(\cdot, \cdot))$.

Efficient Methods for Multi-Class GPs

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$$q(\overline{\mathbf{f}}) = \prod_{k=1}^C \mathcal{N}(\overline{\mathbf{f}}^k|\boldsymbol{\mu}^k, \boldsymbol{\Sigma}^k)$$

$$\overline{\mathbf{f}}^k = (f^k(\overline{\mathbf{x}}_1^k), \ldots, f^k(\overline{\mathbf{x}}_M^k))^\text{T} \qquad \overline{\mathbf{X}}^k = (\overline{\mathbf{x}}_1^k, \ldots, \overline{\mathbf{x}}_M^k)^\text{T}$$

where $q(\overline{\mathbf{f}})$ intuitively approximates $p(\overline{\mathbf{f}}|\mathbf{y})$ and $p(\mathbf{f}|\overline{\mathbf{f}}) = \prod_{k=1}^C p(\mathbf{f}^k|\overline{\mathbf{f}}^k)$.

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Minibatches and stochastic gradients reduce the cost to $\mathcal{O}(CM)$.

Stochastic Variational Inference for Multi-class GPs

Hensman *et al.*, 2015, use a **robust likelihood** function:

$$p(y_i|\mathbf{f}_i) = (1-\epsilon)p_i + \frac{\epsilon}{C-1}(1-p_i) \quad \text{with} \quad p_i = \begin{cases} 1 & \text{if} \quad y_i = arg\,\max_k \quad f^k(\mathbf{x}_i) \\ 0 & \text{otherwise} \end{cases}$$

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- Stochastic optimization of $q(\bar{\mathbf{f}})$ and the hyper-parameters!
- The cost is $\mathcal{O}(CM^3)$ (uses **quadratures**)!

Expectation Propagation (EP)

Let $\boldsymbol{\theta}$ summarize the latent variables of the model.

Approximates $\boxed{p(\boldsymbol{\theta}) \propto p_0(\boldsymbol{\theta}) \prod_{n=1}^{N} f_n(\boldsymbol{\theta})}$ with $\boxed{q(\boldsymbol{\theta}) \propto p_0(\boldsymbol{\theta}) \prod_{n=1}^{N} \tilde{f}_n(\boldsymbol{\theta})}$

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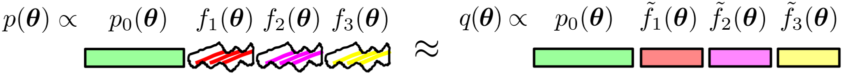

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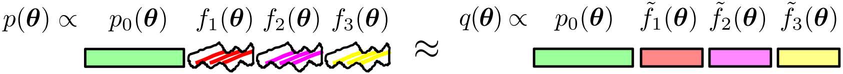

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$$D_{\text{KL}}[p_n || q] \quad \text{for } n = 1, \ldots, N\,, \quad \text{where} \quad \begin{array}{rcl} p_n(\boldsymbol{\theta}) & \propto & f_n(\boldsymbol{\theta}) \prod_{j \neq n} \tilde{f}_j(\boldsymbol{\theta}) \\ q(\boldsymbol{\theta}) & \propto & \tilde{f}_n(\boldsymbol{\theta}) \prod_{j \neq n} \tilde{f}_j(\boldsymbol{\theta}) \end{array}.$$

Model Specification (Villacampa-Calvo and Hernández-Lobato, 2017)

Consider that $y_i = \arg\max_k \; f^k(\mathbf{x}_i)$, which gives the **likelihood**:

$$p(\mathbf{y}|\mathbf{f}) = \prod_{i=1}^{N} p(y_i|\mathbf{f}_i) = \prod_{i=1}^{N} \prod_{k \neq y_i} \Theta(f^{y_i}(\mathbf{x}_i) - f^k(\mathbf{x}_i))$$

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$$p(\bar{\mathbf{f}}|\mathbf{y}) = \frac{\int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\bar{\mathbf{f}})d\mathbf{f}\, p(\bar{\mathbf{f}})}{p(\mathbf{y})} \approx \frac{[\prod_{i=1}^N \int p(y_i|\mathbf{f}_i)p(\mathbf{f}_i|\bar{\mathbf{f}})d\mathbf{f}_i]p(\bar{\mathbf{f}})}{p(\mathbf{y})}$$

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The corresponding **likelihood factors** are:

$$\phi_i(\overline{\mathbf{f}}) = \int \left[\prod_{k \neq y_i} \Theta\left(f_i^{y_i} - f_i^k\right)\right] \prod_{k=1}^C p(f_i^k|\overline{\mathbf{f}}^k)d\mathbf{f}_i$$
$$\approx \prod_{k \neq y_i} p(f_i^{y_i} > f_i^k) = \prod_{k \neq y_i} \Phi(\alpha_i^k)$$

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If $|\mathcal{M}_b| < M$ the **cost** is $\mathcal{O}(CM^3)$.

