Approximate Inference in Deep GPs

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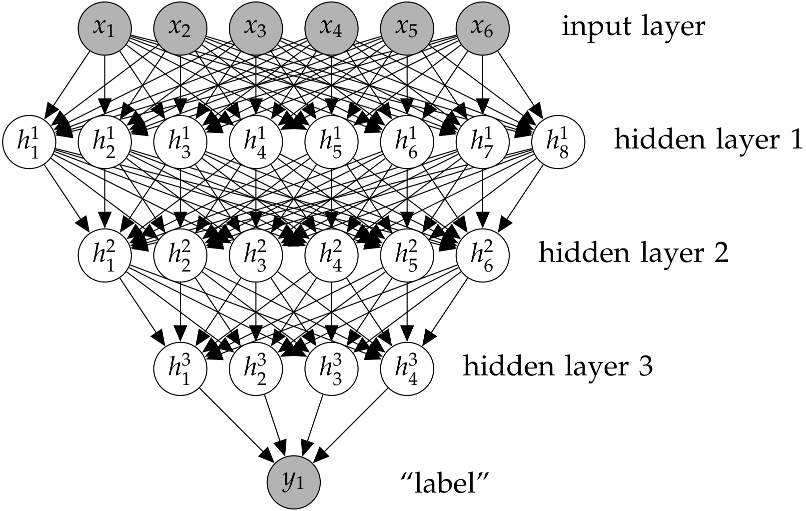
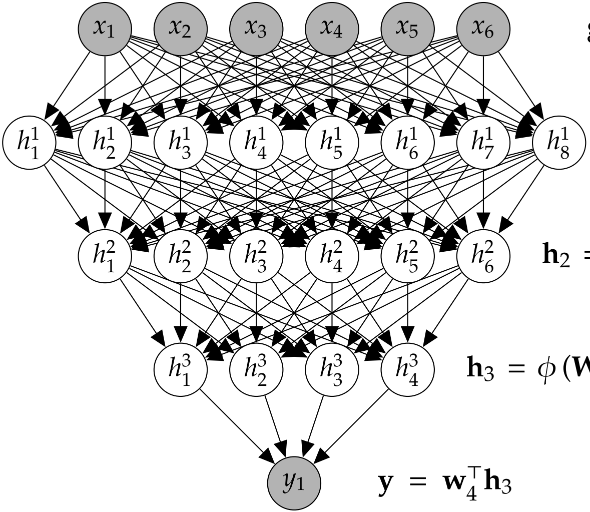
Outline

Deep Neural Network



Deep Neural Network



given $\mathbf{x}$

$$\mathbf{h}_1 = \phi(\mathbf{W}_1\mathbf{x})$$

$$\mathbf{h}_2 = \phi(\mathbf{W}_2\mathbf{h}_1)$$

$$\mathbf{h}_3 = \phi(\mathbf{W}_3\mathbf{h}_2)$$

$$\mathbf{y} = \mathbf{w}_4^\top\mathbf{h}_3$$

Mathematically

$$\begin{aligned}
\mathbf{h}_1 &= \phi\left(\mathbf{W}_1\mathbf{x}\right)\\
\mathbf{h}_2 &= \phi\left(\mathbf{W}_2\mathbf{h}_1\right)\\
\mathbf{h}_3 &= \phi\left(\mathbf{W}_3\mathbf{h}_2\right)\\
\mathbf{y} &= \mathbf{w}_4^\top\mathbf{h}_3
\end{aligned}$$

Overfitting

- Potential problem: if number of nodes in two adjacent layers is big, corresponding **W** is also very big and there is the potential to overfit.
- Proposed solution: "dropout".
- Alternative solution: parameterize **W** with its SVD.

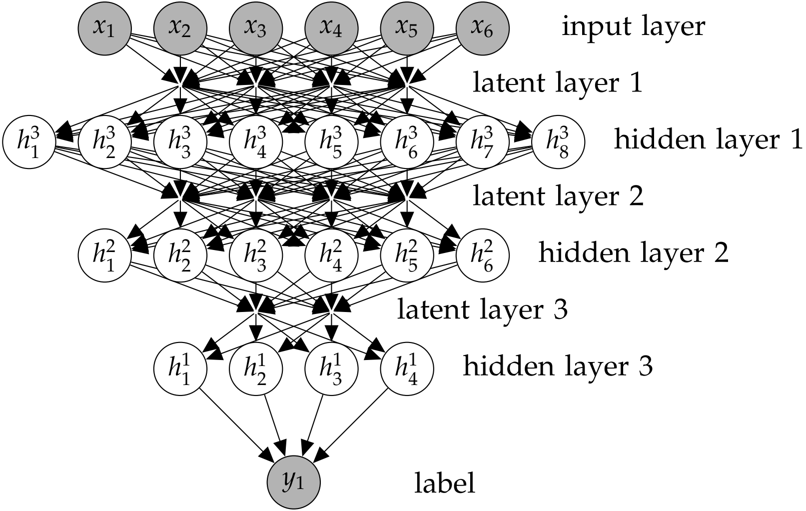
$$\mathbf{W} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^\top$$

or

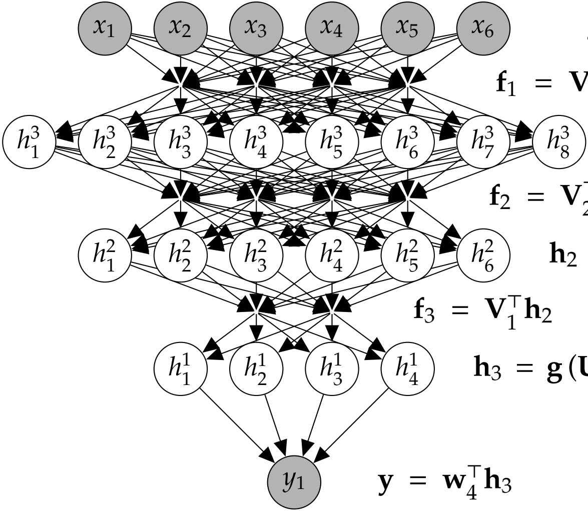
$$\mathbf{W} = \mathbf{U}\mathbf{V}^\top$$

where if $\mathbf{W} \in \Re^{k_1 \times k_2}$ then $\mathbf{U} \in \Re^{k_1 \times q}$ and $\mathbf{V} \in \Re^{k_2 \times q}$, i.e. we have a low rank matrix factorization for the weights.

