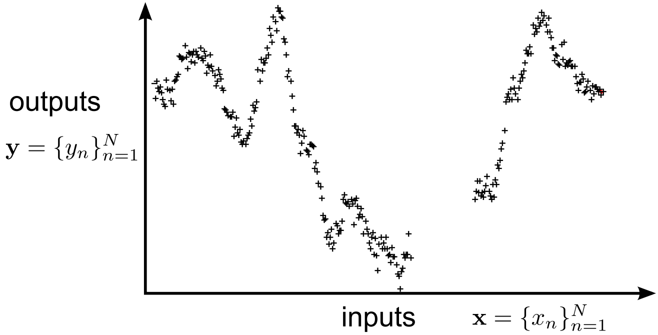
A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation

Dr. Richard E. Turner (ret26@cam.ac.uk)
Computational and Biological Learning Lab, Department of Engineering, University of Cambridge

...joint work with Thang Bui, Cuong Nguyen and Josiah Yan

Motivation: Gaussian Process Regression



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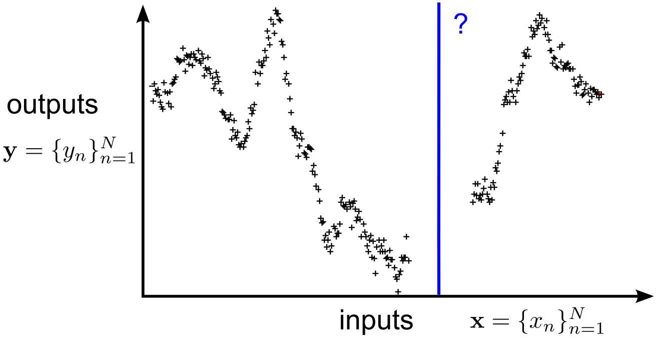
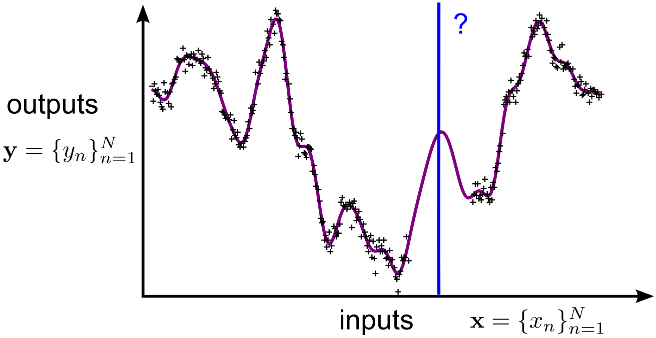


Motivation: Gaussian Process Regression

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

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



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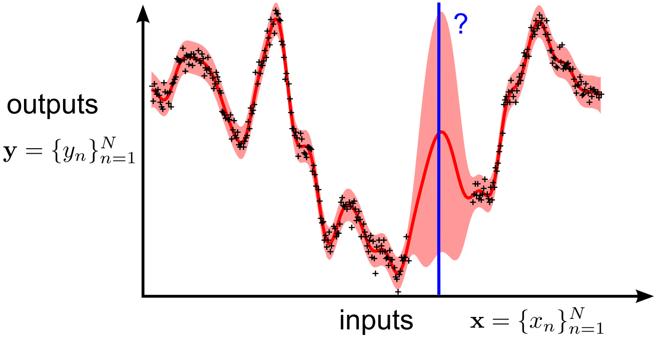
inference & learning →

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

$$p(\mathbf{y}|\mathbf{x}, \theta)$$



Motivation: Gaussian Process Regression

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

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

inference & learning

intractabilities
computational $\mathcal{O}(N^3)$
analytic

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

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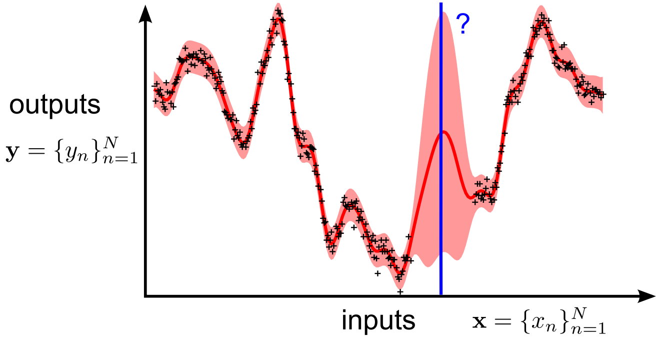