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

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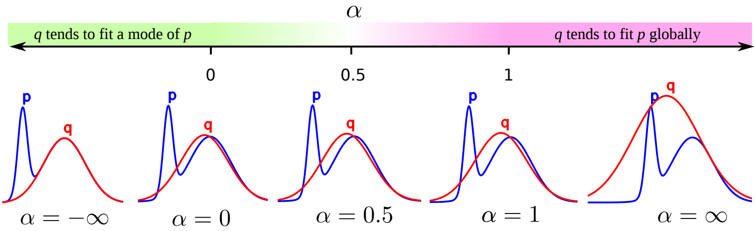

Figure source: (Minka, 2005).

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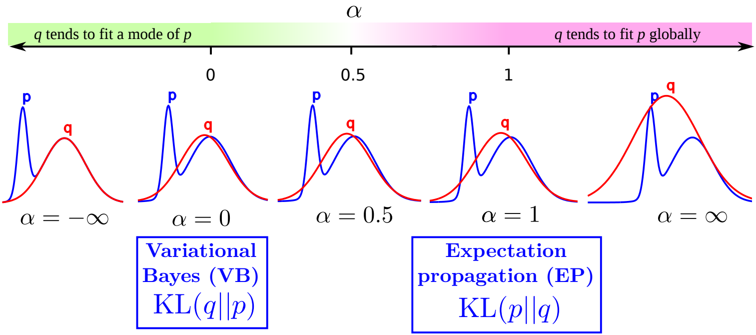

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Local α-divergence minimization (Power EP)

Approximates $p(\boldsymbol{\theta}) \propto p_0(\boldsymbol{\theta}) \prod_{n=1}^{N} f_n(\boldsymbol{\theta})$ with $q(\boldsymbol{\theta}) \propto p_0(\boldsymbol{\theta}) \prod_{n=1}^{N} \tilde{f}_n(\boldsymbol{\theta})$

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$$p(\boldsymbol{\theta}) \propto \; p_0(\boldsymbol{\theta}) \; f_1(\boldsymbol{\theta}) \; f_2(\boldsymbol{\theta}) \; f_3(\boldsymbol{\theta}) \quad \approx \quad q(\boldsymbol{\theta}) \propto \; p_0(\boldsymbol{\theta}) \; \tilde{f}_1(\boldsymbol{\theta}) \; \tilde{f}_2(\boldsymbol{\theta}) \; \tilde{f}_3(\boldsymbol{\theta})$$

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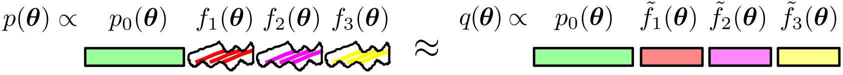

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At convergence $\nabla_{\eta_q} D_\alpha[p_n || q]$ equals zero!

Alternative Algorithms for PEP

The Power-EP approximation to the **evidence** is given by

$$\log Z_{\text{PEP}} = \log Z_q - \log Z_{\text{prior}} + \sum_{n=1}^{N} \frac{1}{\alpha} \log \mathbf{E}_q \left[\left(\frac{f_n(\boldsymbol{\theta})}{\tilde{f}_n(\boldsymbol{\theta})} \right)^{\alpha} \right] \,,$$

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The power-EP solution for q can be obtained by solving

$$\max_{q} \min_{\tilde{f}_1,\ldots,\tilde{f}_N} \log Z_{\text{PEP}} \quad \text{subject to} \quad q(\boldsymbol{\theta}) = p_0(\boldsymbol{\theta}) \prod_{n=1}^{N} \tilde{f}_n(\boldsymbol{\theta}).$$

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Solved with **double-loop** algorithm (Heskes, 2002).

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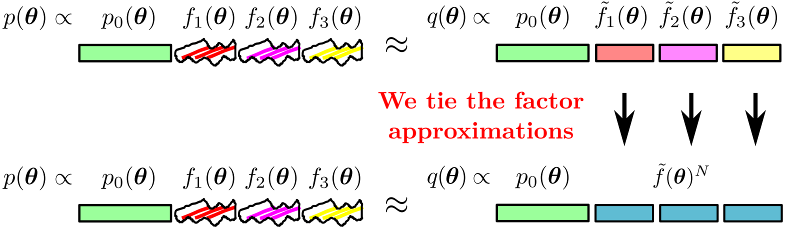

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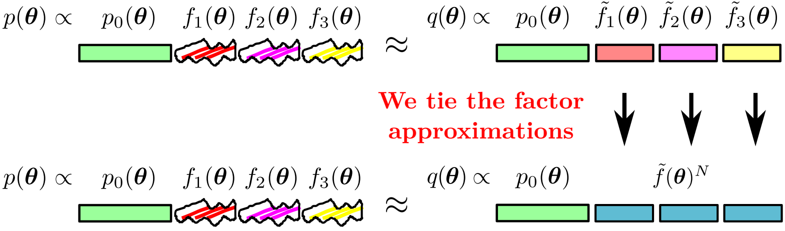

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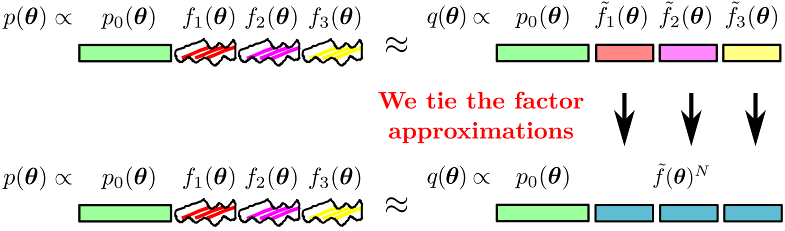