Deep Neural Network



Deep Neural Network



given $\mathbf{x}$

$$\mathbf{f}_1 = \mathbf{V}_1^\top \mathbf{x}$$

$$\mathbf{h}_1 = \mathbf{g}\,(\mathbf{U}_1 \mathbf{f}_1)$$

$$\mathbf{f}_2 = \mathbf{V}_2^\top \mathbf{h}_3$$

$$\mathbf{h}_2 = \mathbf{g}\,(\mathbf{U}_2 \mathbf{f}_2)$$

$$\mathbf{f}_3 = \mathbf{V}_1^\top \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{g}\,(\mathbf{U}_3 \mathbf{f}_3)$$

$$\mathbf{y} = \mathbf{w}_4^\top \mathbf{h}_3$$

Mathematically

$$
\begin{aligned}
\mathbf{f}_1 &= \mathbf{V}_1^\top \mathbf{x} \\
\mathbf{h}_1 &= \phi\left(\mathbf{U}_1 \mathbf{f}_1\right) \\
\mathbf{f}_2 &= \mathbf{V}_2^\top \mathbf{h}_1 \\
\mathbf{h}_2 &= \phi\left(\mathbf{U}_2 \mathbf{f}_2\right) \\
\mathbf{f}_3 &= \mathbf{V}_3^\top \mathbf{h}_2 \\
\mathbf{h}_3 &= \phi\left(\mathbf{U}_3 \mathbf{f}_3\right) \\
\mathbf{y} &= \mathbf{w}_4^\top \mathbf{h}_3
\end{aligned}
$$

A Cascade of Neural Networks

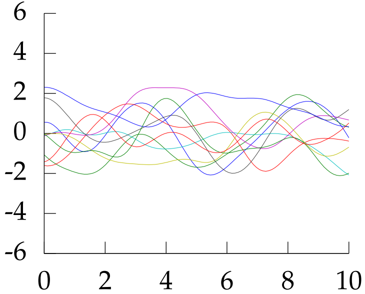
$$
\begin{aligned}
\mathbf{f}_1 &= \mathbf{V}_1^\top \mathbf{x} \\
\mathbf{f}_2 &= \mathbf{V}_2^\top \phi\left(\mathbf{U}_1 \mathbf{f}_1\right) \\
\mathbf{f}_3 &= \mathbf{V}_3^\top \phi\left(\mathbf{U}_2 \mathbf{f}_2\right) \\
\mathbf{y} &= \mathbf{w}_4^\top \mathbf{f}_3
\end{aligned}
$$

Replace Each Neural Network with a Gaussian Process

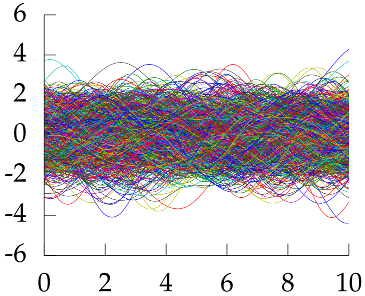
$$
\begin{aligned}
\mathbf{f}_1 &= \mathbf{f}(\mathbf{x}) \\
\mathbf{f}_2 &= \mathbf{f}(\mathbf{f}_1) \\
\mathbf{f}_3 &= \mathbf{f}(\mathbf{f}_2) \\
\mathbf{y} &= \mathbf{f}(\mathbf{f}_3)
\end{aligned}
$$

This is equivalent to Gaussian prior over weights and integrating out all parameters and taking width of each layer to infinity.

Gaussian Processes: Extremely Short Overview



Gaussian Processes: Extremely Short Overview



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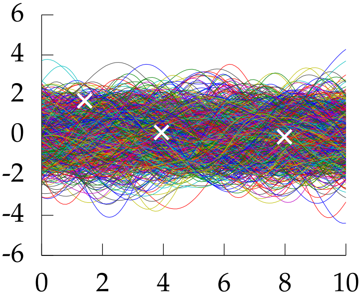
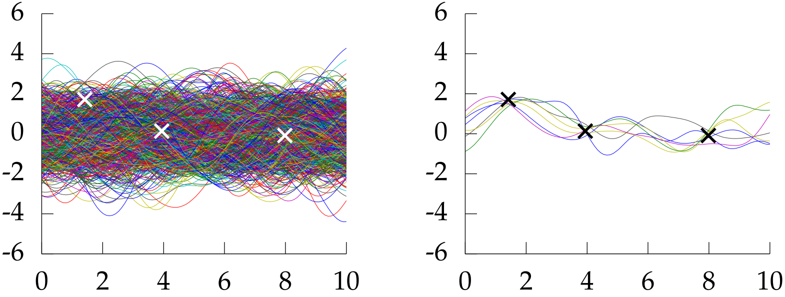


Gaussian Processes: Extremely Short Overview



Outline

Mathematically

- Composite *multivariate* function

$$\mathbf{g}(\mathbf{x}) = \mathbf{f}_5(\mathbf{f}_4(\mathbf{f}_3(\mathbf{f}_2(\mathbf{f}_1(\mathbf{x})))))$$

Why Deep?

- Gaussian processes give priors over functions.
- Elegant properties:
  - e.g. *Derivatives* of process are also Gaussian distributed (if they exist).
- For particular covariance functions they are 'universal approximators', i.e. all functions can have support under the prior.
- Gaussian derivatives might ring alarm bells.
- E.g. a priori they don't believe in function 'jumps'.

Process Composition

- From a process perspective: *process composition*.
- A (new?) way of constructing more complex *processes* based on simpler components.

Note: To retain *Kolmogorov consistency* introduce IBP priors over latent variables in each layer (Zhenwen Dai).

Analysis of Deep GPs

- Duvenaud et al. (2014) Duvenaud et al show that the derivative distribution of the process becomes more *heavy tailed* as number of layers increase.

Difficulty for Probabilistic Approaches

- Propagate a probability distribution through a non-linear mapping.
- Normalisation of distribution becomes intractable.

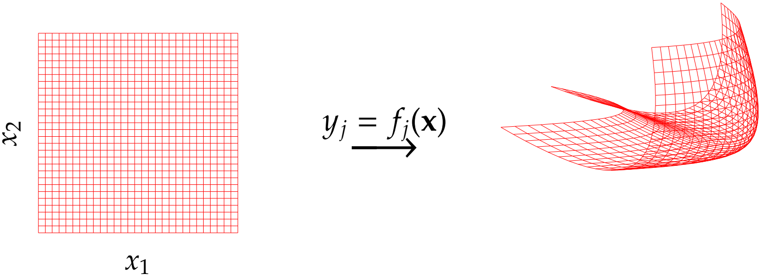


Figure : A three dimensional manifold formed by mapping from a two dimensional space to a three dimensional space.