A Brief History of Gaussian Process Approximations

FITC: Snelson et al. “Sparse Gaussian Processes using Pseudo-inputs”
PITC: Snelson et al. “Local and global sparse Gaussian process approximations”
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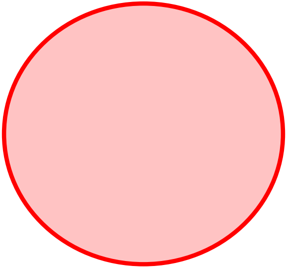
A Brief History of Gaussian Process Approximations

approximate generative model
exact inference

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



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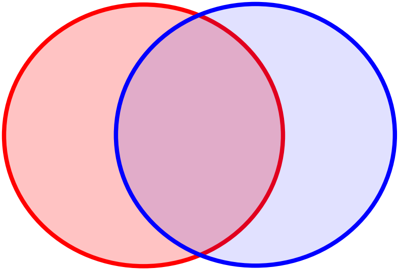

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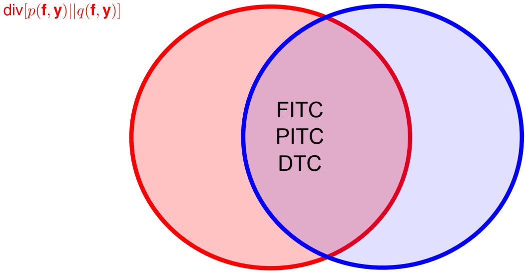

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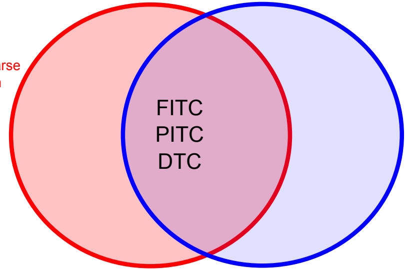

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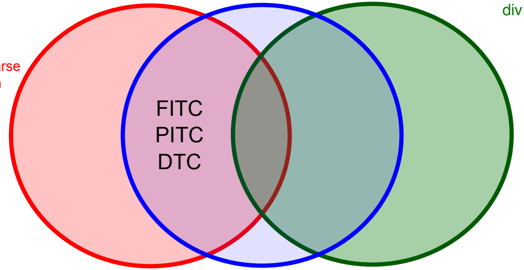

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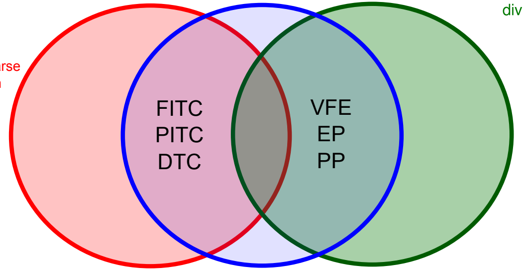

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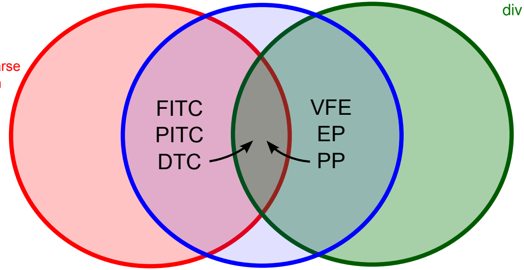

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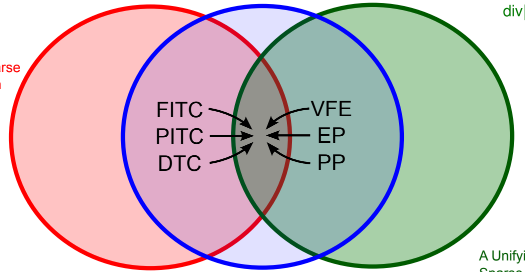

A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation
Bui, Yan and Turner, 2016
(VFE, EP, FITC, PITC ...)

