Sparse Gaussian Process Approximations

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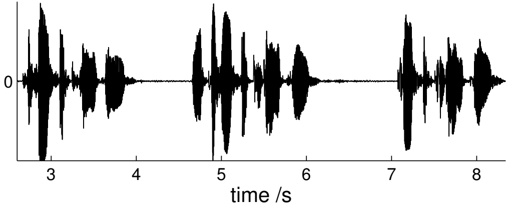
Computational and Biological Learning Lab, Department of Engineering, University of Cambridge

Motivating application 1: Audio modelling

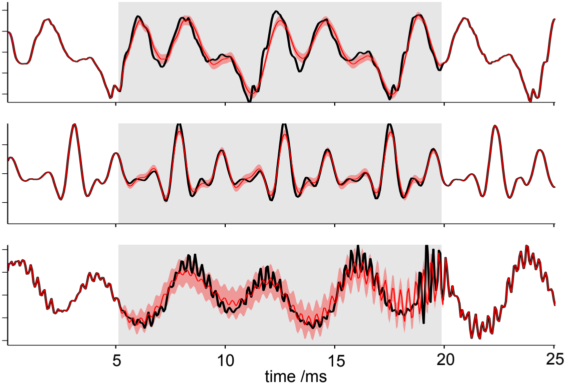
audio time-series data



$y(t)$

$T = 10^5$-10^7 datapoints

reconstruction using a GP model



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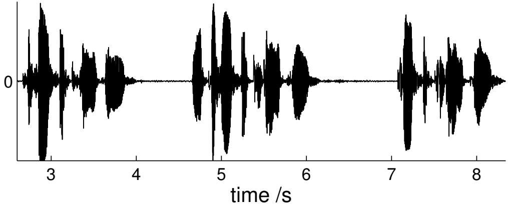

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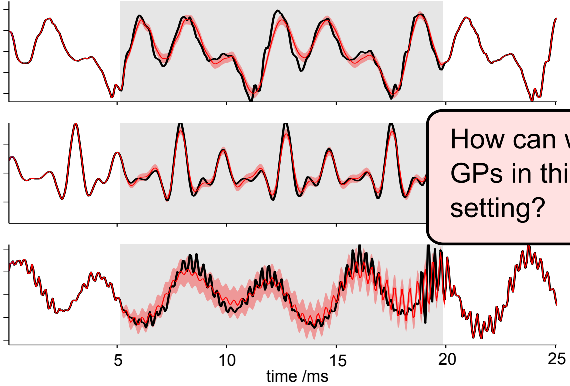
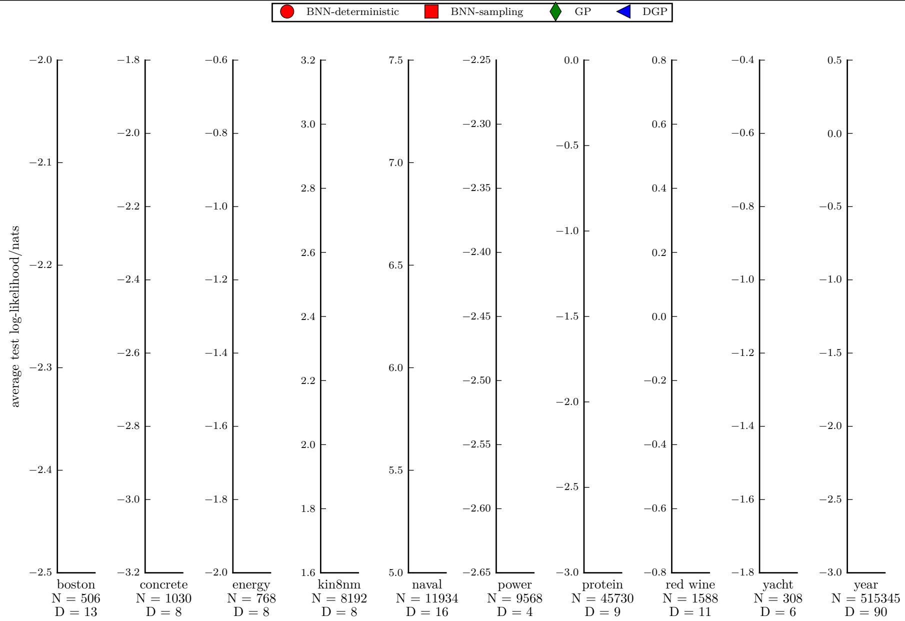
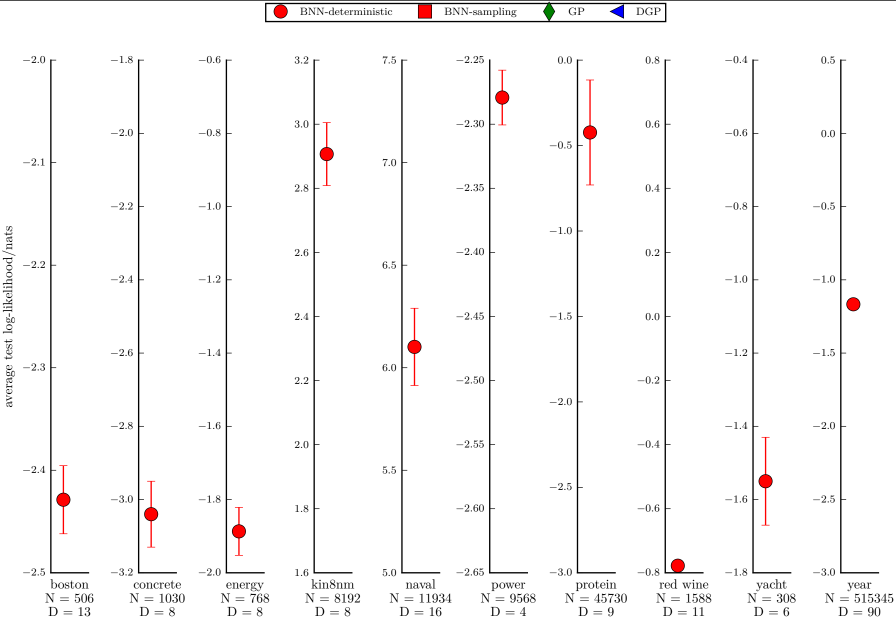


How can we use GPs in this setting?

Motivating application 2: non-linear regression



Motivating application 2: non-linear regression



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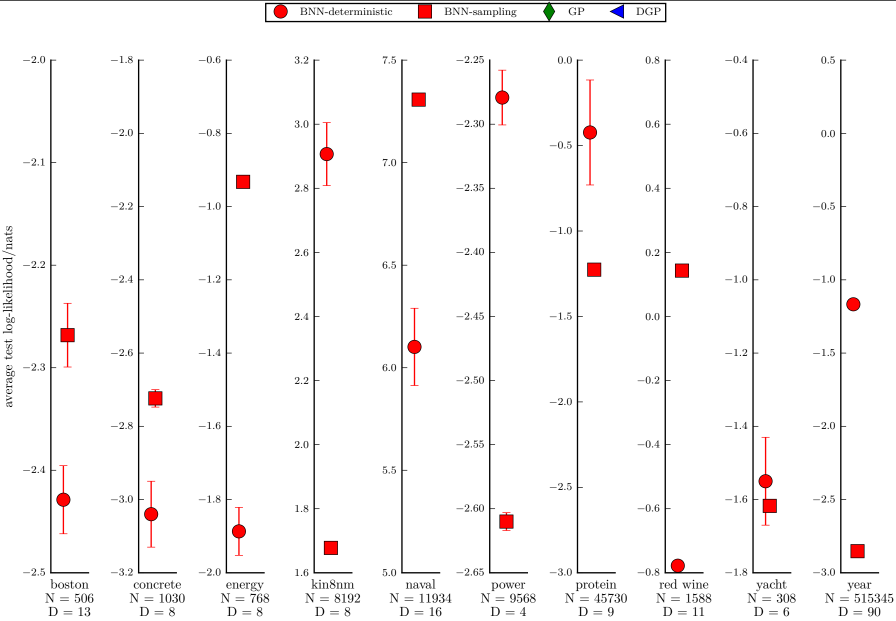

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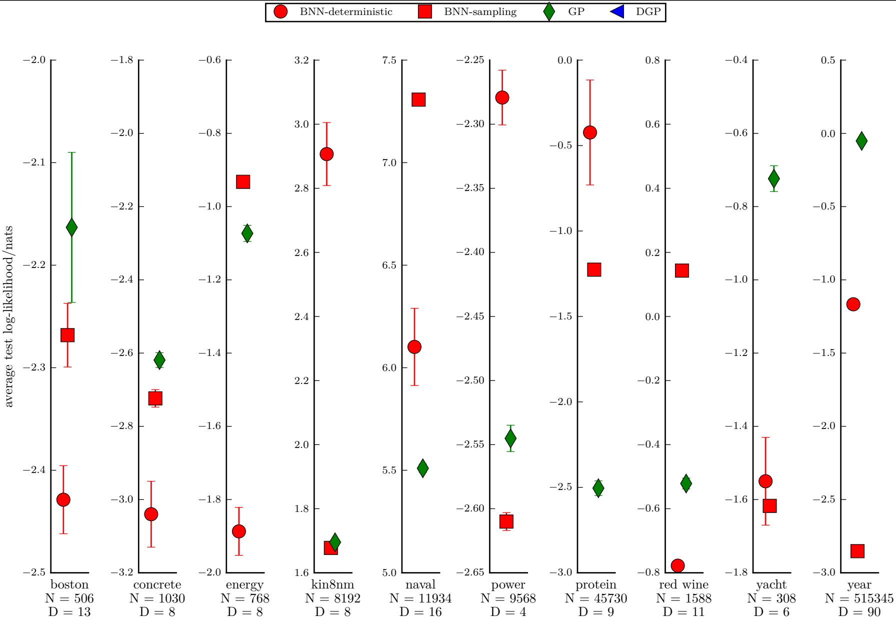