Difficulty for Probabilistic Approaches

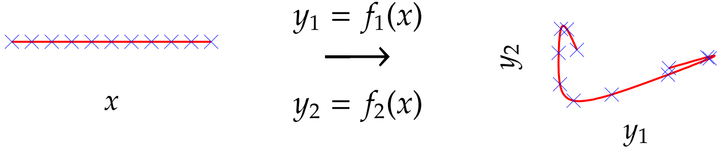


Figure : A string in two dimensions, formed by mapping from one dimension, x, line to a two dimensional space, $[y_1,\ y_2]$ using nonlinear functions $f_1(\cdot)$ and $f_2(\cdot)$.

Difficulty for Probabilistic Approaches

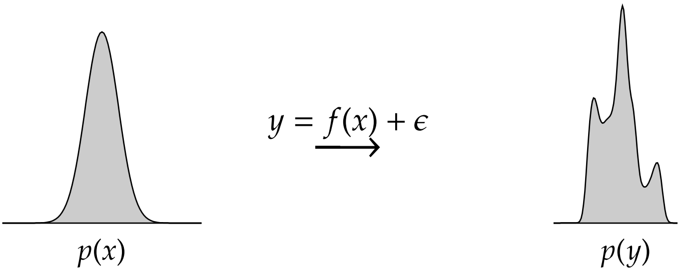


Figure : A Gaussian distribution propagated through a non-linear mapping. $y_i = f(x_i) + \epsilon_i$. $\epsilon \sim \mathcal{N}\left(0, 0.2^2\right)$ and $f(\cdot)$ uses RBF basis, 100 centres between -4 and 4 and $\ell = 0.1$. New distribution over y (right) is multimodal and difficult to normalize.

b

Outline

Introduction

Deep Gaussian Process Models

Flexible Parametric Approximation

Variational Compression

Conclusions

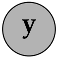
Inducing Variable Approximations

- Date back to (Williams and Seeger, 2001; Smola and Bartlett, 2001; Csató and Opper, 2002; Seeger et al., 2003; Snelson and Ghahramani, 2006). See Quiñonero Candela and Rasmussen (2005) for a review.
- We follow variational perspective of (Titsias, 2009).
- This is an augmented variable method, followed by a collapsed variational approximation (King and Lawrence, 2006; Hensman et al., 2012).

Augmented Variable Model: Not Wrong but Useful?

Augment standard model with a set of m new inducing variables, $\mathbf{u}$.

$$p(\mathbf{y}) = \int p(\mathbf{y}, \mathbf{u}) \mathrm{d}\mathbf{u}$$



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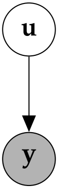
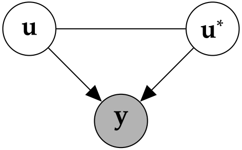
$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{u})p(\mathbf{u})\mathrm{d}\mathbf{u}$$



Augmented Variable Model: Not Wrong but Useful?

Important: Ensure inducing variables are *also* Kolmogorov consistent (we have m^* other inducing variables we are not *yet* using.)

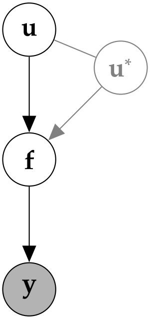
$$p(\mathbf{u}) = \int p(\mathbf{u}, \mathbf{u}^*) \mathrm{d}\mathbf{u}^*$$



Augmented Variable Model: Not Wrong but Useful?

Assume that relationship is through $\mathbf{f}$ (represents 'fundamentals'—push Kolmogorov consistency up to here).

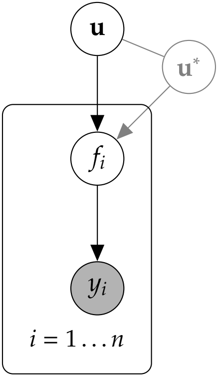
$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})p(\mathbf{u})\mathrm{d}\mathbf{f}\mathrm{d}\mathbf{u}$$



Augmented Variable Model: Not Wrong but Useful?

Convenient to assume factorization (*doesn't* invalidate model—think delta function as worst case).

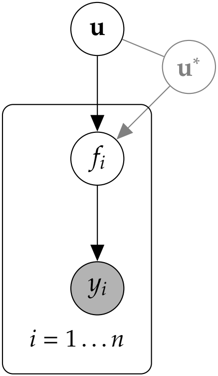
$$p(\mathbf{y}) = \int \prod_{i=1}^{n} p(y_i|f_i)p(\mathbf{f}|\mathbf{u})p(\mathbf{u})\mathrm{d}\mathbf{f}\mathrm{d}\mathbf{u}$$



Augmented Variable Model: Not Wrong but Useful?

Focus on integral over $\mathbf{f}$.

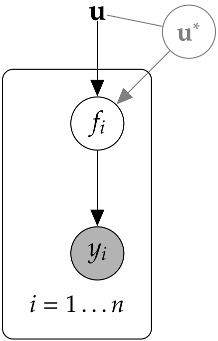
$$p(\mathbf{y}) = \int \int \prod_{i=1}^{n} p(y_i|f_i) p(\mathbf{f}|\mathbf{u}) \mathrm{d}\mathbf{f} p(\mathbf{u}) \mathrm{d}\mathbf{u}$$



Augmented Variable Model: Not Wrong but Useful?

Focus on integral over **f**.

$$p(\mathbf{y}|\mathbf{u}) = \int \prod_{i=1}^{n} p(y_i|f_i)p(\mathbf{f}|\mathbf{u})\mathrm{d}\mathbf{f}$$



Variational Bound on $p(\mathbf{y}|\mathbf{u})$

$$
\begin{aligned}
\log p(\mathbf{y}|\mathbf{u}) &= \log \int p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}|\mathbf{u}) \mathrm{d}\mathbf{f} \\
&= \int q(\mathbf{f}) \log \frac{p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}|\mathbf{u})}{q(\mathbf{f})} \mathrm{d}\mathbf{f} + \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y}, \mathbf{u})\right)
\end{aligned}
$$

Variational Bound on $p(\mathbf{y}|\mathbf{u})$

$$\log p(\mathbf{y}|\mathbf{u}) = \log \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})\mathrm{d}\mathbf{f}$$

$$= \int q(\mathbf{f}) \log \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})}{q(\mathbf{f})}\mathrm{d}\mathbf{f} + \mathrm{KL}\left(q(\mathbf{f})\,\|\,p(\mathbf{f}|\mathbf{y},\mathbf{u})\right)$$