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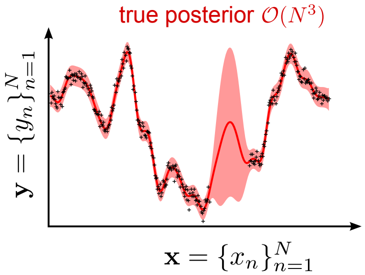
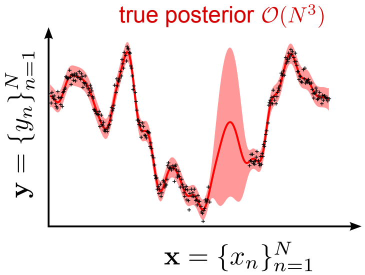
EP pseudo-point approximation

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



EP pseudo-point approximation

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

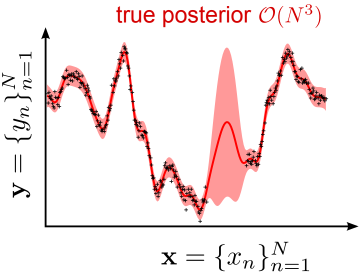


EP pseudo-point approximation

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

marginal likelihood — $p(\mathbf{y}|\mathbf{x}, \theta)$

posterior — $p(f|\mathbf{y}, \mathbf{x}, \theta)$



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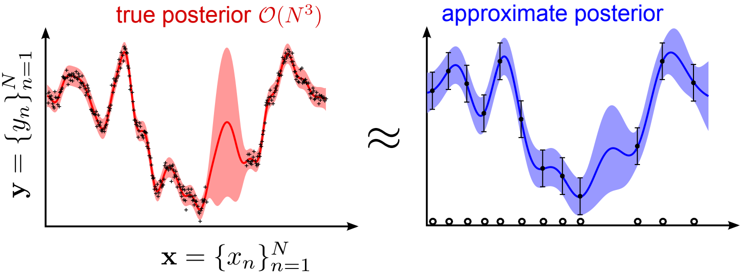
&= \underbrace{p(\mathbf{y}|\mathbf{x}, \theta)}_{\text{marginal likelihood}} \; \underbrace{p(f|\mathbf{y}, \mathbf{x}, \theta)}_{\text{posterior}}
\end{aligned}
$$

$$
q^*(f) = p(f|\theta) \prod_{n=1}^{N} \underline{t_n(f)}
$$



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\qquad
\begin{aligned}
q^*(f) &= p(f|\theta) \prod_{n=1}^{N} \underline{t_n(f)} \\
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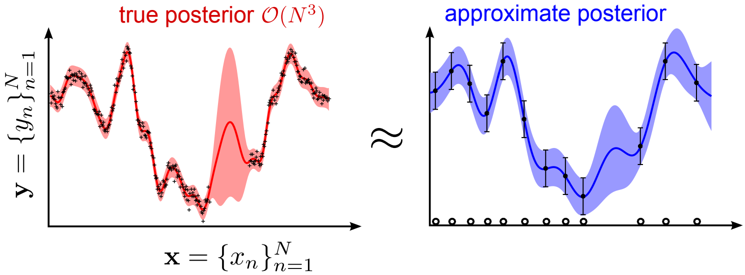
\end{aligned}
$$

marginal likelihood

posterior



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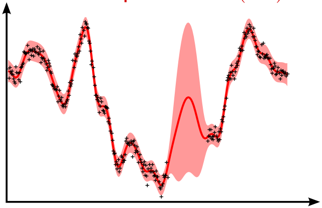
marginal likelihood — posterior

$$q^*(f) = p(f|\theta) \prod_{n=1}^{N} \underline{t_n(f)}$$
$$= \underline{Z_{\mathrm{EP}}}\ \underline{q(f)}$$

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

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

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

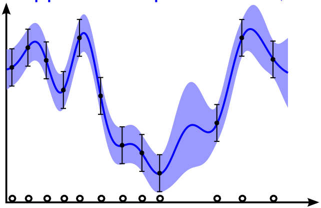


$\mathbf{y} = \{y_n\}_{n=1}^{N}$

$\mathbf{x} = \{x_n\}_{n=1}^{N}$

$\approx$

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



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$$

$$
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q^*(f) &= p(f|\theta) p(\tilde{\mathbf{y}}|\mathbf{u}, \tilde{\Sigma}) \\
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$$