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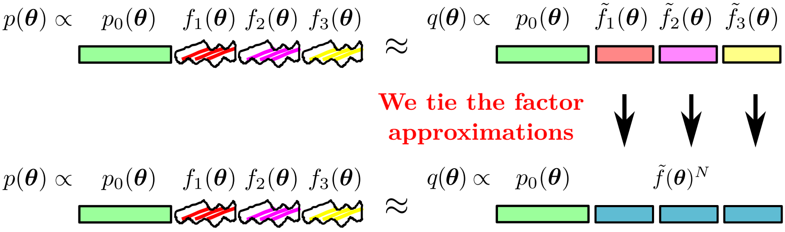

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- **Standard optimization tools** can be used (stochastic gradients).

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Experiments: UCI Datasets

Dataset	#Instances	#Attributes	#Classes
Glass	214	9	6
New-thyroid	215	5	3
Satellite	6435	36	6
Svmguide2	391	20	3
Vehicle	846	18	4
Vowel	540	10	6
Waveform	1000	21	3
Wine	178	13	3

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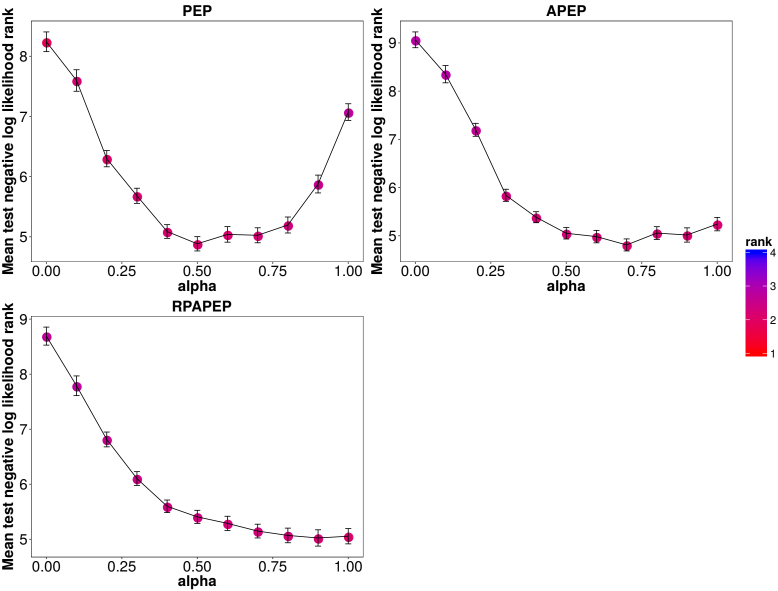
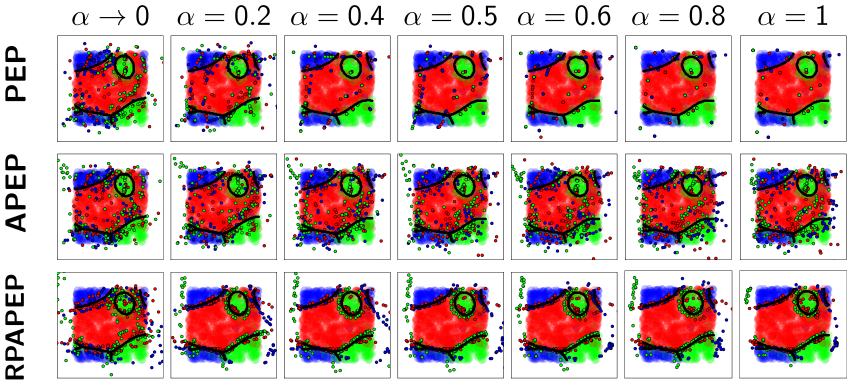
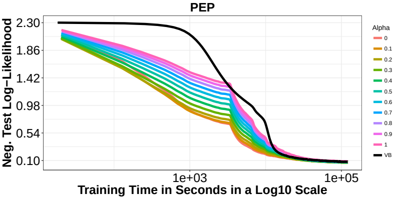


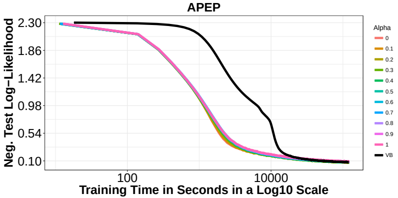
Toy Problem: Inducing Point Locations

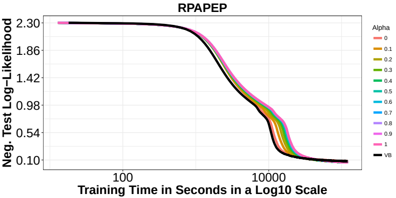


MNIST Dataset

10 classes, 60,000 training instances.