(Titsias, 2009)

- Example, set $q(\mathbf{f}) = p(\mathbf{f}|\mathbf{u})$,

$$\log p(\mathbf{y}|\mathbf{u}) \geq \log \int p(\mathbf{f}|\mathbf{u}) \log p(\mathbf{y}|\mathbf{f})\mathrm{d}\mathbf{f}.$$

$$p(\mathbf{y}|\mathbf{u}) \geq \exp \int p(\mathbf{f}|\mathbf{u}) \log p(\mathbf{y}|\mathbf{f})\mathrm{d}\mathbf{f}.$$

Optimal Compression in Inducing Variables

- Maximizing lower bound minimizes the KL divergence (information gain):

$$\text{KL}\left(p(\mathbf{f}|\mathbf{u})\,\|\,p(\mathbf{f}|\mathbf{y},\mathbf{u})\right) = \int p(\mathbf{f}|\mathbf{u}) \log \frac{p(\mathbf{f}|\mathbf{u})}{p(\mathbf{f}|\mathbf{y},\mathbf{u})} \mathrm{d}\mathbf{u}$$

- This is minimized when the information stored about $\mathbf{y}$ is stored already in $\mathbf{u}$.
- The bound seeks an *optimal compression* from the *information gain* perspective.
- If $\mathbf{u} = \mathbf{f}$ bound is exact ($\mathbf{f}$ d-separates $\mathbf{y}$ from $\mathbf{u}$).

Choice of Inducing Variables

- Optimizing the bound directly not always practical.
- Free to choose whatever heuristics for the inducing variables.
- Can quantify which heuristics perform better through checking lower bound.

Factorizing Likelihoods

- If the likelihood, $p(\mathbf{y}|\mathbf{f})$, factorizes

$$p(\mathbf{y}|\mathbf{u}) \geq \exp \int p(\mathbf{f}|\mathbf{u}) \log \prod_{i=1}^{n} p(y_i|f_i) \mathrm{d}\mathbf{f}.$$

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- Then the bound factorizes.

Factorizing Likelihoods

- If the likelihood, $p(\mathbf{y}|\mathbf{f})$, factorizes

$$p(\mathbf{y}|\mathbf{u}) \geq \prod_{i=1}^{n} \exp \left\langle \log p(y_i|f_i) \right\rangle_{p(f_i|\mathbf{u})}$$

- Then the bound factorizes.

Factorizing Likelihoods

- If the likelihood, $p(\mathbf{y}|\mathbf{f})$, factorizes

$$p(\mathbf{y}|\mathbf{u}) \geq \prod_{i=1}^{n} \exp \left\langle \log p(y_i|f_i) \right\rangle_{p(f_i|\mathbf{u})}$$

- Then the bound factorizes.
- Now need a choice of distributions for **f** and **y**|**f** ...

$$\mathbf{f}, \mathbf{u} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K_{ff}} & \mathbf{K_{fu}} \\ \mathbf{K_{uf}} & \mathbf{K_{uu}} \end{bmatrix}\right)$$

$$\mathbf{y}|\mathbf{f} = \prod_i \mathcal{N}\left(f, \sigma^2\right)$$

Outline

Gaussian $p(y_i|f_i)$

For Gaussian likelihoods:

$$\left\langle \log p(y_i|f_i) \right\rangle_{p(f_i|\mathbf{u})} = -\frac{1}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\left(y_i - \left\langle f_i \right\rangle\right)^2 - \frac{1}{2\sigma^2}\left(\left\langle f_i^2 \right\rangle - \left\langle f_i \right\rangle^2\right)$$

Gaussian $p(y_i|f_i)$

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$$\langle \log p(y_i|f_i) \rangle_{p(f_i|\mathbf{u})} = -\frac{1}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\left(y_i - \langle f_i \rangle\right)^2 - \frac{1}{2\sigma^2}\left(\left\langle f_i^2 \right\rangle - \langle f_i \rangle^2\right)$$

Implying:

$$p(y_i|\mathbf{u}) \geq \exp \langle \log c_i \rangle \mathcal{N}\left(y_i| \langle f_i \rangle, \sigma^2\right)$$

Gaussian Process Over $\mathbf{f}$ and $\mathbf{u}$

Define:

$$q_{i,i} = \text{var}_{p(f_i|\mathbf{u})}(f_i) = \left\langle f_i^2 \right\rangle_{p(f_i|\mathbf{u})} - \left\langle f_i \right\rangle_{p(f_i|\mathbf{u})}^2$$

We can write:

$$c_i = \exp\left(-\frac{q_{i,i}}{2\sigma^2}\right)$$

If joint distribution of $p(\mathbf{f}, \mathbf{u})$ is Gaussian then:

$$q_{i,i} = k_{i,i} - \mathbf{k}_{i,\mathbf{u}}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{k}_{i,\mathbf{u}}$$

c_i is not a function of $\mathbf{u}$ but *is* a function of $\mathbf{X}_{\mathbf{u}}$.

Total Conditional Variance

- The sum of $q_{i,i}$ is the *total conditional variance*.
- If conditional density $p(\mathbf{f}|\mathbf{u})$ is Gaussian then it has covariance
$$\mathbf{Q} = \mathbf{K}_{\mathbf{ff}} - \mathbf{K}_{\mathbf{fu}}\mathbf{K}_{\mathbf{uu}}^{-1}\mathbf{K}_{\mathbf{uf}}$$
- $\text{tr}\left(\mathbf{Q}\right) = \sum_i q_{i,i}$ is known as total variance.
- Because it is on conditional distribution we call it *total conditional variance*.

Capacity of a Density

- Measure the 'capacity of a density'.
- Determinant of covariance represents 'volume' of density.
- log determinant is entropy: sum of *log* eigenvalues of covariance.
- trace of covariance is total variance: sum of eigenvalues of covariance.
- $\lambda > \log \lambda$ then total conditional variance upper bounds entropy.