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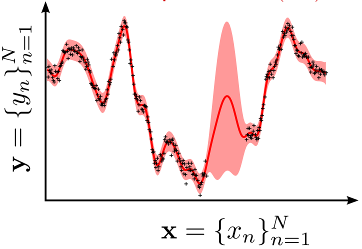

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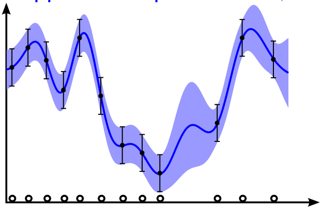

EP pseudo-point approximation

$$p^*(f) = p(f, \mathbf{y}|\mathbf{x}, \theta) = p(f|\theta) \prod_{n=1}^{N} \underline{p(y_n|f, x_n, \theta)} = \underbrace{p(\mathbf{y}|\mathbf{x}, \theta)}_{\text{marginal likelihood}} \; \underbrace{p(f|\mathbf{y}, \mathbf{x}, \theta)}_{\text{posterior}}$$

$$q^*(f) = p(f|\theta) p(\tilde{\mathbf{y}}|\mathbf{u}, \tilde{\Sigma}) = p(f|\theta) \prod_{n=1}^{N} \underline{t_n(f)} = \underline{Z_{\text{EP}}} \; \underline{q(f)}$$

exact joint of new GP regression model

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

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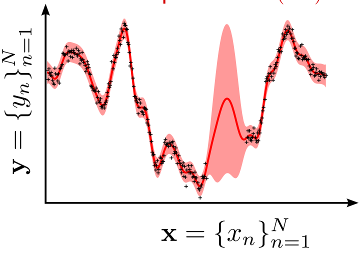
true posterior $\mathcal{O}(N^3)$



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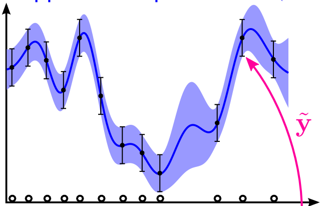
approximate posterior $\mathcal{O}(NM^2)$



input locations of 'pseudo' data $\tilde{\mathbf{x}}$

outputs and covariance 'pseudo' data

EP algorithm

EP algorithm

1. remove

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

cavity

take out one pseudo-observation likelihood

EP algorithm

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

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take out one pseudo-observation likelihood

2. include

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

tilted

add in one true observation likelihood

EP algorithm

1. remove

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add in one true observation likelihood

KL between unnormalised stochastic processes

3. project

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

project onto approximating family

EP algorithm

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KL between unnormalised stochastic processes

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

project onto approximating family

4. update

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

update pseudo-observation likelihood

EP algorithm

1. remove

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

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project onto approximating family

1. minimum: moments matched at pseudo-inputs $\mathcal{O}(NM^2)$
2. Gaussian regression: matches moments everywhere

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update pseudo-observation likelihood

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project onto approximating family

1. minimum: moments matched at pseudo-inputs $\mathcal{O}(NM^2)$
2. Gaussian regression: matches moments everywhere

4. update

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

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

update pseudo-observation likelihood

rank 1

Fixed points of EP = FITC approximation

$$t_n(\mathbf{u}) = p(y_n|\mathbf{u}, x_n, \theta) = \mathcal{N}(y_n; \mathrm{K}_{f_n\mathbf{u}}\mathrm{K}_{\mathbf{uu}}^{-1}\mathbf{u}; \mathrm{K}_{f_nf_n} - \mathrm{K}_{f_n\mathbf{u}}\mathrm{K}_{\mathbf{uu}}^{-1}\mathrm{K}_{\mathbf{u}f_n} + \sigma_y^2)$$

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$$q^*(f) = p(f)\prod_{n=1}^{N} t_n(\mathbf{u})$$

suppressed θ & x_n

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$$q^*(f) = p(f)\prod_{n=1}^{N} t_n(\mathbf{u}) = p(f_{\neq\mathbf{u}}|\mathbf{u})p(\mathbf{u})\prod_{n=1}^{N} p(y_n|\mathbf{u})$$