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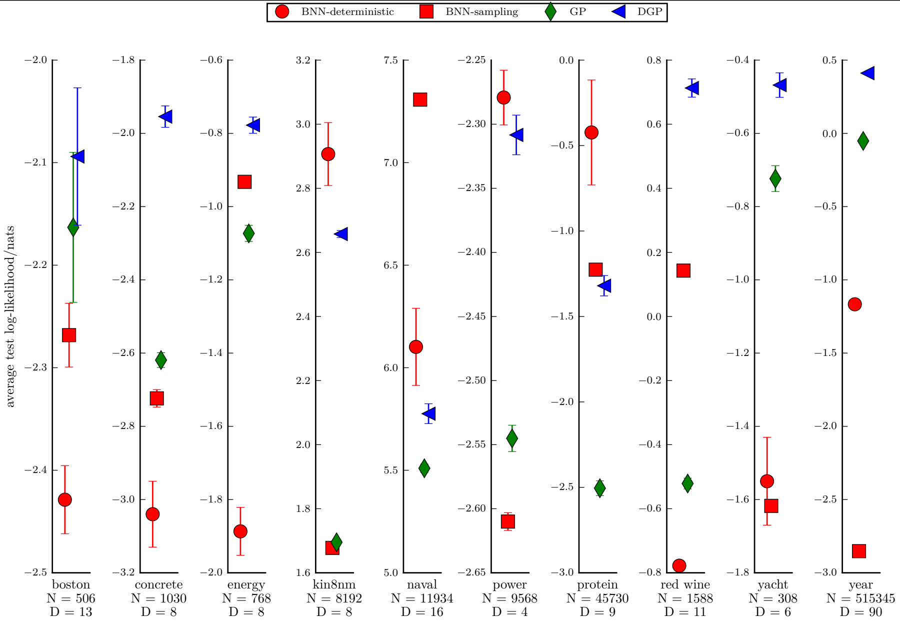
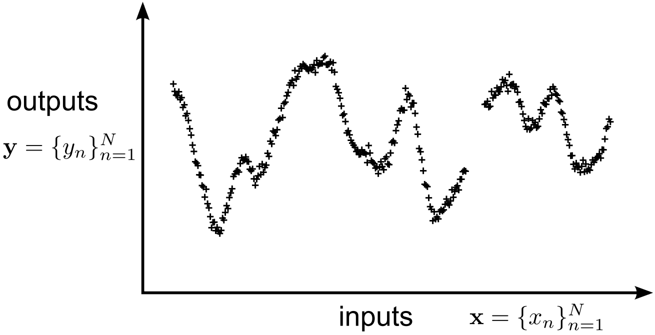


Motivation: Gaussian Process Regression



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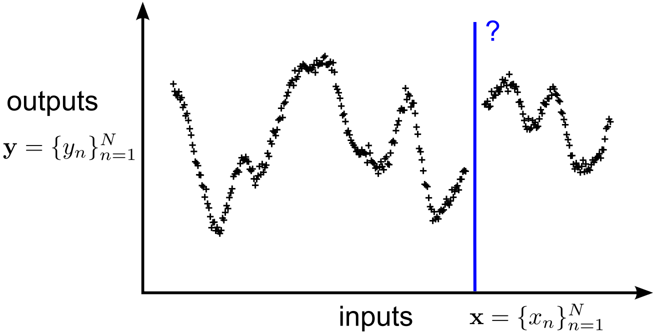

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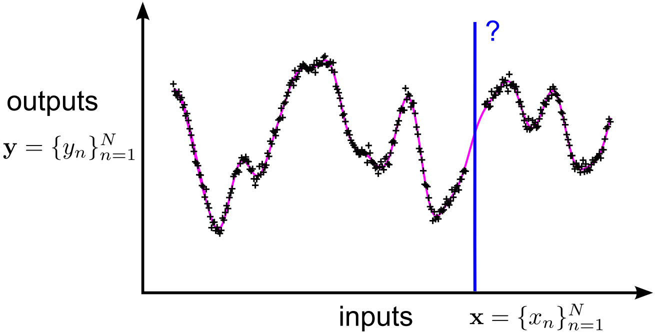
$$p(f|\theta) = \mathcal{GP}(f; 0, \mathrm{K}_\theta)$$

$$p(y_n|f, x_n, \theta)$$



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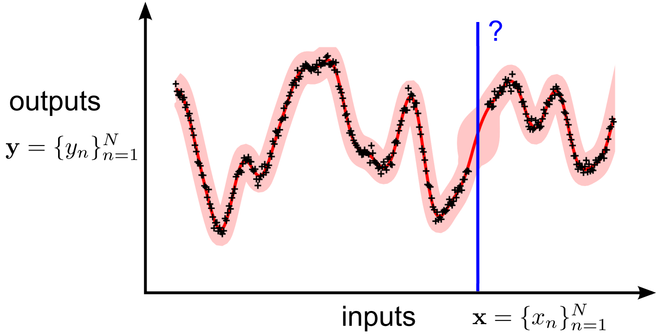
$$p(y_n|f, x_n, \theta) \xrightarrow{\text{inference \& learning}} p(\mathbf{y}|\mathbf{x}, \theta)$$



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intractabilities
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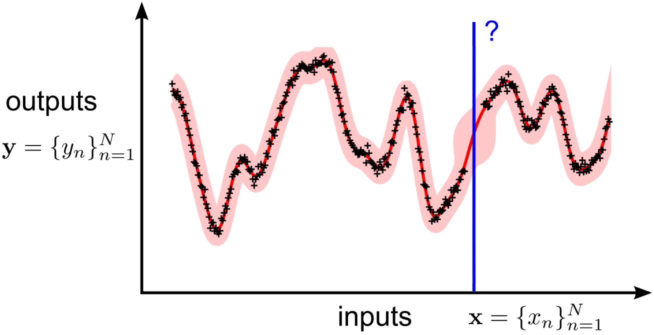

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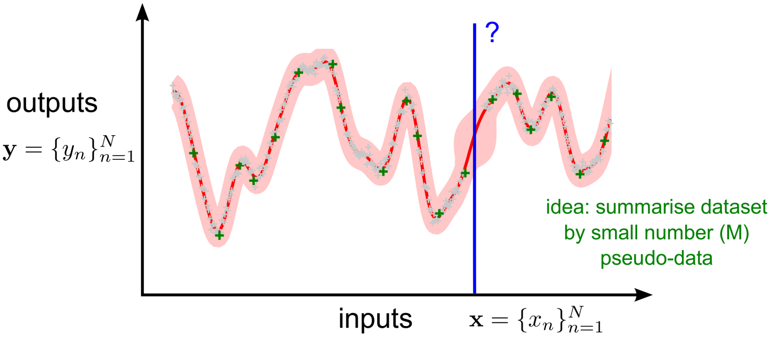

A Brief History of Gaussian Process Approximations

FITC: Snelson et al. “Sparse Gaussian Processes using Pseudo-inputs”
PITC: Snelson et al. “Local and global sparse Gaussian process approximations”
EP: Csato and Opper 2002 / Qi et al. "Sparse-posterior Gaussian Processes for general likelihoods.”
VFE: Titsias “Variational Learning of Inducing Variables in Sparse Gaussian Processes”
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approximate generative model
exact inference

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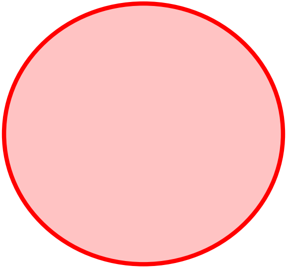

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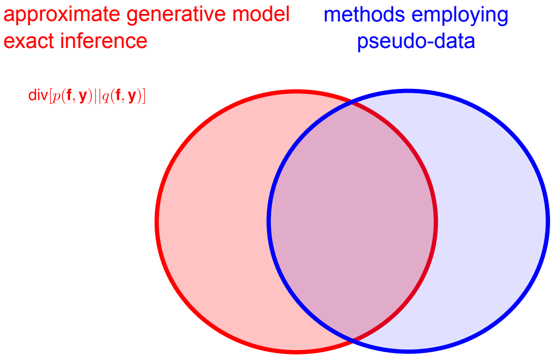

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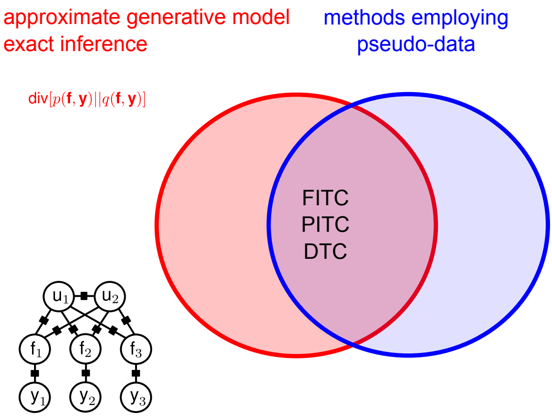

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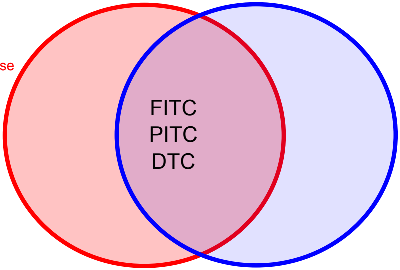
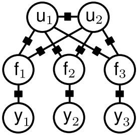
A Unifying View of Sparse Approximate Gaussian Process Regression Quinonero-Candela & Rasmussen, 2005 (FITC, PITC, DTC)





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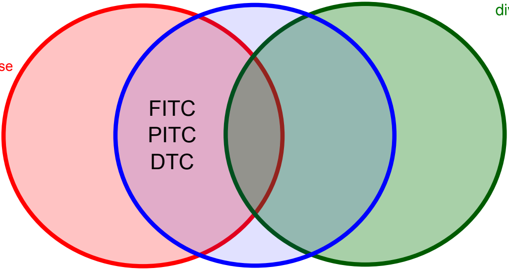

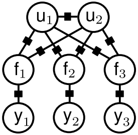

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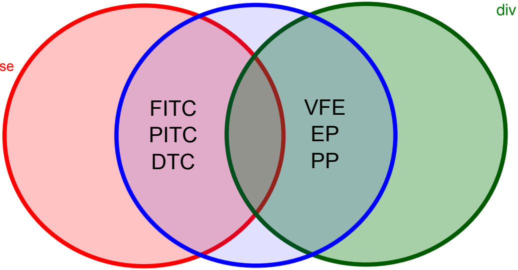

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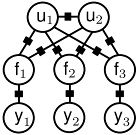

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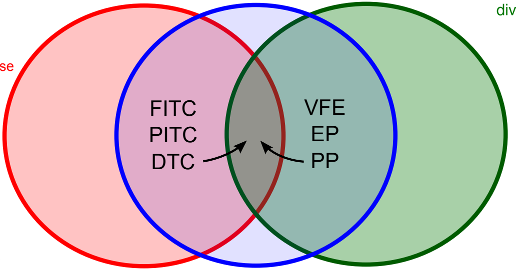

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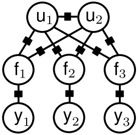

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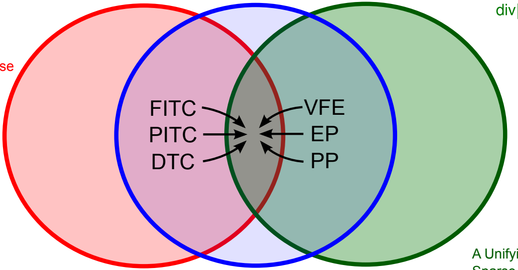

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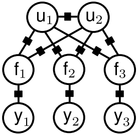

A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation
Bui, Yan and Turner, 2016
(VFE, EP, FITC, PITC ...)