Alternative View

Exponentiated total variance bounds determinant.

$$|\mathbf{Q}| < \exp \operatorname{tr}(\mathbf{Q})$$

Because

$$\prod_{i=1}^{k} \lambda_i < \prod_{i=1}^{k} \exp(\lambda_i)$$

where $\{\lambda_i\}_{i=1}^{k}$ are the *positive* eigenvalues of $\mathbf{Q}$ This in turn implies

$$|\mathbf{Q}| < \prod_{i=1}^{k} \exp(q_{i,i})$$

Communication Channel

- Conditional density $p(\mathbf{f}|\mathbf{u})$ can be seen as a *communication channel*.
- Normally we have:

$$\text{Transmitter} \xrightarrow{\mathbf{u}} \underset{\text{Channel}}{p(\mathbf{f}|\mathbf{u})} \xrightarrow{\mathbf{f}} \text{Receiver}$$

  and we control $p(\mathbf{u})$ (the source density).
- *Here* we can also control the transmission channel $p(\mathbf{f}|\mathbf{u})$.

Lower Bound on Likelihood

Substitute variational bound into marginal likelihood:

$$p(\mathbf{y}) \geq \prod_{i=1}^{n} c_i \int \mathcal{N}\left(\mathbf{y}|\left\langle \mathbf{f} \right\rangle, \sigma^2\mathbf{I}\right) p(\mathbf{u}) \mathrm{d}\mathbf{u}$$

Note that:

$$\left\langle \mathbf{f} \right\rangle_{p(\mathbf{f}|\mathbf{u})} = \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}$$

is *linearly* dependent on $\mathbf{u}$.

Deterministic Training Conditional

Making the marginalization of $\mathbf{u}$ straightforward. In the Gaussian case:

$$p(\mathbf{u}) = \mathcal{N}\left(\mathbf{u}|\mathbf{0}, \mathbf{K}_{\mathbf{u},\mathbf{u}}\right)$$

$$\int p(\mathbf{y}|\mathbf{u})p(\mathbf{u})\mathrm{d}\mathbf{u} \geq \prod_{i=1}^{n} c_i \int \mathcal{N}\left(\mathbf{y}|\mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}, \sigma^2\right)\mathcal{N}\left(\mathbf{u}|\mathbf{0}, \mathbf{K}_{\mathbf{u},\mathbf{u}}\right)\mathrm{d}\mathbf{u}$$

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Maximize log of the bound to find covariance function parameters,

$$L \geq \sum_{i=1}^{n} \log c_i + \log \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \sigma^2\mathbf{I} + \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{u},\mathbf{f},}\right)$$

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Deterministic Training Conditional

Making the marginalization of $\mathbf{u}$ straightforward. In the Gaussian case:

$$p(\mathbf{u}) = \mathcal{N}\left(\mathbf{u}|\mathbf{0}, \mathbf{K}_{\mathbf{u},\mathbf{u}}\right)$$

$$\int p(\mathbf{y}|\mathbf{u})p(\mathbf{u})\mathrm{d}\mathbf{u} \geq \prod_{i=1}^{n} c_i \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \sigma^2\mathbf{I} + \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{u},\mathbf{f}}\right)$$

Maximize log of the bound to find covariance function parameters,

$$L \approx \log \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \sigma^2\mathbf{I} + \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{u},\mathbf{f},}\right)$$

- If the bound is normalized, the c_i terms are removed.

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Maximize log of the bound to find covariance function parameters,

- If the bound is normalized, the c_i terms are removed.
- This results in the projected process approximation (Rasmussen and Williams, 2006) or DTC (Quiñonero Candela and Rasmussen, 2005). Proposed by (Smola and Bartlett, 2001; Seeger et al., 2003; Csató and Opper, 2002; Csató, 2002).

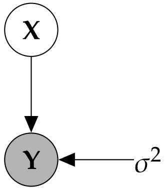
Selecting Data Dimensionality

- GP-LVM Provides probabilistic non-linear dimensionality reduction.
- How to select the dimensionality?
- Need to estimate marginal likelihood.
- In standard GP-LVM it increases with increasing q.

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.

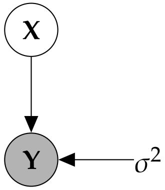


$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over *latent space*, **X**.



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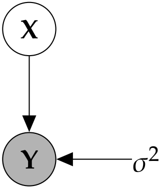


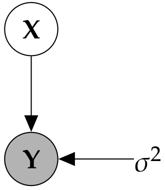
$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \alpha_i^{-2}\mathbf{I}\right)$$

Integrate Mapping Function and Latent Variables

Bayesian GP-LVM

- Start with a standard GP-LVM.
- Apply standard latent variable approach:
  - Define Gaussian prior over *latent space*, $\mathbf{X}$.
  - Integrate out *latent variables*.
  - Unfortunately integration is intractable.



$$p(\mathbf{Y}|\mathbf{X}) = \prod_{j=1}^{p} \mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0}, \mathbf{K}\right)$$

$$p(\mathbf{X}) = \prod_{j=1}^{q} \mathcal{N}\left(\mathbf{x}_{:,j}|\mathbf{0}, \alpha_i^{-2}\mathbf{I}\right)$$

$$p(\mathbf{Y}|\boldsymbol{\alpha}) = ??$$

Standard Variational Approach Fails

- Standard variational bound has the form:

$$\mathcal{L} = \left\langle \log p(\mathbf{y}|\mathbf{X}) \right\rangle_{q(\mathbf{X})} + \mathrm{KL}\left(q(\mathbf{X}) \,\|\, p(\mathbf{X}) \right)$$

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- Requires expectation of $\log p(\mathbf{y}|\mathbf{X})$ under $q(\mathbf{X})$.

$$\log p(\mathbf{y}|\mathbf{X}) = -\frac{1}{2}\mathbf{y}^\top \left(\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}\right)^{-1} \mathbf{y} - \frac{1}{2}\log\left|\mathbf{K}_{\mathbf{f},\mathbf{f}} + \sigma^2\mathbf{I}\right| - \frac{n}{2}\log 2\pi$$

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- Extremely difficult to compute because $\mathbf{K}_{\mathbf{f},\mathbf{f}}$ is dependent on $\mathbf{X}$ and appears in the inverse.

Variational Bayesian GP-LVM

- Consider collapsed variational bound,

$$p(\mathbf{y}) \geq \prod_{i=1}^{n} c_i \int \mathcal{N}\left(\mathbf{y}|\left\langle \mathbf{f} \right\rangle, \sigma^2\mathbf{I}\right) p(\mathbf{u}) \mathrm{d}\mathbf{u}$$

Variational Bayesian GP-LVM

- Consider collapsed variational bound,

$$p(\mathbf{y}|\mathbf{X}) \geq \prod_{i=1}^{n} c_i \int \mathcal{N}\left(\mathbf{y}|\left\langle \mathbf{f} \right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2\mathbf{I}\right) p(\mathbf{u}) \mathrm{d}\mathbf{u}$$

Variational Bayesian GP-LVM

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Variational Bayesian GP-LVM

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- Apply variational lower bound to the inner integral.