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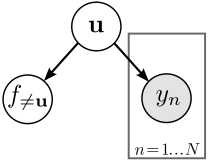
suppressed θ & x_n

$q^*(f)$



Fixed points of EP = FITC approximation

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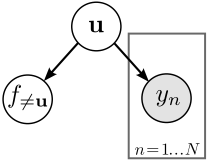
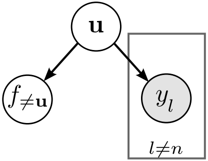


$$q^{\backslash n}(f) = \frac{q^*(f)}{t_n(\mathbf{u})}$$



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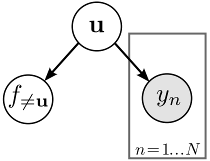

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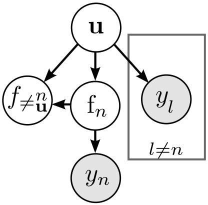

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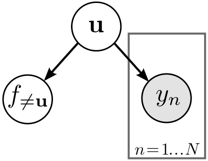

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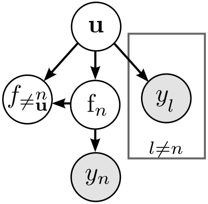

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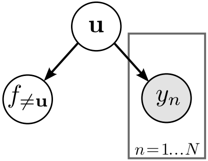

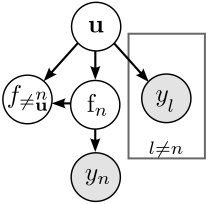

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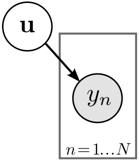

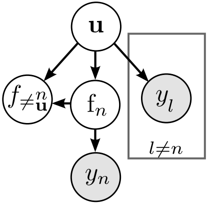

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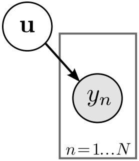

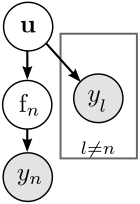

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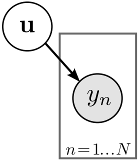

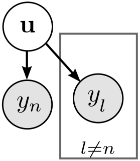

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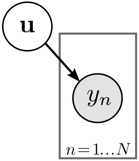

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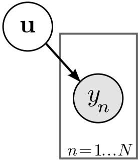

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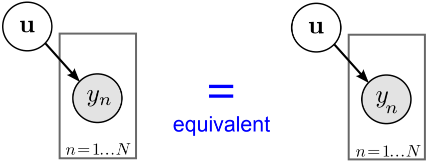

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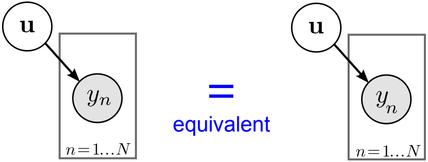

Csato & Opper (2002)

Qi, Abdel-Gawad & Minka (2010)

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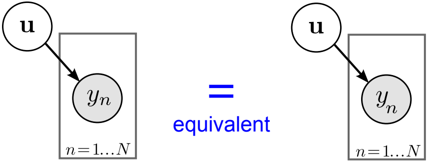

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Interpretation resolves philosophical issues with FITC (increase M with N)
FITC likelihood > GP likelihood => EP over-estimates (marginal) likelihood

EP algorithm

1. remove

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

cavity

take out one pseudo-observation likelihood

2. include

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

tilted

add in one true observation likelihood

KL between unnormalised stochastic processes

3. project

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

project onto approximating family

1. minimum: moments matched at pseudo-inputs $\mathcal{O}(NM^2)$
2. Gaussian regression: matches moments everywhere

4. update

$$t_n(\mathbf{u}) = \frac{q^*(f)}{q^{\backslash n}(f)}$$
$$= z_n \mathcal{N}(\mathrm{K}_{f_n \mathbf{u}} \mathrm{K}_{\mathbf{uu}}^{-1} \mathbf{u}; g_n, v_n)$$

update pseudo-observation likelihood

rank 1

Power EP algorithm (as tractable as EP)