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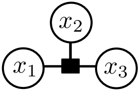
Factor Graphs: introduction / reminder

factor graph examples

$$p(x_1, x_2, x_3) = g(x_1, x_2, x_3)$$



$$p(x_1, x_2, x_3) = g_1(x_1, x_2) g_2(x_2, x_3)$$

$x_3 \perp x_1 | x_2$

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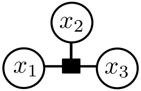

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$x_3 \perp x_1 | x_2$

what is the minimal factor graph for this multivariate Gaussian?

$$p(\mathbf{x}|\mu, \Sigma) = \mathcal{N}(\mathbf{x}; \mu, \Sigma)$$ 4 dimensional

$$\Sigma = \begin{bmatrix} 1 & 1/2 & 1/2 & 1/4 \\ 1/2 & 5/4 & 1/4 & 1/8 \\ 1/2 & 1/4 & 5/4 & 5/8 \\ 1/4 & 1/8 & 5/8 & 21/16 \end{bmatrix} \quad \Sigma^{-1} = \begin{bmatrix} 1.5 & -1/2 & -1/2 & 0 \\ -1/2 & 1 & 0 & 0 \\ -1/2 & 0 & 5/4 & -1/2 \\ 0 & 0 & -1/2 & 1 \end{bmatrix}$$

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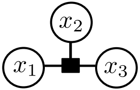

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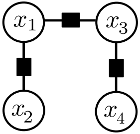
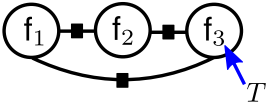
solution:



Fully independent training conditional (FITC) approximation

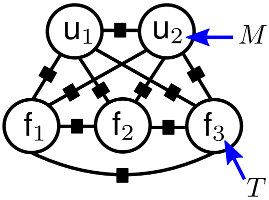


construct new generative model (with pseudo-data)
cheaper to perform exact learning and inference
calibrated to original

Fully independent training conditional (FITC) approximation

1. augment model with M<T pseudo data

$$p(\mathbf{f},\mathbf{u}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix}; \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \mathsf{K}_{\mathbf{ff}} & \mathsf{K}_{\mathbf{fu}} \\ \mathsf{K}_{\mathbf{uf}} & \mathsf{K}_{\mathbf{uu}} \end{bmatrix}\right)$$



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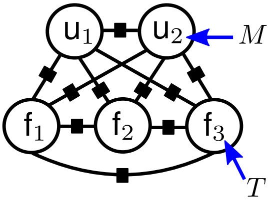

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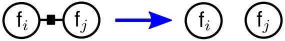
2. remove some of the dependencies
   (results in simpler model)



all factors

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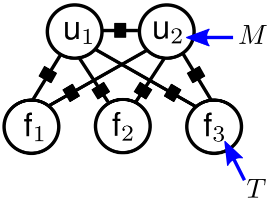

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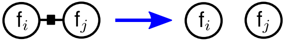

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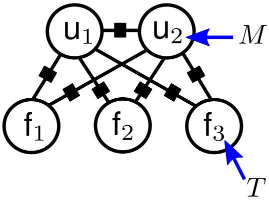

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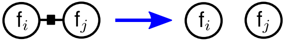

all factors

3. calibrate model
   (e.g. using KL divergence, many choices)

$$\underset{q(\mathbf{u}),\{q(\mathsf{f}_t|\mathbf{u})\}_{t=1}^{T}}{\arg\min} \mathrm{KL}\left(p(\mathbf{f},\mathbf{u})\,||\,q(\mathbf{u})\prod_{t=1}^{T} q(\mathsf{f}_t|\mathbf{u})\right) \implies \begin{aligned} q(\mathbf{u}) &= p(\mathbf{u})\\ q(\mathsf{f}_t|\mathbf{u}) &= p(\mathsf{f}_t|\mathbf{u})\end{aligned}$$

equal to exact conditionals

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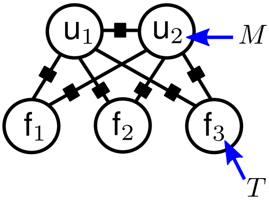
calibrated to original

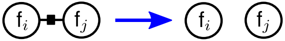
Fully independent training conditional (FITC) approximation

1. augment model with M<T pseudo data

$$p(\mathbf{f},\mathbf{u}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix}; \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \mathsf{K}_{\mathbf{ff}} & \mathsf{K}_{\mathbf{fu}} \\ \mathsf{K}_{\mathbf{uf}} & \mathsf{K}_{\mathbf{uu}} \end{bmatrix}\right)$$



2. remove some of the dependencies
   (results in simpler model)



all factors

3. calibrate model
   (e.g. using KL divergence, many choices)

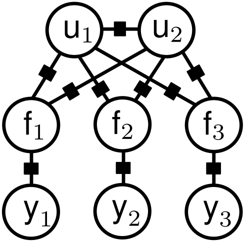
$$\underset{q(\mathbf{u}),\{q(\mathsf{f}_t|\mathbf{u})\}_{t=1}^{T}}{\arg\min} \mathrm{KL}\left(p(\mathbf{f},\mathbf{u})||q(\mathbf{u})\prod_{t=1}^{T} q(\mathsf{f}_t|\mathbf{u})\right) \implies \begin{array}{c} q(\mathbf{u}) = p(\mathbf{u}) \\ q(\mathsf{f}_t|\mathbf{u}) = p(\mathsf{f}_t|\mathbf{u}) \end{array}$$

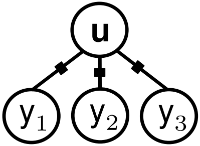
equal to exact conditionals

construct new generative model (with pseudo-data)
cheaper to perform exact learning and inference
calibrated to original

indirect posterior approximation

Fully independent training conditional (FITC) approximation





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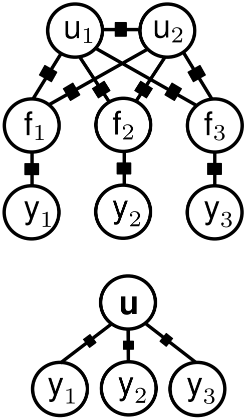

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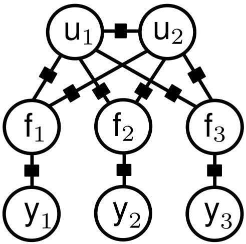

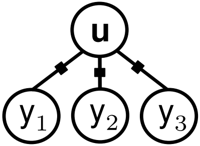

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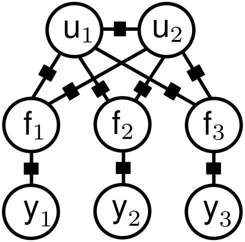
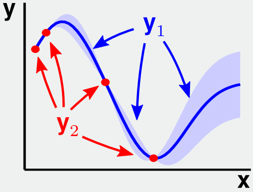
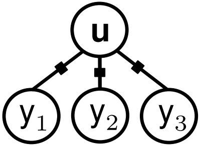


How do we make predictions?

$$p(\mathbf{y}_1|\mathbf{y}_2) = \mathcal{N}(\mathbf{y}_1; \Sigma_{12}\Sigma_{22}^{-1}\mathbf{y}_2, \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^{\intercal})$$





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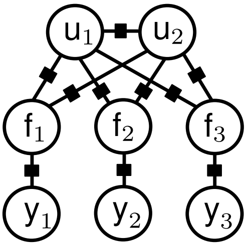

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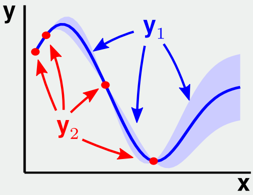

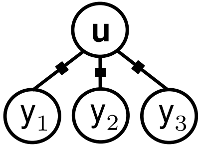

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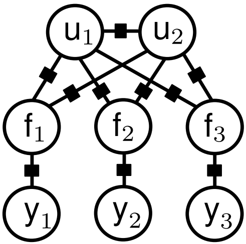

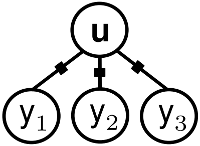

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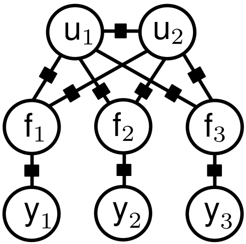

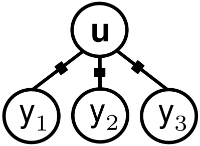

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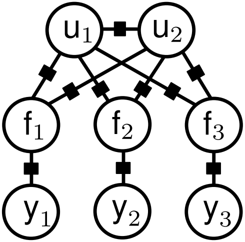

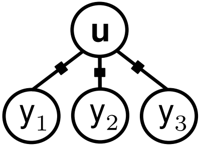

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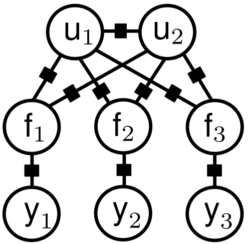
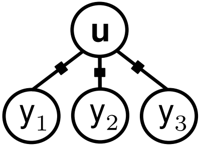
cost of computing likelihood is $\mathcal{O}(TM^2)$





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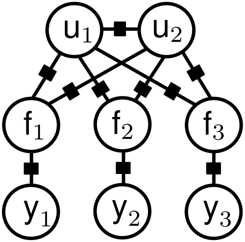

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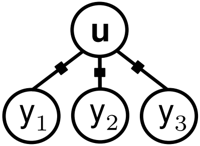

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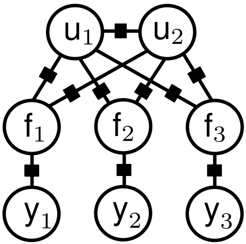

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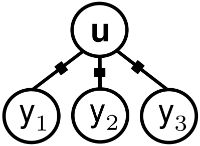

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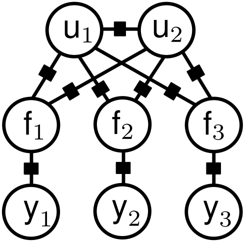

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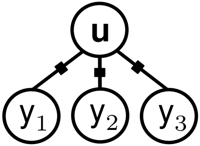

original variances along diagonal: stops variances collapsing

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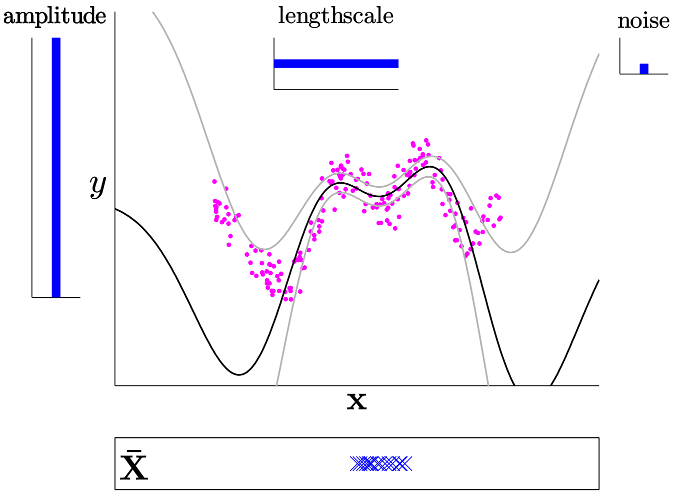
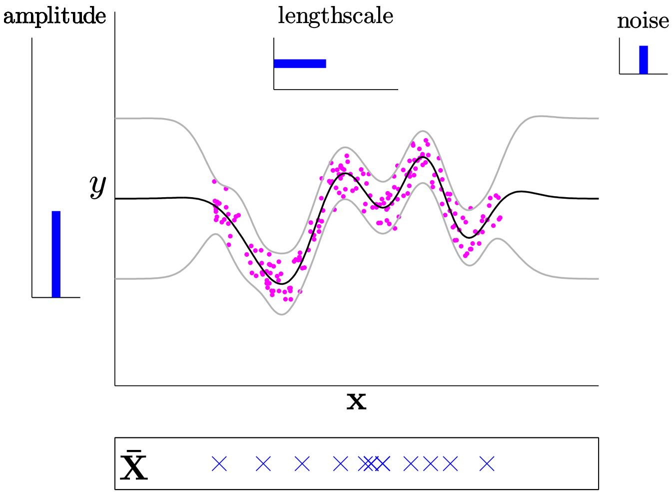
FITC: Demo (Snelson)