Variational Bayesian GP-LVM

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- Apply variational lower bound to the inner integral.

$$\int \prod_{i=1}^{n} c_i \mathcal{N}\left(\mathbf{y}|\left\langle \mathbf{f} \right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2\mathbf{I}\right) p(\mathbf{X})\mathrm{d}\mathbf{X}$$

$$\geq \left\langle \sum_{i=1}^{n} \log c_i \right\rangle_{q(\mathbf{X})} + \left\langle \log \mathcal{N}\left(\mathbf{y}|\left\langle \mathbf{f} \right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2\mathbf{I}\right) \right\rangle_{q(\mathbf{X})} + \mathrm{KL}\left(q(\mathbf{X}) \,\|\, p(\mathbf{X})\right)$$

Variational Bayesian GP-LVM

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$$\int p(\mathbf{y}|\mathbf{X})p(\mathbf{X})\mathrm{d}\mathbf{X} \geq \int \prod_{i=1}^{n} c_i \mathcal{N}\left(\mathbf{y}|\left\langle\mathbf{f}\right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2\mathbf{I}\right) p(\mathbf{X})\mathrm{d}\mathbf{X}p(\mathbf{u})\mathrm{d}\mathbf{u}$$

- Apply variational lower bound to the inner integral.

$$\begin{aligned}\int \prod_{i=1}^{n} c_i \mathcal{N}\left(\mathbf{y}|\left\langle\mathbf{f}\right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2\mathbf{I}\right)p(\mathbf{X})\mathrm{d}\mathbf{X} \\ &\geq \left\langle \sum_{i=1}^{n} \log c_i \right\rangle_{q(\mathbf{X})} \\ &\quad + \left\langle \log \mathcal{N}\left(\mathbf{y}|\left\langle\mathbf{f}\right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X})}, \sigma^2\mathbf{I}\right)\right\rangle_{q(\mathbf{X})} \\ &\quad + \mathrm{KL}\left(q(\mathbf{X}) \,\|\, p(\mathbf{X})\right)\end{aligned}$$

- Which is analytically tractable for Gaussian $q(\mathbf{X})$ and some covariance functions.

Required Expectations

- Need expectations under $q(\mathbf{X})$ of:

$$\log c_i = \frac{1}{2\sigma^2}\left[k_{i,i} - \mathbf{k}_{i,\mathbf{u}}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{k}_{i,\mathbf{u}}\right]$$

and

$$\log \mathcal{N}\left(\mathbf{y}|\left\langle \mathbf{f}\right\rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{Y})}, \sigma^2\mathbf{I}\right) = -\frac{1}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\left(y_i - \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\right)^2$$

- This requires the expectations

$$\left\langle \mathbf{K}_{\mathbf{f},\mathbf{u}}\right\rangle_{q(\mathbf{X})}$$

and

$$\left\langle \mathbf{K}_{\mathbf{f},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{u},\mathbf{f}}\right\rangle_{q(\mathbf{X})}$$

which can be computed analytically for some covariance functions.

Variational Compression

(Damianou and Lawrence, 2013)

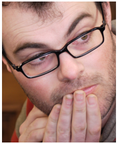
- Augment each layer with inducing variables $\mathbf{u}_i$.
- Apply variational compression,

$$p(\mathbf{y}, \{\mathbf{f}_i\}_{i=1}^{\ell-1}|\{\mathbf{u}_i\}_{i=1}^{\ell}, \mathbf{X}) \geq \tilde{p}(\mathbf{y}|\mathbf{u}_\ell, \mathbf{f}_{\ell-1}) \prod_{i=2}^{\ell-1} \tilde{p}(\mathbf{f}_i|\mathbf{u}_i, \mathbf{f}_{i-1}) \tilde{p}(\mathbf{f}_1|\mathbf{u}_i, \mathbf{X})$$
$$\times \exp\left(\sum_{i=1}^{\ell} -\frac{1}{2\sigma_i^2} \text{tr}\left(\boldsymbol{\Sigma}_i\right)\right) \quad (1)$$

where

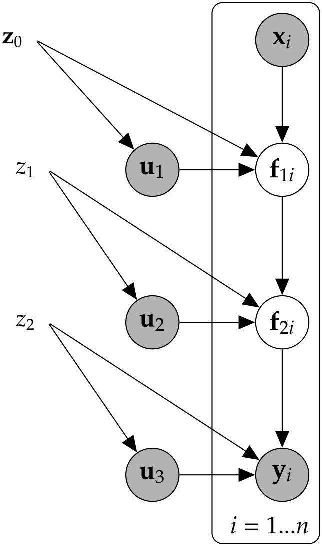
$$\tilde{p}(\mathbf{f}_i|\mathbf{u}_i, \mathbf{f}_{i-1}) = \mathcal{N}\left(\mathbf{f}_i|\mathbf{K}_{\mathbf{f}_i\mathbf{u}_i}\mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1}\mathbf{u}_i, \sigma_i^2\mathbf{I}\right).$$

Nested Variational Compression



(Hensman and Lawrence, 2014)

- By sustaining explicity distributions over inducing variables James Hensman has developed a nested variatnt of variational compression.
- Exciting thing: it mathematically looks like a deep neural network, but with inducing variables in the place of basis functions.
- Additional complexity control term in the objective function.



$\mathbf{z}_0$
z_1
z_2
$\mathbf{u}_1$
$\mathbf{u}_2$
$\mathbf{u}_3$
$\mathbf{x}_i$
$\mathbf{f}_{1i}$
$\mathbf{f}_{2i}$
$\mathbf{y}_i$
$i = 1...n$

Nested Bound

$$
\begin{aligned}
\log p(\mathbf{y}|\mathbf{X}) \geq &- \frac{1}{\sigma_1^2}\mathrm{tr}\left(\boldsymbol{\Sigma}_1\right) - \sum_{i=2}^{\ell} \frac{1}{2\sigma_i^2}\left(\psi_i - \mathrm{tr}\left(\boldsymbol{\Phi}_i \mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1}\right)\right) \\
&- \sum_{i=1}^{\ell} \mathrm{KL}\left(q(\mathbf{u}_i) \,\|\, p(\mathbf{u}_i)\right) \\
&- \sum_{i=2}^{\ell} \frac{1}{2\sigma_i^2}\mathrm{tr}\left((\boldsymbol{\Phi}_i - \boldsymbol{\Psi}_i^\top \boldsymbol{\Psi}_i)\mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1} \left\langle \mathbf{u}_i\mathbf{u}_i^\top \right\rangle_{q(\mathbf{u}_i)} \mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1}\right) \\
&+ \log \mathcal{N}\left(\mathbf{y}|\boldsymbol{\Psi}_\ell \mathbf{K}_{\mathbf{u}_\ell\mathbf{u}_\ell}^{-1}\mathbf{m}_\ell, \sigma_\ell^2 \mathbf{I}\right) \qquad (2)
\end{aligned}
$$