1. remove

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

cavity

take out fraction of pseudo-observation likelihood

2. include

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

tilted

add in fraction of true observation likelihood

KL between unnormalised stochastic processes

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

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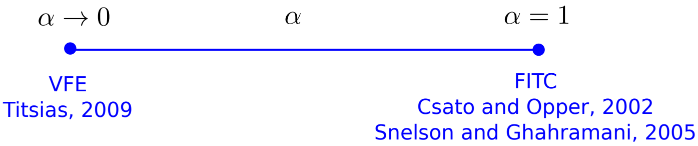
Power EP: a unifying framework



$$t_n(\mathbf{u}) = \mathcal{N}(\mathbf{K}_{\mathrm{f}_n\mathbf{u}}\mathbf{K}_{\mathbf{uu}}^{-1}\mathbf{u}; y_n, \alpha D_{\mathrm{f}_n\mathrm{f}_n} + \sigma_y^2)$$

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$$\log \mathcal{Z}_{\mathrm{PEP}} = -\frac{N}{2}\log(2\pi) - \frac{1}{2}\log|\overline{\mathbf{K}}_{\mathbf{ff}}| - \frac{1}{2}\mathbf{y}^\intercal\overline{\mathbf{K}}_{\mathbf{ff}}^{-1}\mathbf{y} + \frac{1-\alpha}{2\alpha}\sum_n \log\left(1 + \alpha D_{\mathrm{f}_n\mathrm{f}_n}/\sigma_y^2\right)$$

$$\overline{\mathbf{K}}_{\mathbf{ff}} = \mathbf{Q}_{\mathbf{ff}} + \alpha\mathrm{diag}(\mathbf{D}_{\mathbf{ff}}) + \sigma_y^2\mathrm{I} \qquad \mathbf{D}_{\mathbf{ff}} = \mathbf{K}_{\mathbf{ff}} - \mathbf{Q}_{\mathbf{ff}}$$

Power EP: a unifying framework

Approximate blocks of data: structured approximations

$$p^*(f) = p(f, \mathbf{y}|\mathbf{x}, \theta) = p(f|\theta) \prod_{k=1}^{K} \prod_{n \in \mathcal{K}_n} p(y_n|f, x_n, \theta)$$

Power EP: a unifying framework

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$\alpha = 1$

PITC / BCM
Schwaighofer & Tresp, 2002,
Snelson 2006,

$\alpha \to 0$

VFE
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Place pseudo-data in different space: interdomain transformations

$g(z) = \int w(z, z') f(z') \mathrm{d}z'$ (linear transform)

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pseudo-data
in new space

$g = \{\mathbf{u}, g_{\neq \mathbf{u}}\}$

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$\alpha = 1$

PITC / BCM
Schwaighofer & Tresp, 2002,
Snelson 2006,

$\alpha \to 0$

VFE
Titsias, 2009

Place pseudo-data in different space: interdomain transformations

$$g(z) = \int w(z, z') f(z') \mathrm{d}z'$$ (linear transform)