Initialize adversarially: amplitude and lengthscale too big
noise too small
pseudo-inputs bunched up

FITC: Demo (Snelson)



Pseudo-inputs and hyperparameters optimized

Fully independent training conditional (FITC) approximation

- parametric (although cleverly so)
- if I see more data, should I add extra pseudo-data?
  - unnatural from a generative modelling perspective
  - natural from a prediction perspective (posterior gets more complex)

$\Longrightarrow$ **lost elegant separation of model, inference and approximation**

- example of **prior approximation**

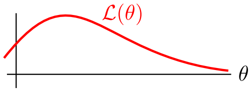
Extensions:

- inter-domain GP (pseudo-data in a different space)
- partially independent training conditional and tree-structured approximations

Variational free-energy method (VFE)

lower bound the likelihood

$$\color{red}{\mathcal{L}(\theta)} = \log p(\mathbf{y}|\theta) = \log \int \mathsf{d}f\ p(\mathbf{y}, f|\theta)$$



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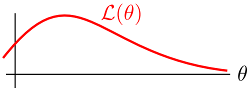

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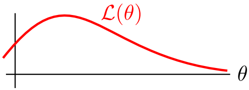

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$$= \log \int \mathsf{d}f\ p(\mathbf{y}, f|\theta) \frac{q(f)}{q(f)} \geq \int \mathsf{d}f\ q(f) \log \frac{p(\mathbf{y}, f|\theta)}{q(f)}$$

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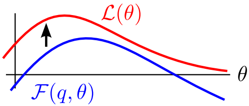

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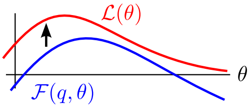

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$$\mathcal{F}(\theta) = \int \mathsf{d}f \; q(f) \log \frac{p(f|\mathbf{y}, \theta) p(\mathbf{y}|\theta)}{q(f)}$$

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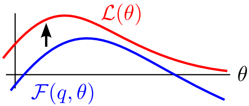

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$$\mathcal{F}(\theta) = \int \mathrm{d}f \; q(f) \log \frac{p(f|\mathbf{y},\theta)p(\mathbf{y}|\theta)}{q(f)} = \log p(\mathbf{y}|\theta) - \underbrace{\mathbf{KL}}_{\text{KL between stochastic processes}}(q(f)||p(f|\mathbf{y}))$$

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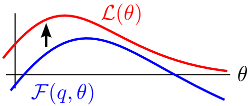

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assume approximate posterior factorisation with special form

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Variational free-energy method (VFE)

$$\mathcal{F}(\theta) \;=\; \log p(\mathbf{y}|\theta) - \mathbf{KL}(q(f)||p(f|\mathbf{y}))$$

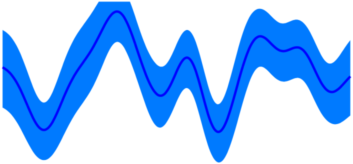
approximate posterior

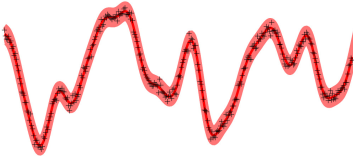
$$q(f) = p(f_{\neq \mathbf{u}}|\mathbf{u})q(\mathbf{u})$$

true posterior

$$p(f|\mathbf{y})$$

KL





Variational free-energy method (VFE)

$$\mathcal{F}(\theta) = \log p(\mathbf{y}|\theta) - \mathbf{KL}(q(f)||p(f|\mathbf{y}))$$

same form as prediction from GP-regression

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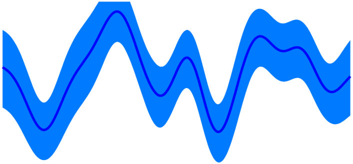

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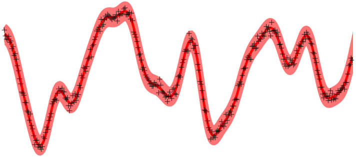

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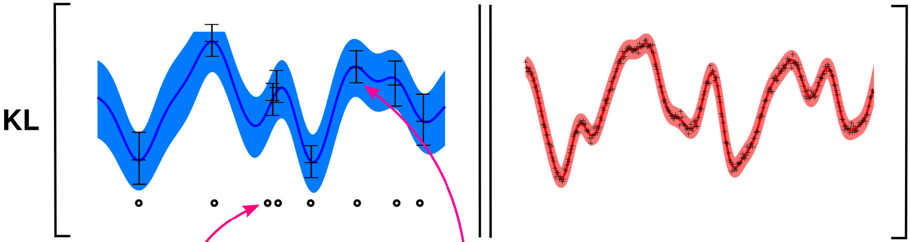


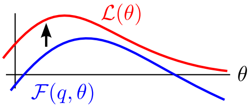
inputs locations of 'pseudo' data

output locations and covariance 'pseudo' data

optimise variational free-energy wrt to these variational parameters

Variational free-energy method (VFE)

lower bound the likelihood



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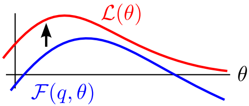

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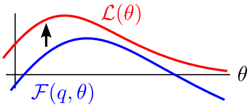

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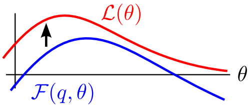

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Variational free-energy method (VFE)

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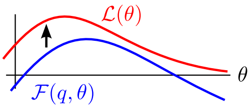

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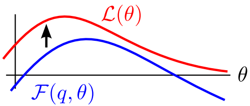

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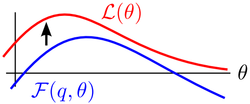
average of quadratic form

KL between two multivariate Gaussians

Variational free-energy method (VFE)

lower bound the likelihood



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Variational free-energy method (VFE)

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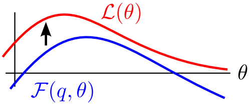

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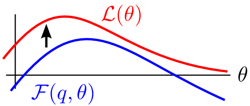
$q^*(\mathbf{u}) \propto p(\mathbf{u}) \mathcal{N}(\mathbf{y}; \mathsf{K}_{\mathsf{fu}} \mathsf{K}_{\mathsf{uu}}^{-1} \mathbf{u}, \sigma_{\mathsf{y}}^2 \mathsf{I})$ (DTC)

Variational free-energy method (VFE)

lower bound the likelihood



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$$\mathcal{F}(q^*,\theta) = \log \mathcal{N}(\mathbf{y}; \mathbf{0}, \mathsf{K}_{\mathsf{fu}}\mathsf{K}_{\mathsf{uu}}^{-1}\mathsf{K}_{\mathsf{uf}}, \sigma_{\mathsf{y}}^2\mathsf{I}) - \frac{1}{2\sigma_{\mathsf{y}}^2}\mathrm{trace}(\mathsf{K}_{\mathsf{ff}} - \mathsf{K}_{\mathsf{fu}}\mathsf{K}_{\mathsf{uu}}^{-1}\mathsf{K}_{\mathsf{uf}})$$

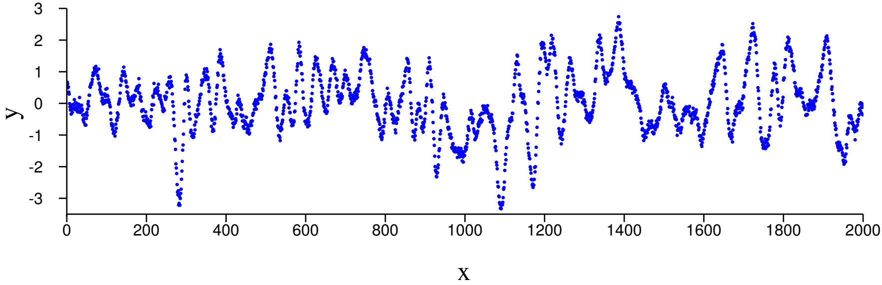
DTC like

uncertainty based correction

Summary of VFE method

- optimisation of pseudo point inputs: **VFE has better guarantees than FITC**
- variational methods known to **underfit** (and have other **biases**)
- **no augmentation required: target is posterior over functions, which includes inducing variables**
  - pseudo-input locations are pure variational parameters (do not parameterise the generative model like they do in FITC)
  - coherent way of adding pseudo-data: more complex posteriors require more computational resources (more pseudo-points)
- Rule of thumb:
  VFE returns better mean estimates
  FITC returns better error-bar estimates
- **how should we select M = number of pseudo-points?**

How do we select M = number of pseudo-data?