Nested Bound

$$
\begin{aligned}
\log p(\mathbf{y}|\mathbf{X}) \geq & -\frac{1}{\sigma_1^2}\mathrm{tr}\left(\boldsymbol{\Sigma}_1\right) - \sum_{i=2}^{\ell}\frac{1}{2\sigma_i^2}\left(\psi_i - \mathrm{tr}\left(\boldsymbol{\Phi}_i\mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1}\right)\right) \\
& - \sum_{i=1}^{\ell}\mathrm{KL}\left(q(\mathbf{u}_i)\,\|\,p(\mathbf{u}_i)\right) \\
& - \sum_{i=2}^{\ell}\frac{1}{2\sigma_i^2}\mathrm{tr}\left((\boldsymbol{\Phi}_i - \boldsymbol{\Psi}_i^\top\boldsymbol{\Psi}_i)\mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1}\left\langle\mathbf{u}_i\mathbf{u}_i^\top\right\rangle_{q(\mathbf{u}_i)}\mathbf{K}_{\mathbf{u}_i\mathbf{u}_i}^{-1}\right) \\
& + \log\mathcal{N}\left(\mathbf{y}|\boldsymbol{\Psi}_\ell\mathbf{K}_{\mathbf{u}_\ell\mathbf{u}_\ell}^{-1}\mathbf{m}_\ell, \sigma_\ell^2\mathbf{I}\right) \qquad (2)
\end{aligned}
$$

Required Expectations

$$\log \mathcal{N}\left(\mathbf{y}|\boldsymbol{\Psi}_\ell \mathbf{K}_{\mathbf{u}_\ell \mathbf{u}_\ell}^{-1} \mathbf{m}_\ell, \sigma_\ell^2 \mathbf{I}\right)$$

where

Required Expectations

$$\log \mathcal{N}\left(\mathbf{y}|\boldsymbol{\Psi}_\ell \mathbf{K}_{\mathbf{u}_\ell\mathbf{u}_\ell}^{-1}\mathbf{m}_\ell, \sigma_\ell^2\mathbf{I}\right)$$

where

$$\boldsymbol{\Psi}_i = \left\langle \mathbf{K}_{\mathbf{f}_i\mathbf{u}_i} \right\rangle_{q(\mathbf{f}_{i-1})}$$

where elements of $\mathbf{K}_{\mathbf{f}_i\mathbf{u}_i}$ are

$$k_{f_i u_i'}(\mathbf{f}_{i-1}, \mathbf{z}_i')$$

Required Expectations

$$\log \mathcal{N}\left(\mathbf{y}|\boldsymbol{\Psi}_\ell \mathbf{K}_{\mathbf{u}_\ell \mathbf{u}_\ell}^{-1}\mathbf{m}_\ell, \sigma_\ell^2 \mathbf{I}\right)$$

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$$\boldsymbol{\Psi}_i = \left\langle \mathbf{K}_{\mathbf{f}_i \mathbf{u}_i} \right\rangle_{q(\mathbf{f}_{i-1})}$$

where elements of $\mathbf{K}_{\mathbf{f}_i \mathbf{u}_i}$ are

$$k_{f_i u_i'}(\mathbf{f}_{i-1}, \mathbf{z}_i')$$

And

$$q(\mathbf{f}_1) = \int \tilde{p}(\mathbf{f}_1|\mathbf{u}_1, \mathbf{X}) q(\mathbf{u}_1) \mathrm{d}\mathbf{u}_1,$$

$$q(\mathbf{f}_i) = \int \tilde{p}(\mathbf{f}_i|\mathbf{u}_i, \mathbf{f}_{i-1}) q(\mathbf{u}_i) q(\mathbf{f}_{i-1}) \mathrm{d}\mathbf{u}_i \mathrm{d}\mathbf{f}_i,$$

Required Expectations

$$\log \mathcal{N}\left(\mathbf{y}|\boldsymbol{\Psi}_\ell \mathbf{K}_{\mathbf{u}_\ell \mathbf{u}_\ell}^{-1}\mathbf{m}_\ell, \sigma_\ell^2 \mathbf{I}\right)$$

where

$$\boldsymbol{\Psi}_i = \left\langle \mathbf{K}_{\mathbf{f}_i \mathbf{u}_i} \right\rangle_{q(\mathbf{f}_{i-1})}$$

where elements of $\mathbf{K}_{\mathbf{f}_i \mathbf{u}_i}$ are

$$k_{f_i u_i'}(\mathbf{f}_{i-1}, \mathbf{z}_i')$$

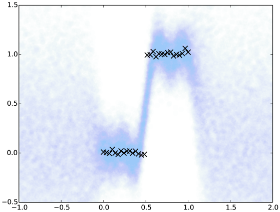
And

$$q(\mathbf{f}_1) = \int \tilde{p}(\mathbf{f}_1|\mathbf{u}_1, \mathbf{X})q(\mathbf{u}_1)\mathrm{d}\mathbf{u}_1,$$

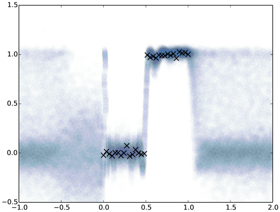
$$q(\mathbf{f}_i) = \int \tilde{p}(\mathbf{f}_i|\mathbf{u}_i, \mathbf{f}_{i-1})q(\mathbf{u}_i)q(\mathbf{f}_{i-1})\mathrm{d}\mathbf{u}_i\mathrm{d}\mathbf{f}_i,$$

cf wake sleep algorithm. recognition network and generation network (Hinton et al., 1995).