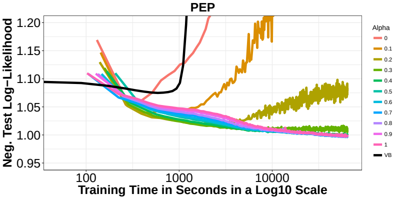


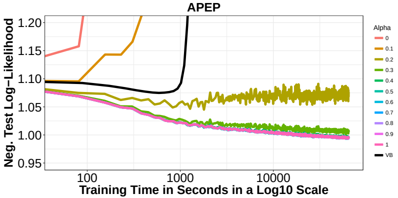


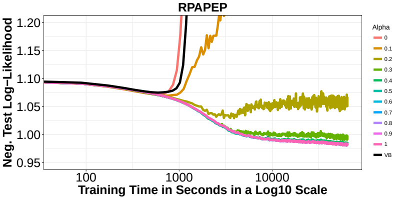


Airline Delays

3 classes, 2 million training instances.







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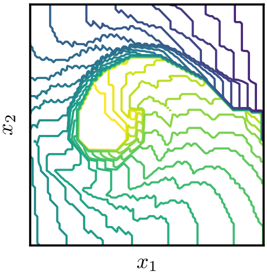
- VB sometimes gives **bad test log-likelihoods**.

Motivation for Deep Gaussian Processes

Target function



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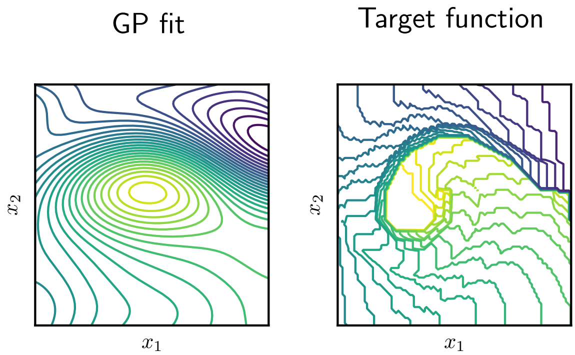

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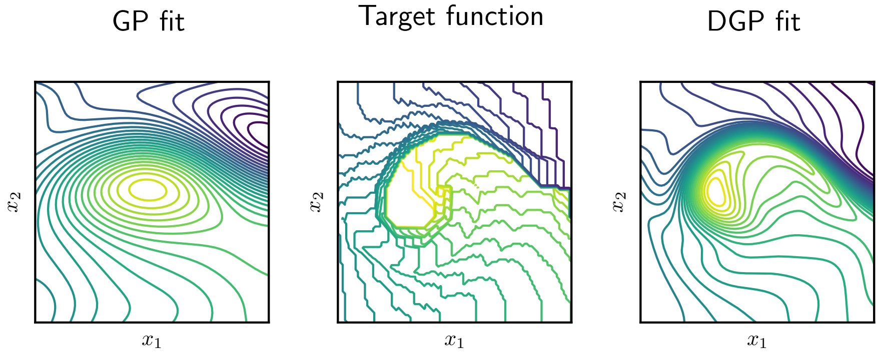
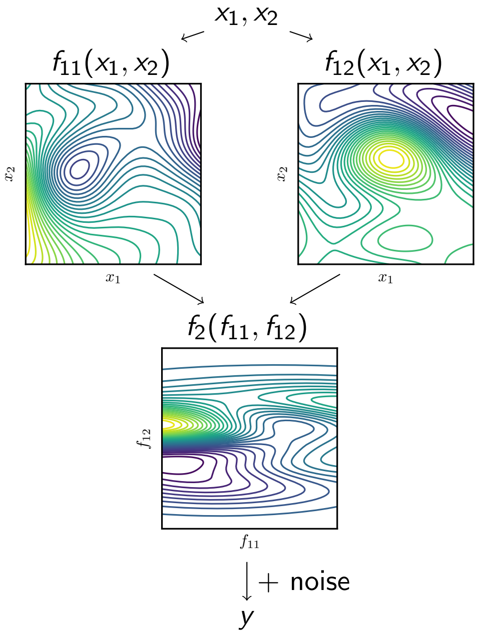


How do deep GPs work?



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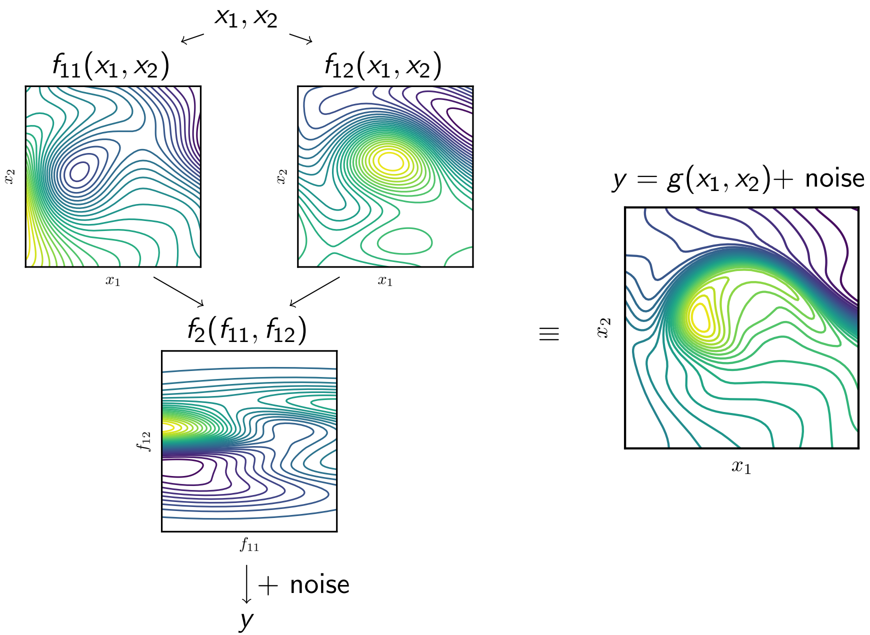