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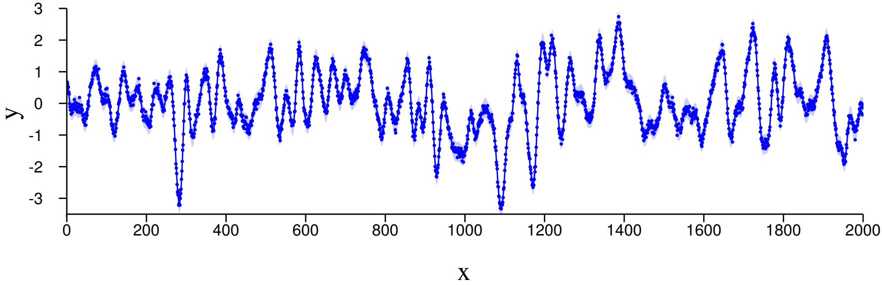

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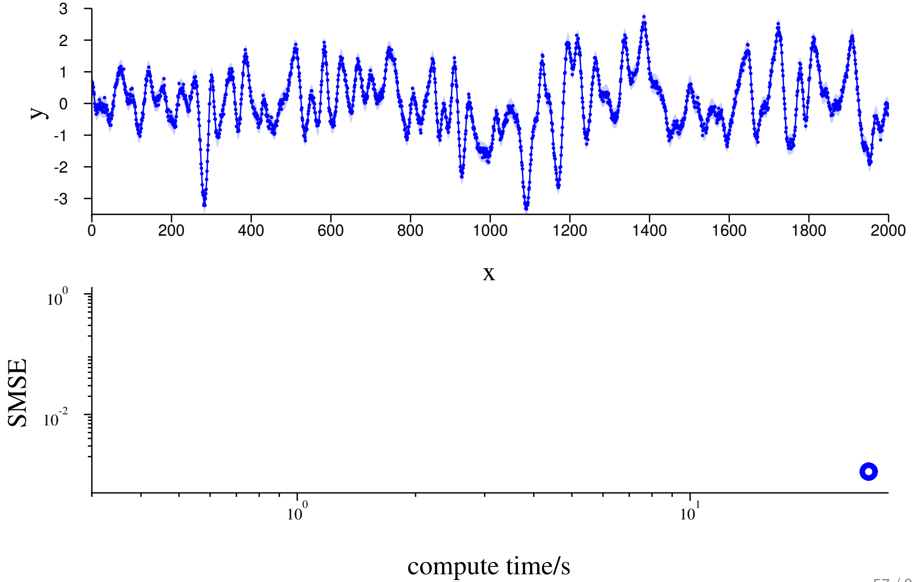

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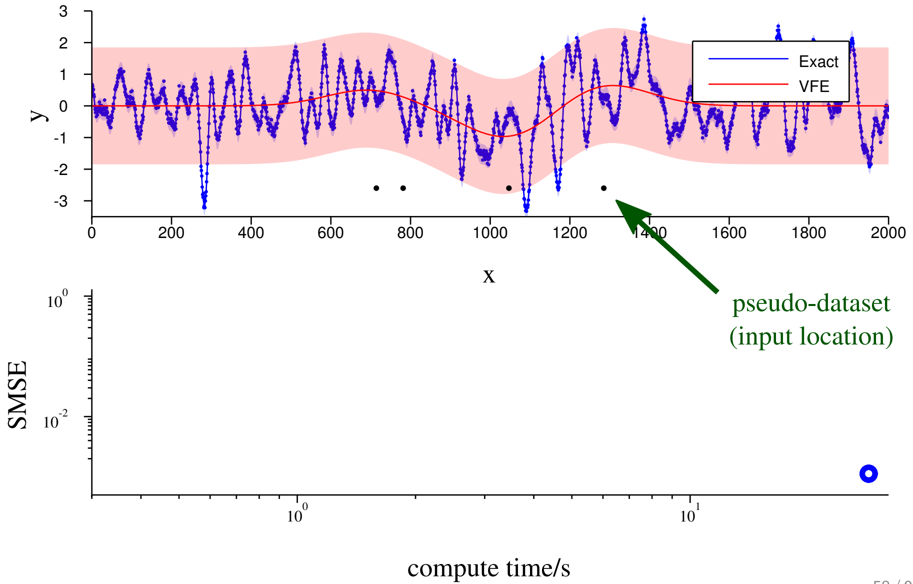

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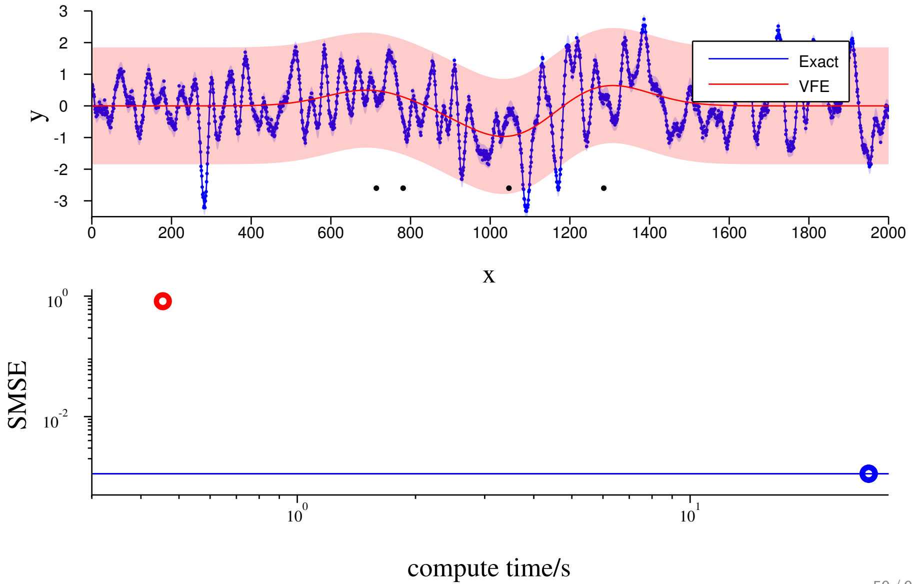

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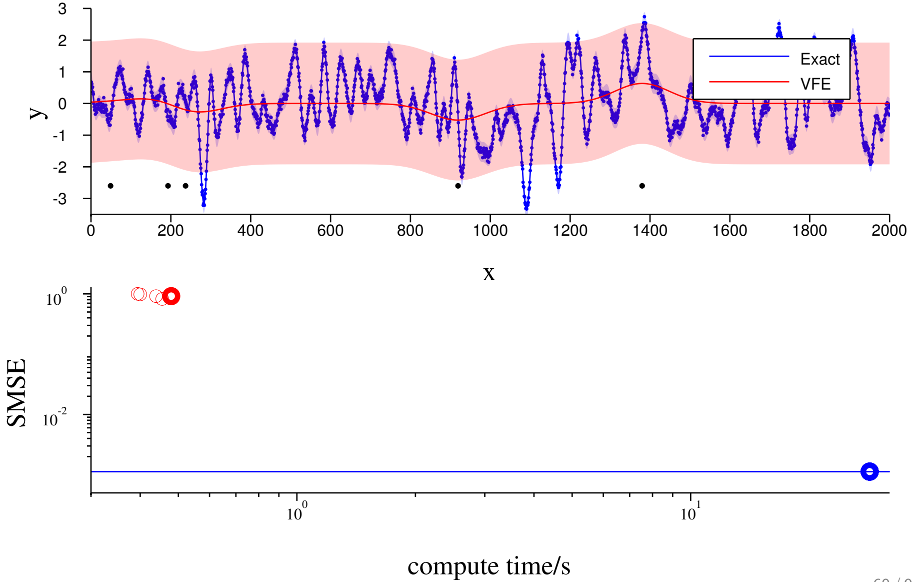

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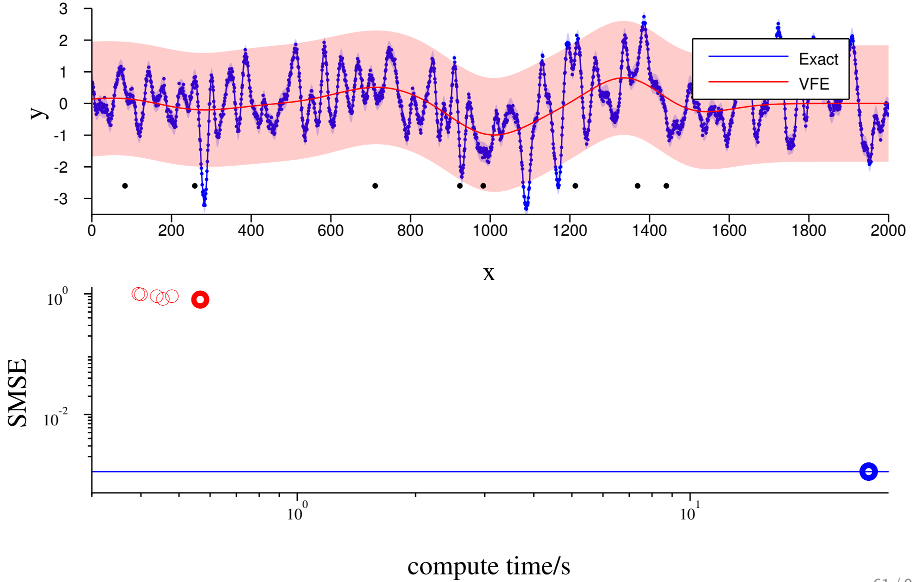

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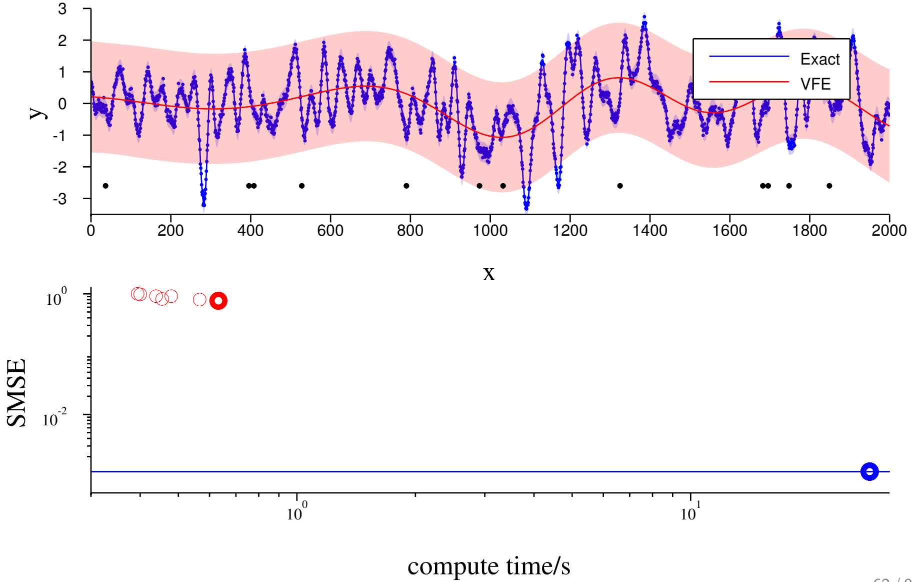

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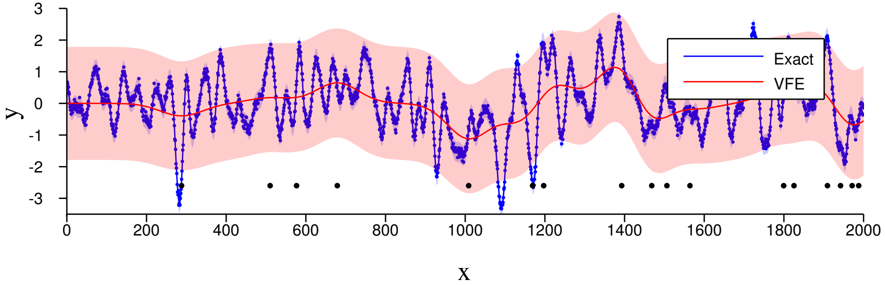