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

$$q^*(f, g) = p(f, g|\theta) \prod_{n=1}^{N} t_n(\mathbf{u})$$

pseudo-data in new space $g = \{\mathbf{u}, g_{\neq \mathbf{u}}\}$

$\alpha = 1$

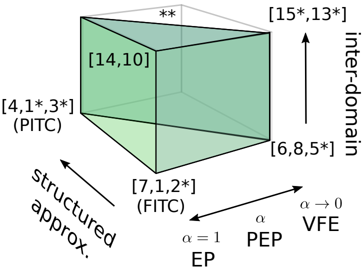
Figueiras-Vidal & Lázaro-Gredilla 2009

$\alpha \to 0$

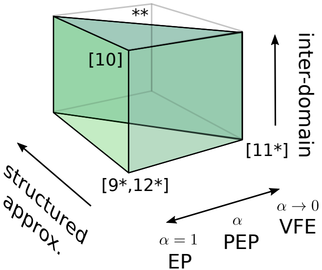
Tobar et al. 2015
Matthews et al, 2016

Power EP: a unifying framework

GP Regression



GP Classification



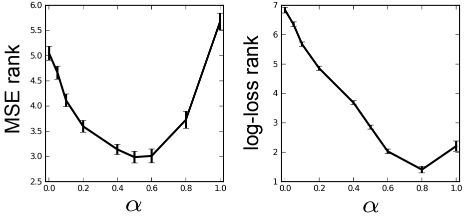
[1] Quiñonero-Candela et al. 2005
[2] Snelson et al., 2005
[3] Snelson, 2006
[4] Schwaighofer, 2002
[5] Titsias, 2009
[6] Csató, 2002
[7] Csató et al., 2002
[8] Seeger et al., 2003
[9] Naish-Guzman et al, 2007
[10] Qi et al., 2010
[11] Hensman et al., 2015
[12] Hernández-Lobato et al., 2016
[13] Matthews et al., 2016
[14] Figueiras-Vidal et al., 2009
[15] Alverez et al. 2010

* = optimised pseudo-inputs

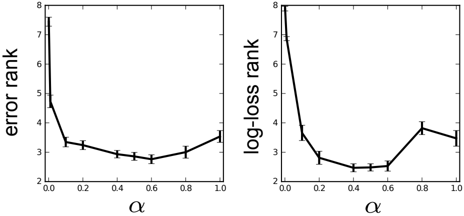
** = structured versions of VFE recover VFE (Remark 5)

How should I set the power parameter α?

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

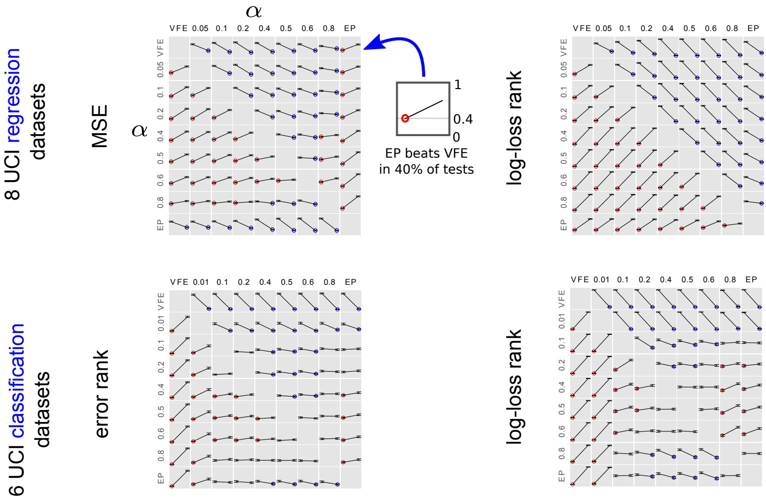


6 UCI classification datasets
20 random splits
M = 10, 50, 100
hypers and inducing
inputs optimised



α = 0.5 does well on average

How should I set the power parameter α?



α = 0.5 does well on average

Goal: Online posterior update (using old posterior and new data batch).

Two new innovations for **online learning and inducing input optimisation**

1. naïve approach: use previous approximate posterior as prior

$$\overbrace{q^{(\text{new})}(f)}^{\text{new posterior}} \approx \overbrace{p(\mathbf{y}^{(\text{new})}|f)}^{\text{new likelihood}} \;\; \overbrace{q^{(\text{old})}(f)}^{\text{old posterior}}$$

Streaming / Online Sparse Approximations

Goal: Online posterior update (using old posterior and new data batch).

Two new innovations for **online learning and inducing input optimisation**

1. better approach: only take likelihood terms from old posterior

$$\overbrace{q^{(\text{new})}(f)}^{\text{new posterior}} \approx \overbrace{p(\mathbf{y}^{(\text{new})}|f)}^{\text{new likelihood}} \overbrace{\frac{q^{(\text{old})}(f)}{p(f|\theta^{(\text{old})})}}^{\text{old likelihoods}} \overbrace{p(f|\theta^{(\text{new})})}^{\text{original prior}}$$

Streaming / Online Sparse Approximations

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2. naïve approach: use same pseudo-points throughout

$$q^{(\text{old})}(f) = p(f_{\neq \mathbf{u}}|\mathbf{u}, \theta^{(\text{old})})q(\mathbf{u})$$
$$q^{(\text{new})}(f) = p(f_{\neq \mathbf{u}}|\mathbf{u}, \theta^{(\text{new})})q(\mathbf{u})$$

Streaming / Online Sparse Approximations

Goal: Online posterior update (using old posterior and new data batch).