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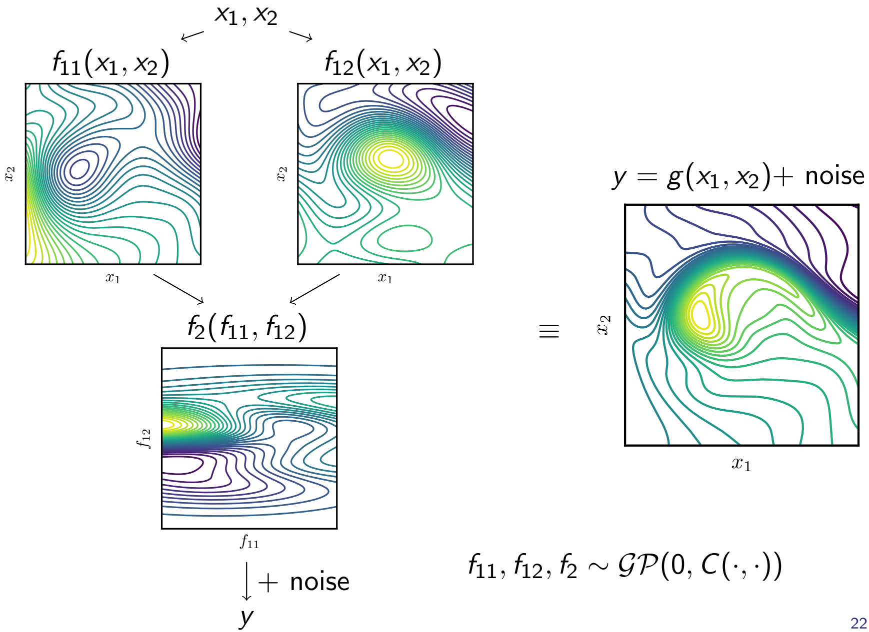
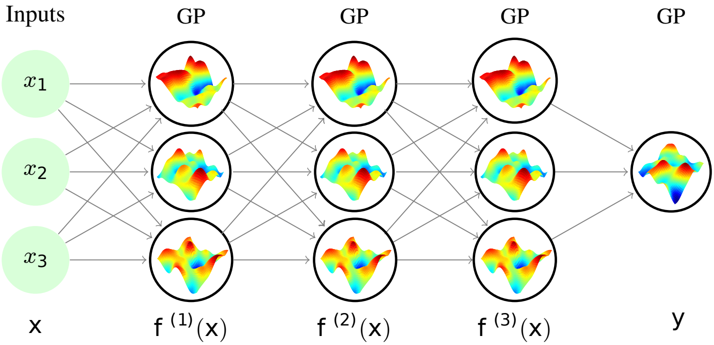


$$f_{11}, f_{12}, f_2 \sim \mathcal{GP}(0, C(\cdot, \cdot))$$

Deep GPs as Deep Neural Networks



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Advantages:

- useful input warping: automatic, nonparametric kernel design
- repair damage done by sparse approximations to GPs
- more accurate predictions and better uncertainty estimates

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Drawbacks:

- require complicated approximate inference methods
- high computational cost

Bayesian inference

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

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

- GP priors
- Likelihood function
- Marginal likelihood

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

Inducing Points Representation

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

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

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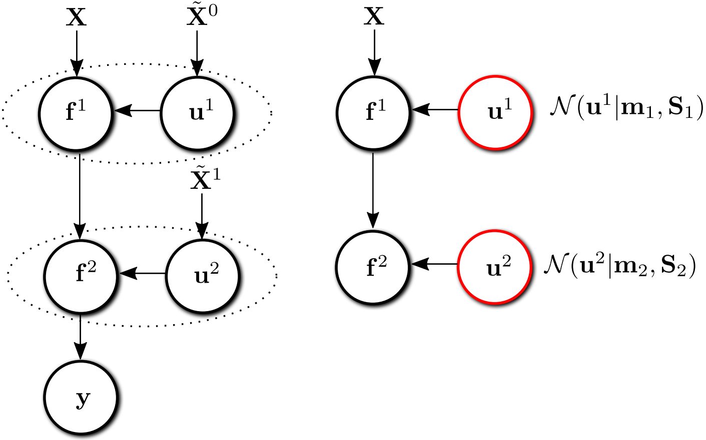
Given u or a Gaussian for u, f is fully specified!

Deep Gaussian Process Joint Distribution.

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

Prob. Graphical Model and Posterior Approx.