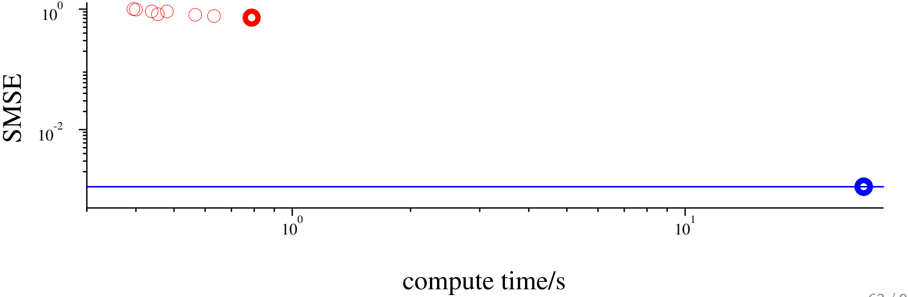

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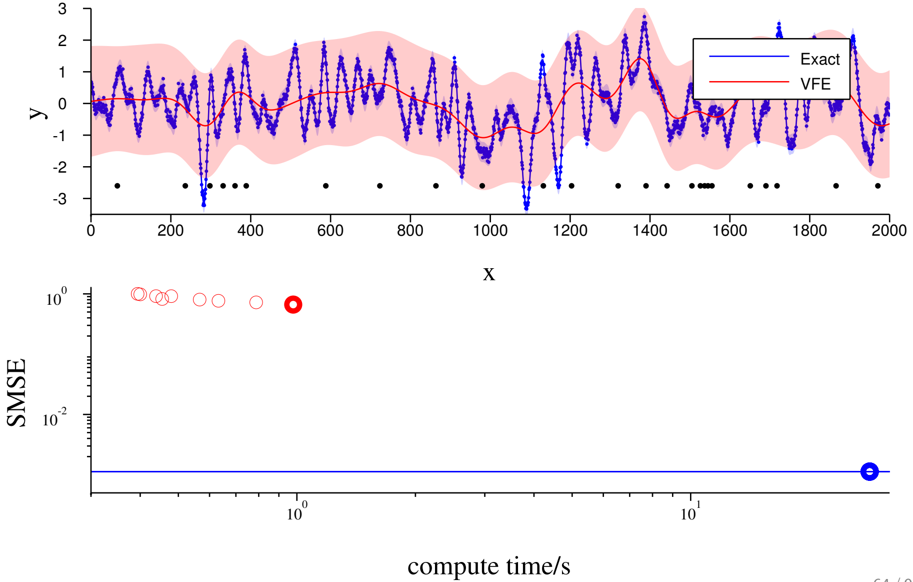

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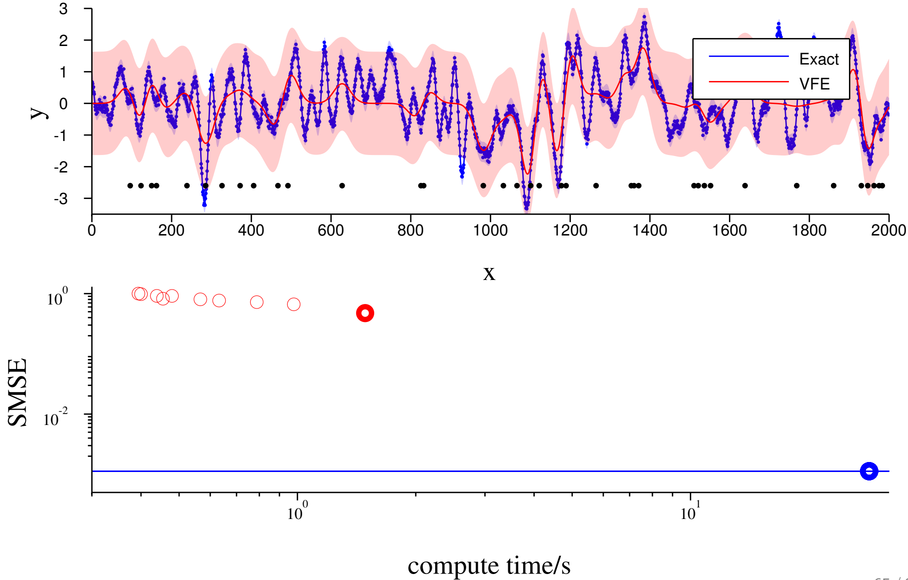

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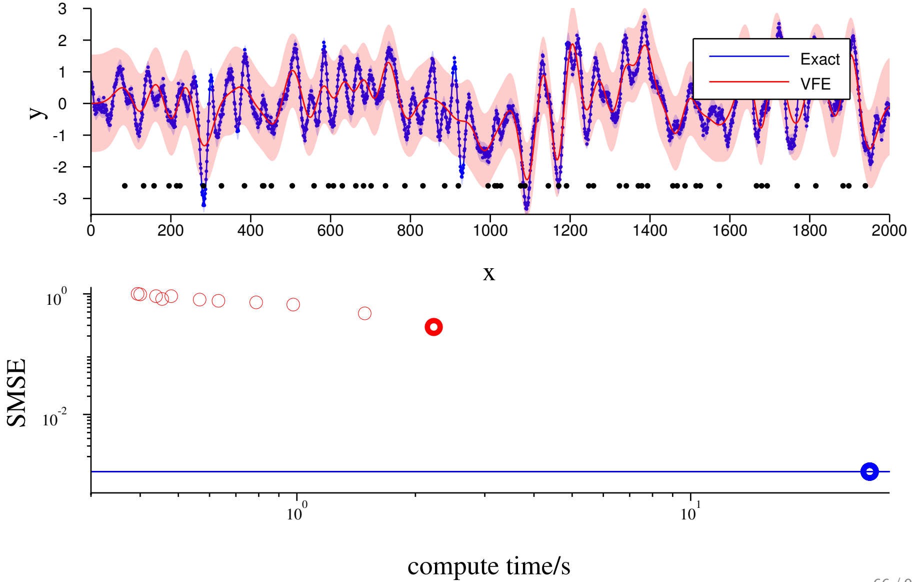

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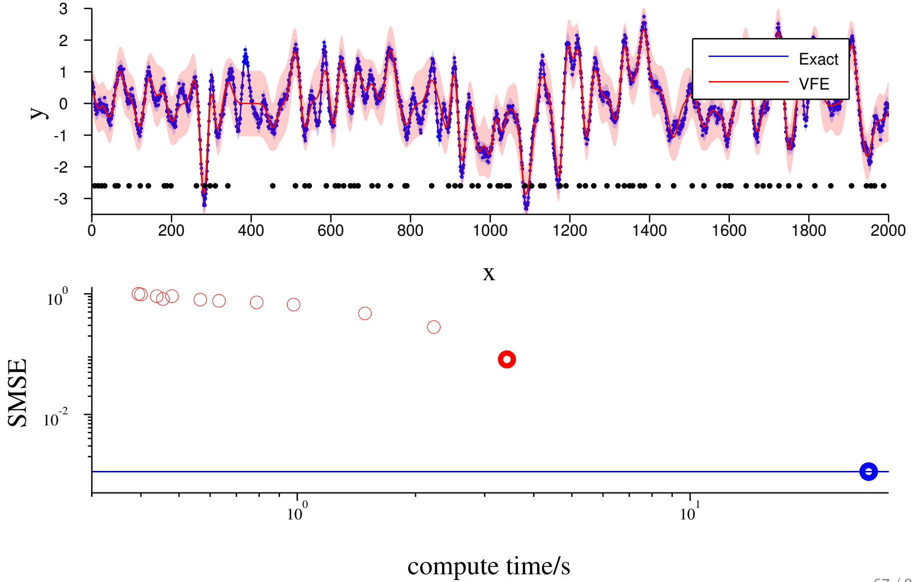

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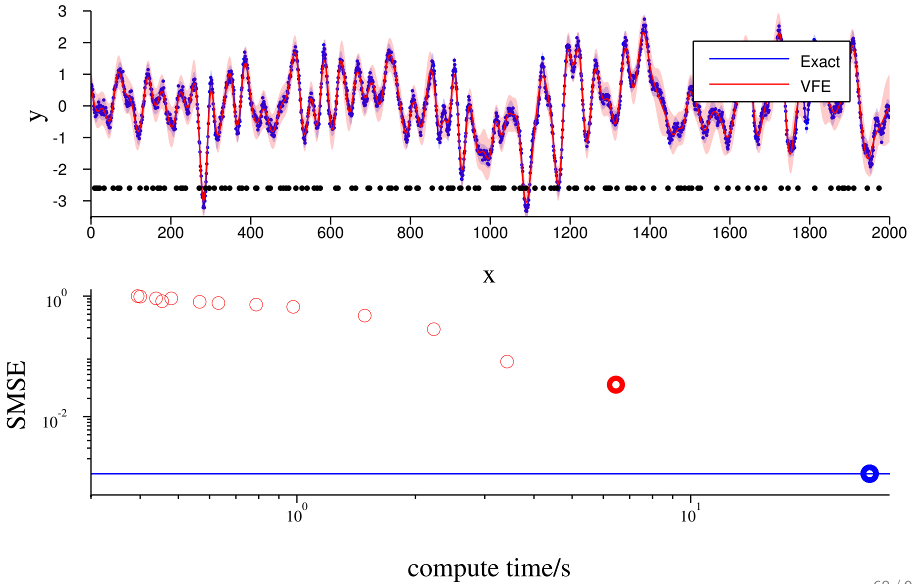

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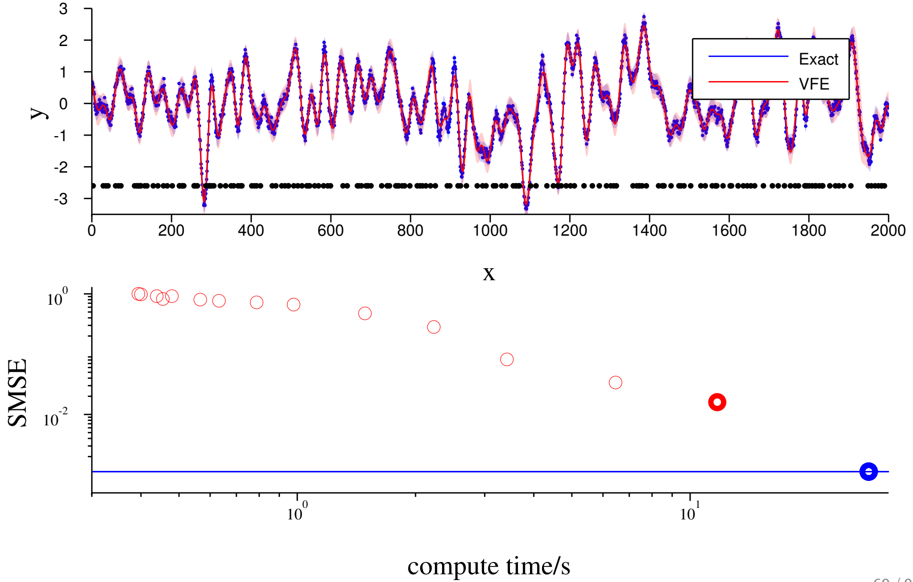