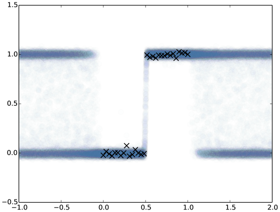
Derivative Tails Increase with Layers: Step Function



(a) GP

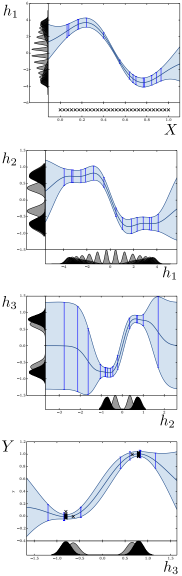


(b) 2 layers

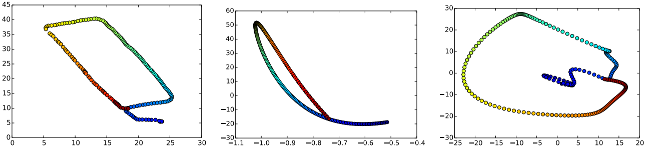


(c) 4 layers

Values in Hidden Layers



Loop Detection in Robotics



(d) True path (e) Hidden layer 1 (f) Hidden layer 2

- Dynamically constrained model
- Correctly detects the loop
- Learns temporal continuity and corner-like features in different layers

Data fit for Loop Closure

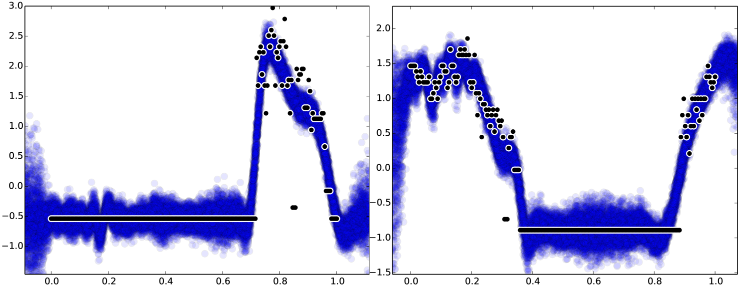
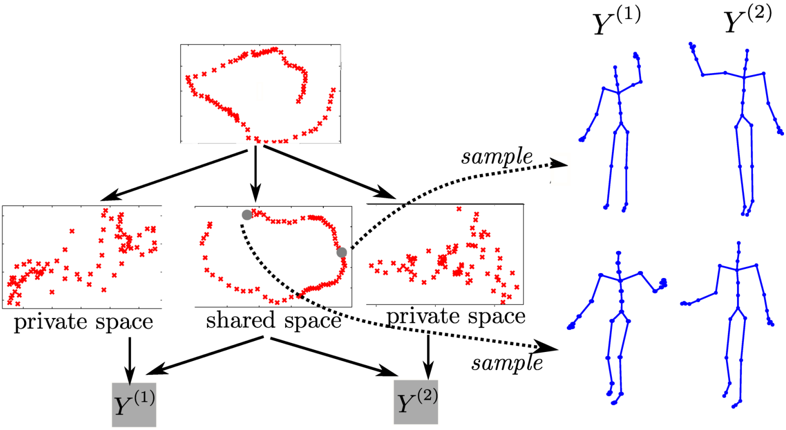


Figure : Example data fits for 2 of the 30 output dimensions

Motion Capture

- ‘High five’ data.
- Model learns structure between two interacting subjects.

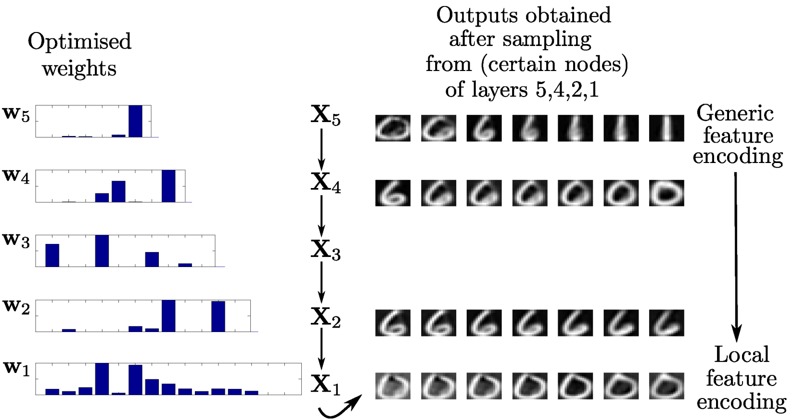
Deep hierarchies – motion capture



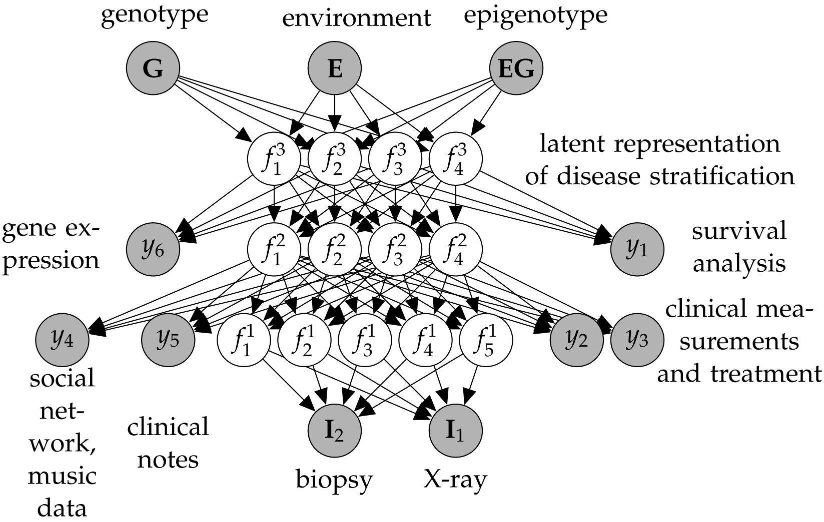
Digits Data Set

- Are deep hierarchies justified for small data sets?
- We can lower bound the evidence for different depths.
- For 150 6s, 0s and 1s from MNIST we found at least 5 layers are required.

Deep hierarchies – MNIST



Deep Health



genotype
environment
epigenotype
G
E
EG
f_1^3 f_2^3 f_3^3 f_4^3
latent representation of disease stratification
gene expression
y_6
f_1^2 f_2^2 f_3^2 f_4^2
y_1
survival analysis
clinical measurements and treatment
y_4 y_5
f_1^1 f_2^1 f_3^1 f_4^1 f_5^1
y_2 y_3
social network, music data
clinical notes
$\mathbf{I}_2$
$\mathbf{I}_1$
biopsy
X-ray

Summary

- Deep Gaussian Processes allow unsupervised and supervised deep learning.
- They can be easily adapted to handle multitask learning.
- Data dimensionality turns out to not be a computational bottleneck.
- Variational compression algorithms show promise for scaling these models to *massive* data sets.

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