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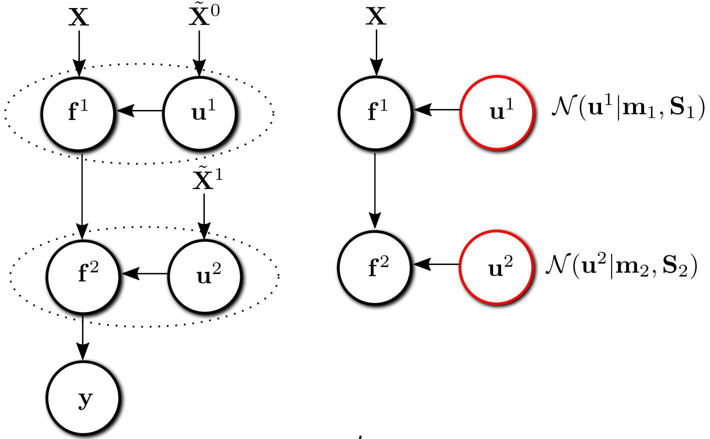

$$q(\{\mathbf{f}^l, \mathbf{u}^l\}_{l=1}^{L}) = \prod_{l=1}^{L} p(\mathbf{f}^l|\mathbf{u}^l)\, q(\mathbf{u}^l)$$

- Fixed
- Tuneable

Variational Inference for Deep GPs

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

(Salimbeni, 2017)

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Equivalent to maximizing:

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

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

(Salimbeni, 2017)

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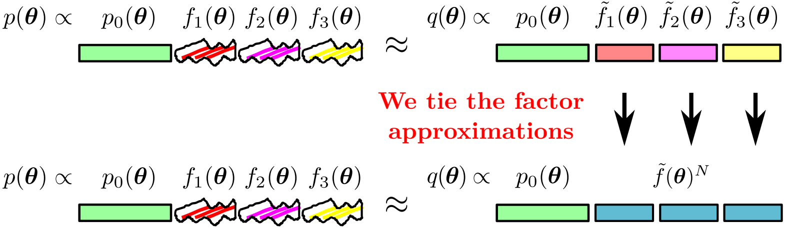

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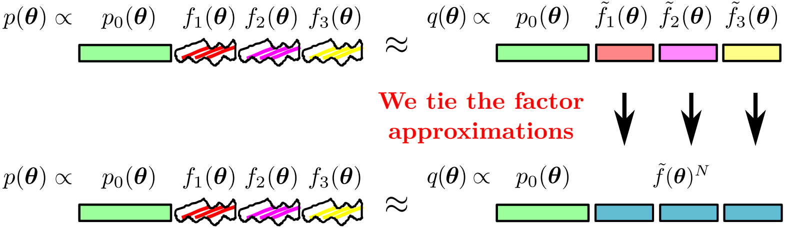

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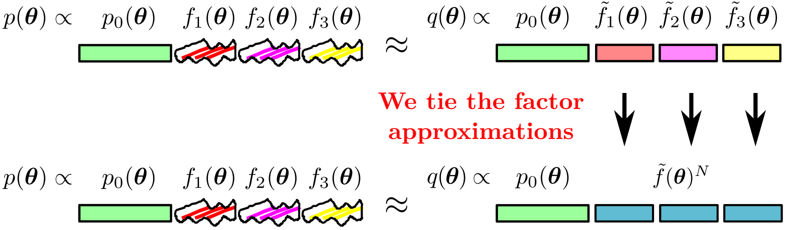
Approximate Expectation Propagation



- $\max_{q} \min_{\tilde{f}_1,\ldots,\tilde{f}_N}$ problem $\rightarrow$ $\max_{q}$ problem, **no double-loop needed!**
- **Memory saving** scales as $\mathcal{O}(N)$.

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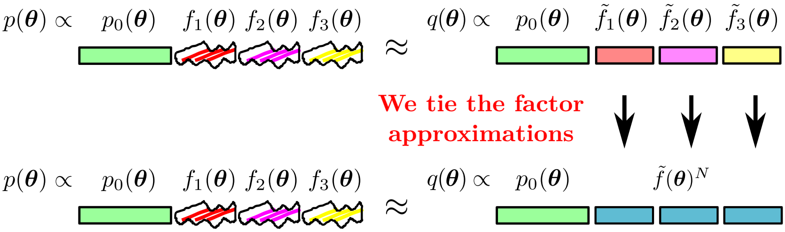

- $\max_q \min_{\tilde{f}_1,\dots,\tilde{f}_N}$ problem $\rightarrow$ $\max_q$ problem, **no double-loop needed!**
- **Memory saving** scales as $\mathcal{O}(N)$.
- **Standard optimization tools** can be used (stochastic gradients).

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One only needs to optimize

$$\log Z_{\mathrm{EP}} = \log Z_q - \log Z_{\mathrm{prior}} + \sum_{n=1}^{N} \log \mathbf{E}_q \left[\left(\frac{f_n(\boldsymbol{\theta})}{\tilde{f}(\boldsymbol{\theta})} \right) \right] .$$

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But this requires integrating the exact likelihood factors (**intractable**).

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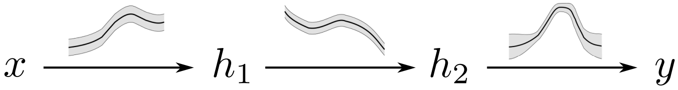
For some kernels it is possible to compute the moments of the GP predictive distribution with random Gaussian inputs!