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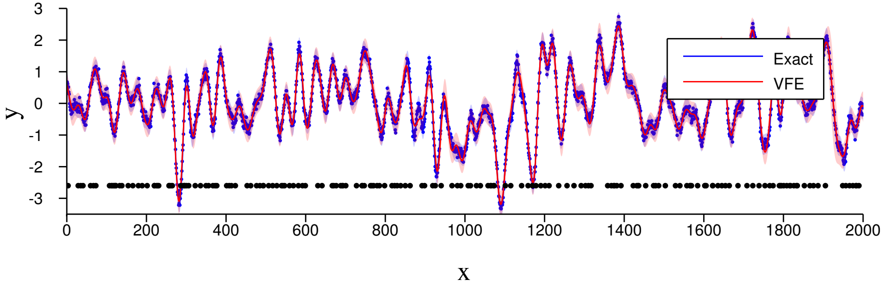

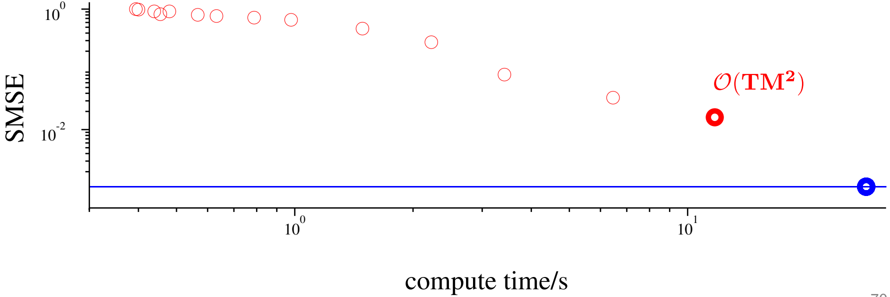

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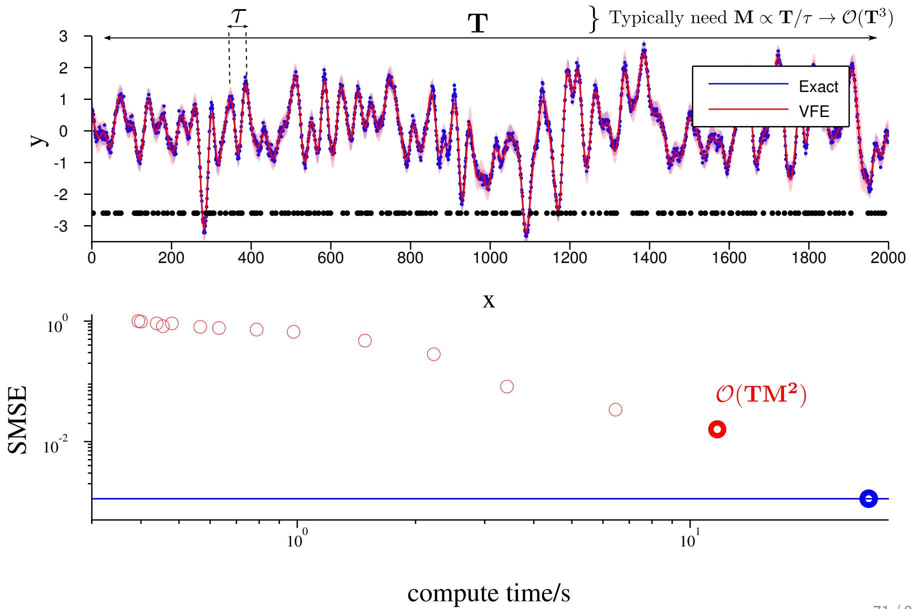


Power Expectation Propagation and Gaussian Processes

A Brief History of Gaussian Process Approximations

approximate generative model
exact inference

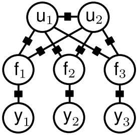
methods employing
pseudo-data

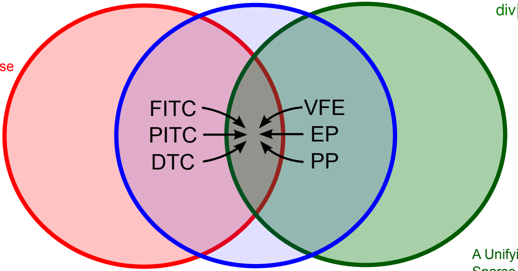
exact generative model
approximate inference

div$[p(\mathbf{f}, \mathbf{y}) || q(\mathbf{f}, \mathbf{y})]$

div$[p(\mathbf{f}|\mathbf{y}) || q(\mathbf{f})]$

A Unifying View of Sparse Approximate Gaussian Process Regression
Quinonero-Candela & Rasmussen, 2005
(FITC, PITC, DTC)





A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation
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(VFE, EP, FITC, PITC ...)

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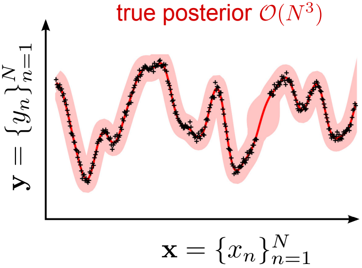
EP pseudo-point approximation

$$p^*(f) = \; p(f, \mathbf{y}|\mathbf{x}, \theta)$$



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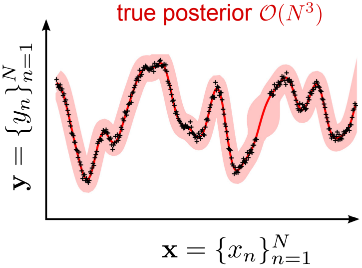
$$\begin{aligned} p^*(f) &= p(f, \mathbf{y}|\mathbf{x}, \theta) \\ &= p(f|\theta) \prod_{n=1}^{N} \underline{p(y_n|f, x_n, \theta)} \end{aligned}$$



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$$= p(f|\theta) \prod_{n=1}^{N} p(y_n|f, x_n, \theta)$$
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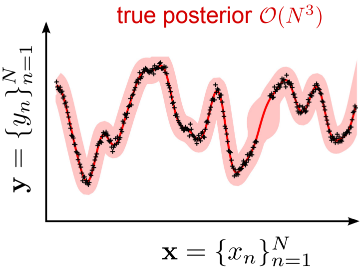

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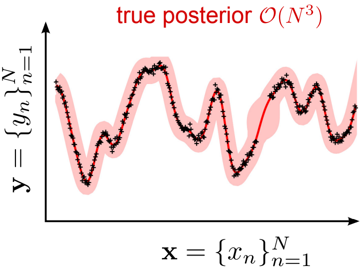
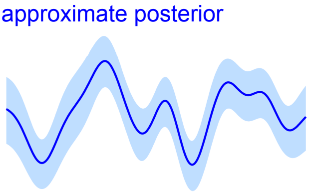


$\approx$



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$$p^*(f) = p(f, \mathbf{y}|\mathbf{x}, \theta)$$

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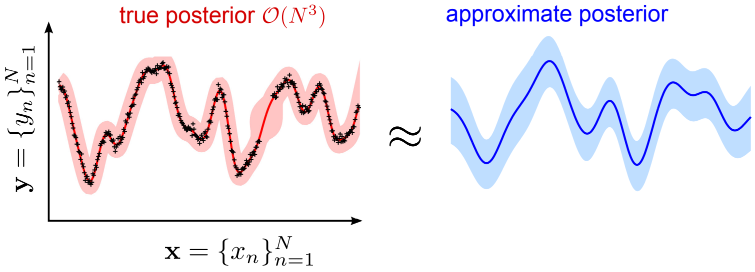
$$= \underbrace{p(\mathbf{y}|\mathbf{x}, \theta)}_{\text{marginal likelihood}} \; \underbrace{p(f|\mathbf{y}, \mathbf{x}, \theta)}_{\text{posterior}} \qquad = \underline{Z_{\mathrm{EP}}} \; \underline{q(f)}$$



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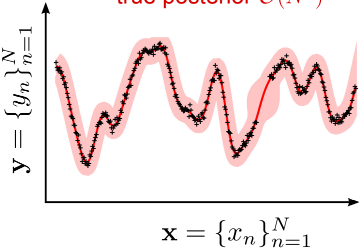
$$t_n(f) = \mathcal{N}(\mathbf{u}; \mu_n, \Sigma_n)$$

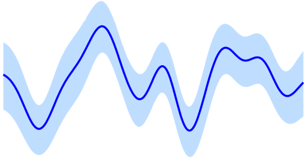
$$\dim(\mathbf{u}) = M \quad f = \{\mathbf{u}, f_{\neq \mathbf{u}}\}$$

true posterior $\mathcal{O}(N^3)$



$\approx$

approximate posterior $\mathcal{O}(NM^2)$



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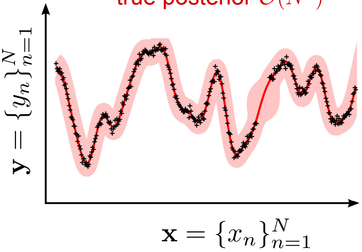

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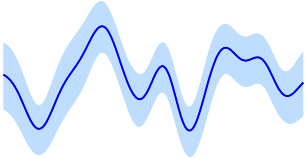

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exact joint of new GP regression model

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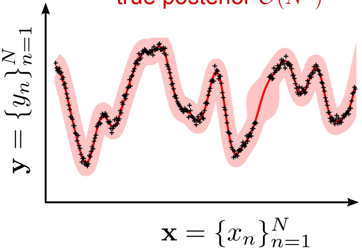

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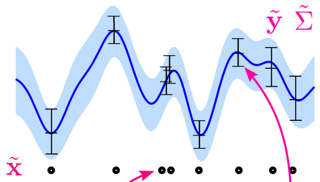

input locations of 'pseudo' data

outputs and covariance 'pseudo' data

EP algorithm

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1. remove

$$q^{\setminus n}(f) = \frac{q^*(f)}{t_n(\mathbf{u})}$$

cavity

take out one pseudo-observation likelihood

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$$q^*(f) = \underset{q^*(f)}{\operatorname{argmin}} \operatorname{KL}\left[p_n^{\text{tilt}}(f) || q^*(f)\right]$$

project onto approximating family

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update pseudo-observation likelihood

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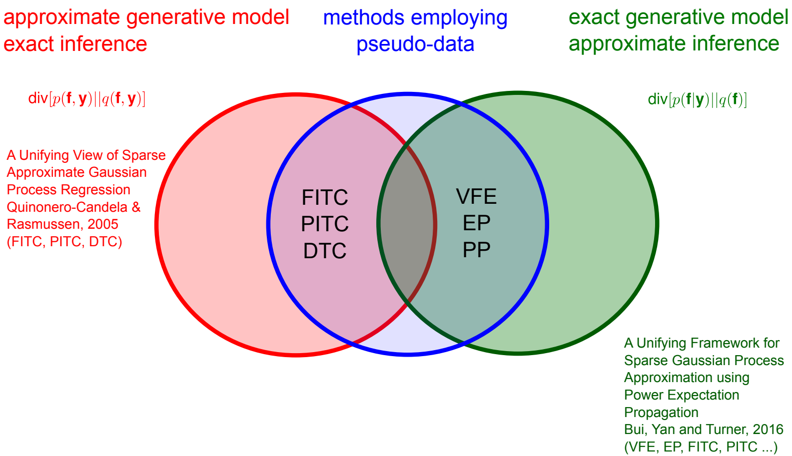
A Brief History of Gaussian Process Approximations