Iterative Gaussian Approximations



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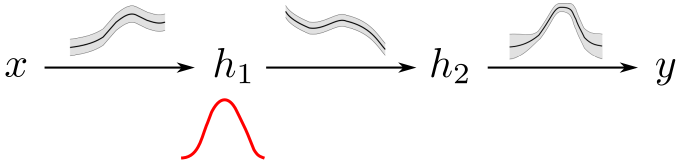

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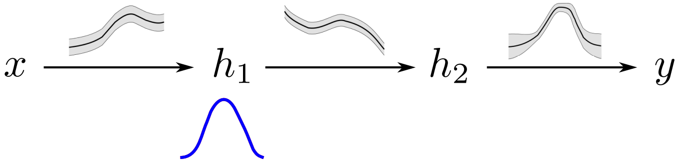

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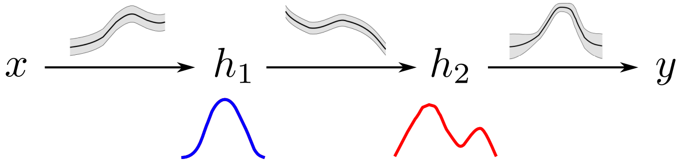

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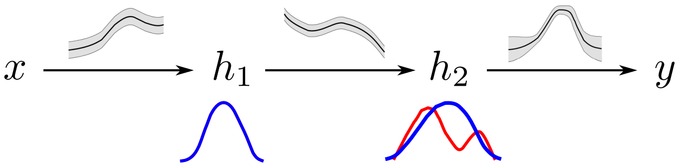

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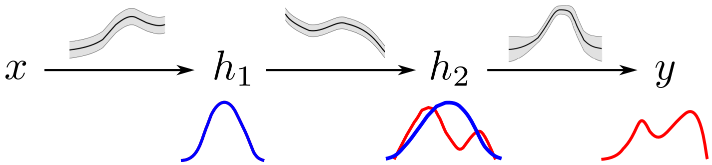

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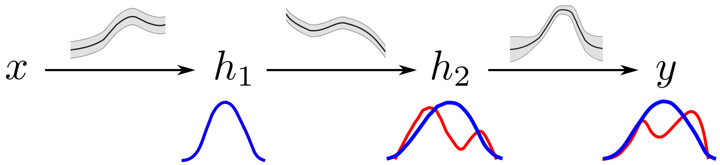

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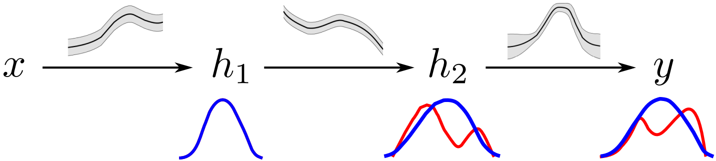

This approach allows to approximate the required expectations!

α-divergence Minimization for Deep GPs

One only needs to optimize the approximate Power EP objective:

$$\log Z_{\mathsf{EP}} = \log Z_q - \log Z_{\mathsf{prior}} + \frac{1}{\alpha} \sum_{n=1}^{N} \log \mathbf{E}_q \left[\left(\frac{f_n(\boldsymbol{\theta})}{\tilde{f}(\boldsymbol{\theta})} \right)^{\alpha} \right] .$$

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We suggest to use a Monte Carlo approach similar to that of VI.

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Expected to give better results than the Gaussian approximation!

Monte Carlo Approximation

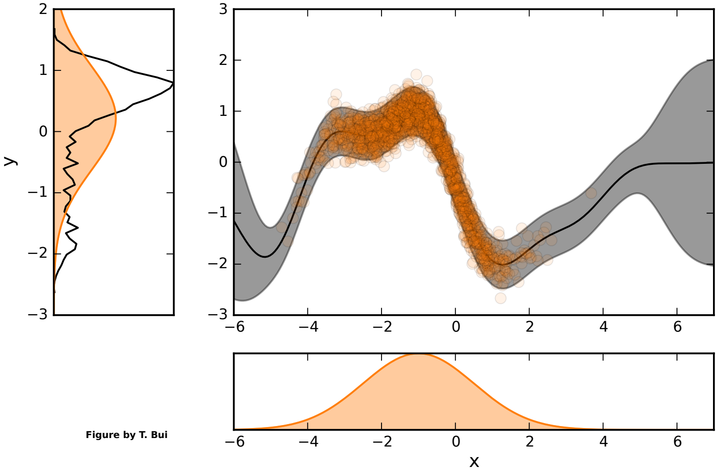
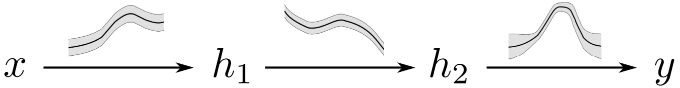


Figure by T. Bui

The predictive distribution with random Gaussian inputs may be very different from Gaussian!

Monte Carlo Approximation



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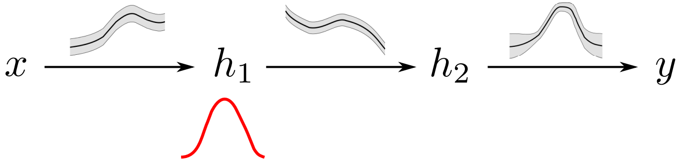

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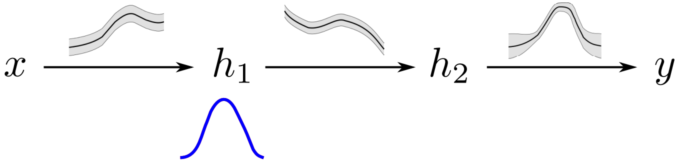

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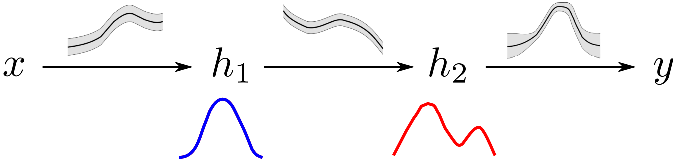

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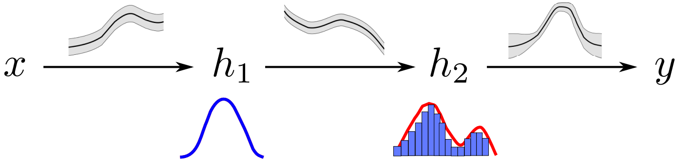

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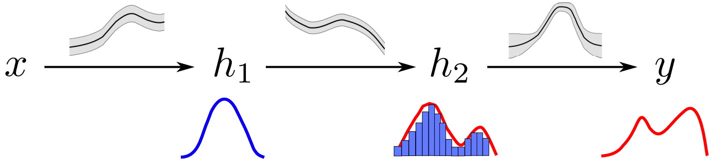

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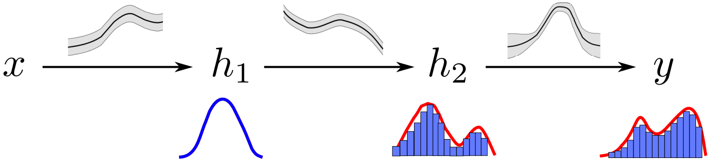

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The required expectation is approximated as:

$$\frac{1}{\alpha}\log \mathbb{E}_q\left[\left(\frac{f_n(\boldsymbol{\theta})}{\tilde{f}(\boldsymbol{\theta})}\right)^{\alpha}\right] \approx \frac{1}{\alpha}\log\left(\frac{1}{S}\sum_{s=1}^{S} p(y_i|f_{i,s}^{L})\right) - \frac{g_q}{\alpha} + \frac{g_{q_{\text{cav}}^{\alpha}}}{\alpha}$$

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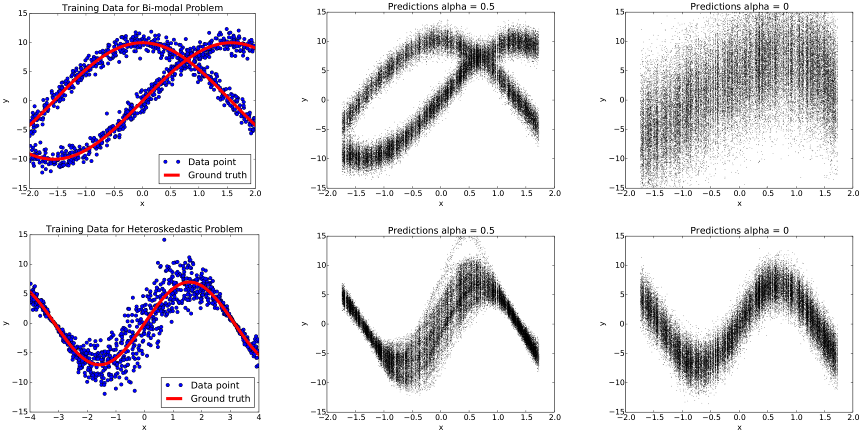
This is a biased estimate, but the bias goes to zero as the number of samples S increases.

Expected Benefits of α-divergence Minimization

Similar to those of Bayesian neural networks...



(Depeweg et al., 2016)

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Future Work:

- Carry out experiments to assess the benefits of alpha divergence minimization for Deep GPs.

Thank you for your attention!

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Specific Application of PEP to Multi-class GPC

The likelihood factors are the same as those of the VI approach:

$$p(y_i|\mathbf{f}_i) = (1-\epsilon)p_i + \frac{\epsilon}{C-1}(1-p_i) \quad \text{with} \quad p_i = \begin{cases} 1 & \text{if} \quad y_i = arg\,\max\limits_k \quad f^k(\mathbf{x}_i) \\ 0 & \text{otherwise} \end{cases}$$

The posterior approximation is:

$$q(\mathbf{f}, \bar{\mathbf{f}}) = p(\mathbf{f}|\bar{\mathbf{f}})q(\bar{\mathbf{f}})$$

At each step of PEP we have to update $\tilde{\phi}_i$ to minimize:

$$\text{KL}\left[p(y_i|\mathbf{f}_i)^\alpha p(\mathbf{f}|\bar{\mathbf{f}}) \frac{q(\bar{\mathbf{f}})}{\tilde{\phi}_i^\alpha} \,||\, p(\mathbf{f}|\bar{\mathbf{f}})q(\bar{\mathbf{f}}) \right]$$

Done by matching the moments of $\bar{\mathbf{f}}$! Requires quadratures!