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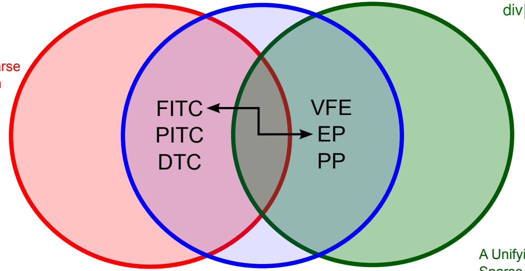

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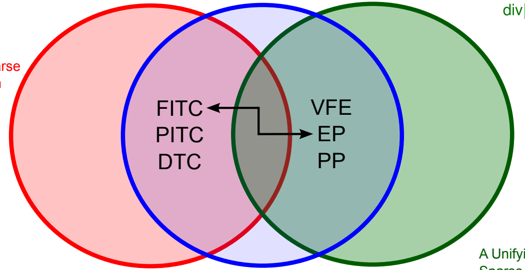

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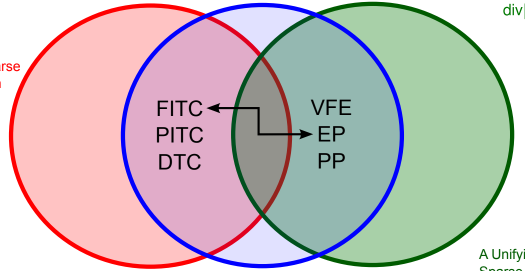

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interpretation resolves issues with FITC:
why does it work so well?
are we allowed to increase M with N

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EP algorithm

1. remove

$$q^{\setminus n}(f) = \frac{q^*(f)}{t_n(\mathbf{u})}$$

cavity

take out one pseudo-observation likelihood

2. include

$$p_n^{\text{tilt}}(f) = q^{\setminus n}(f) p(y_n | f, x_n, \theta)$$

tilted

add in one true observation likelihood

KL between unnormalised stochastic processes

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$$= z_n \mathcal{N}(\mathrm{K}_{f_n \mathbf{u}} \mathrm{K}_{\mathbf{uu}}^{-1} \mathbf{u}; g_n, v_n)$$

update pseudo-observation likelihood

rank 1

Power EP algorithm (as tractable as EP)

1. remove

cavity

$$q^{\backslash n}(f) = \frac{q^*(f)}{t_n(\mathbf{u})^{\alpha}}$$

take out fraction of pseudo-observation likelihood

2. include

tilted

$$p_n^{\text{tilt}}(f) = q^{\backslash n}(f) p(y_n | f, x_n, \theta)^{\alpha}$$

add in fraction of true observation likelihood

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update pseudo-observation likelihood

rank 1

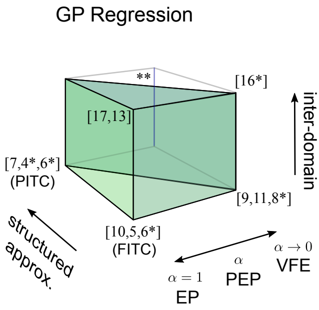
Power EP: a unifying framework

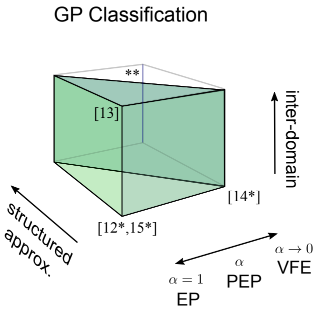
$\alpha \to 0$ α $\alpha = 1$

VFE
Titsias, 2009

FITC
Csato and Opper, 2002
Snelson and Ghahramani, 2005

Power EP: a unifying framework





[4] Quiñonero-Candela et al. 2005
[5] Snelson et al., 2005
[6] Snelson, 2006
[7] Schwaighofer, 2002

[8] Titsias, 2009
[9] Csató, 2002
[10] Csató et al., 2002
[11] Seeger et al., 2003

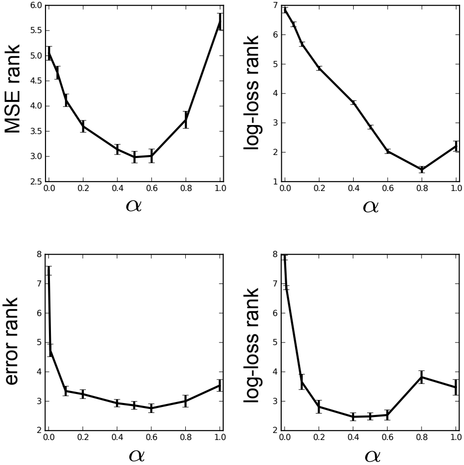
[12] Naish-Guzman et al, 2007
[13] Qi et al., 2010
[14] Hensman et al., 2015
[15] Hernández-Lobato et al., 2016
[16] Matthews et al., 2016
[17] Figueiras-Vidal et al., 2009

* = optimised pseudo-inputs
** = structured versions of VFE recover VFE

How should I set the power parameter α?

8 UCI regression datasets
20 random splits
M = 0 - 200
hypers and inducing
inputs optimised

6 UCI classification datasets
20 random splits
M = 10, 50, 100
hypers and inducing
inputs optimised



α = 0.5 does well on average

Approximate inference in GPs:

- A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation, arXiv preprint 2016

Scalable Approximate inference:

- Stochastic Expectation Propagation, NIPS 2015
- Black-box α-divergence Minimization, ICML 2016

Deep Gaussian Processes (incl. comparisons to Bayesian Neural Networks and GPs):

- Deep Gaussian Processes for Regression using Approximate Expectation Propagation, ICML 2016

GP regression: introducing notation

Q1. What's the formal justification for how we were using GPs for regression?

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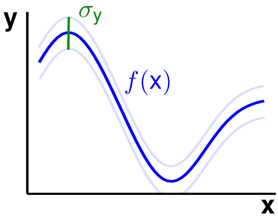
generative model (like non-linear regression)

$\mathsf{y}(\mathsf{x}) = f(\mathsf{x}) + \epsilon \sigma_{\mathsf{y}}$

$p(\epsilon) = \mathcal{N}(0, 1)$



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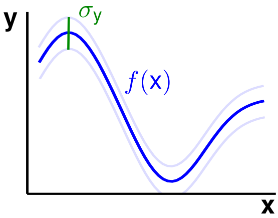

place GP prior over the non-linear function

$$p(f(\mathsf{x})|\theta) = \mathcal{GP}(0, \mathsf{K}(\mathsf{x}, \mathsf{x}'))$$

$$\mathsf{K}(\mathsf{x}, \mathsf{x}') = \sigma^2 \exp\left(-\frac{1}{2l^2}(\mathsf{x} - \mathsf{x}')^2\right)$$ (smoothly wiggling functions expected)

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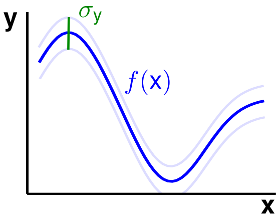

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sum of Gaussian variables = Gaussian: induces a GP over $\mathsf{y}(\mathsf{x})$

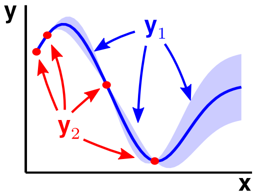
$p(\mathsf{y}(\mathsf{x})|\theta) = \mathcal{GP}(0, \mathsf{K}(\mathsf{x}, \mathsf{x}') + \mathrm{I}\sigma_{\mathsf{y}}^2)$

GP regression: introducing notation

Q3. How do we make predictions?

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

$$p(\mathbf{y}_1|\mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$



$$\Longrightarrow \quad p(\mathbf{y}_1|\mathbf{y}_2) = \mathcal{N}(\mathbf{a} + \mathsf{B}\mathsf{C}^{-1}(\mathbf{y}_2 - \mathbf{b}), \mathsf{A} - \mathsf{B}\mathsf{C}^{-1}\mathsf{B}^\top)$$

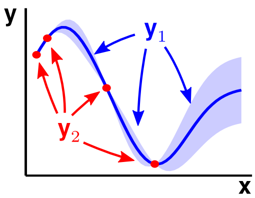
predictive mean

$$\mu_{\mathbf{y}_1|\mathbf{y}_2} = \mathbf{a} + \mathsf{B}\mathsf{C}^{-1}(\mathbf{y}_2 - \mathbf{b})$$

GP regression: introducing notation

Q3. How do we make predictions?

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



$$p(\mathbf{y}_1|\mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$

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

predictive mean

$$\begin{aligned}\mu_{\mathbf{y}_1|\mathbf{y}_2} &= \mathbf{a} + \mathsf{B}\mathsf{C}^{-1}(\mathbf{y}_2 - \mathbf{b}) \\ &= \mathsf{B}\mathsf{C}^{-1}\mathbf{y}_2 \\ &= \mathsf{W}\mathbf{y}_2\end{aligned}$$

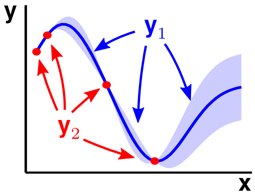
linear in the data

GP regression: introducing notation

Q3. How do we make predictions?

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

$$p(\mathbf{y}_1|\mathbf{y}_2) = \frac{p(\mathbf{y}_1, \mathbf{y}_2)}{p(\mathbf{y}_2)}$$



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

predictive mean

$$\mu_{\mathbf{y}_1|\mathbf{y}_2} = \mathbf{a} + \mathsf{BC}^{-1}(\mathbf{y}_2 - \mathbf{b})$$
$$= \mathsf{BC}^{-1}\mathbf{y}_2$$
$$= \mathsf{W}\mathbf{y}_2$$

linear in the data

predictive covariance

$$\Sigma_{\mathbf{y}_1|\mathbf{y}_2} = \mathsf{A} - \mathsf{BC}^{-1}\mathsf{B}^\mathsf{T}$$

predictive uncertainty = prior uncertainty − reduction in uncertainty

predictions more confident than prior

A brief introduction to the Kullback-Leibler divergence

$$\mathcal{KL}(p_1(z)||p_2(z)) = \sum_z p_1(z) \log \frac{p_1(z)}{p_2(z)}$$

Important properties:

- Gibb's inequality: $\mathcal{KL}(p_1(z)||p_2(z)) \geq 0$, equality at $p_1(z) = p_2(z)$
  - proof via Jensen's inequality or differentiation (see MacKay pg. 35)
- Non-symmetric: $\mathcal{KL}(p_1(z)||p_2(z)) \neq \mathcal{KL}(p_2(z)||p_1(z))$
  - hence named *divergence* and not *distance*

Example:

- binary variables $z \in \{0, 1\}$
- $p(z = 1) = 0.8$ and $q(z = 1) = \rho$