Two new innovations for **online learning and inducing input optimisation**

1. better approach: only take likelihood terms from old posterior

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2. better approach: decouple sets of pseudo-points

$$q^{(\text{old})}(f) = p(f_{\neq \mathbf{u}^{(\text{old})}}|\mathbf{u}^{(\text{old})}, \theta^{(\text{old})})\, q(\mathbf{u}^{(\text{old})})$$
$$q^{(\text{new})}(f) = p(f_{\neq \mathbf{u}^{(\text{new})}}|\mathbf{u}^{(\text{new})}, \theta^{(\text{new})})\, q(\mathbf{u}^{(\text{new})})$$

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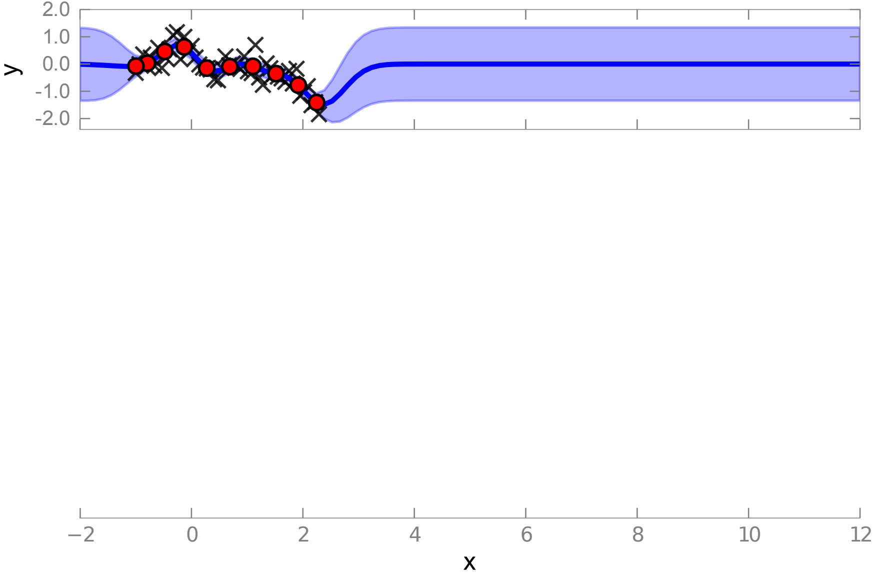
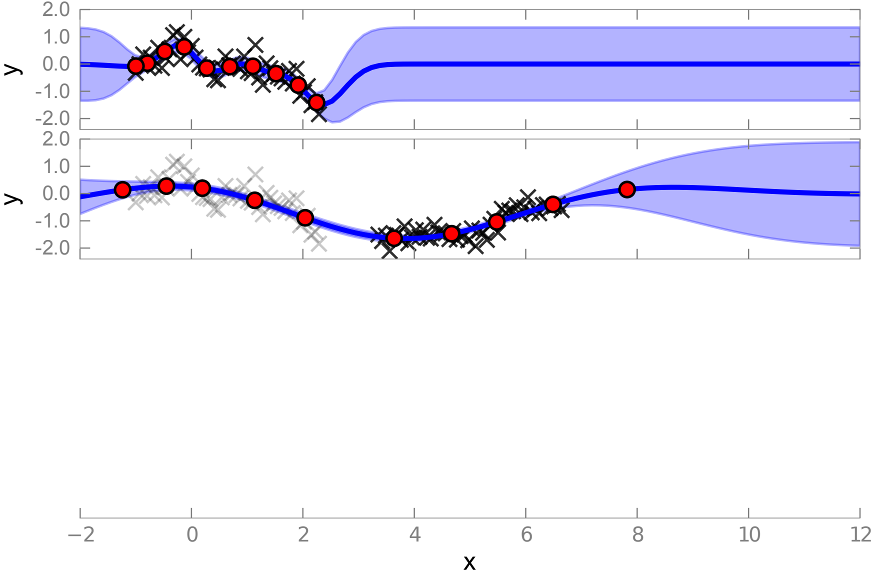
VFE is now the best Power EP method (inducing point clumping)

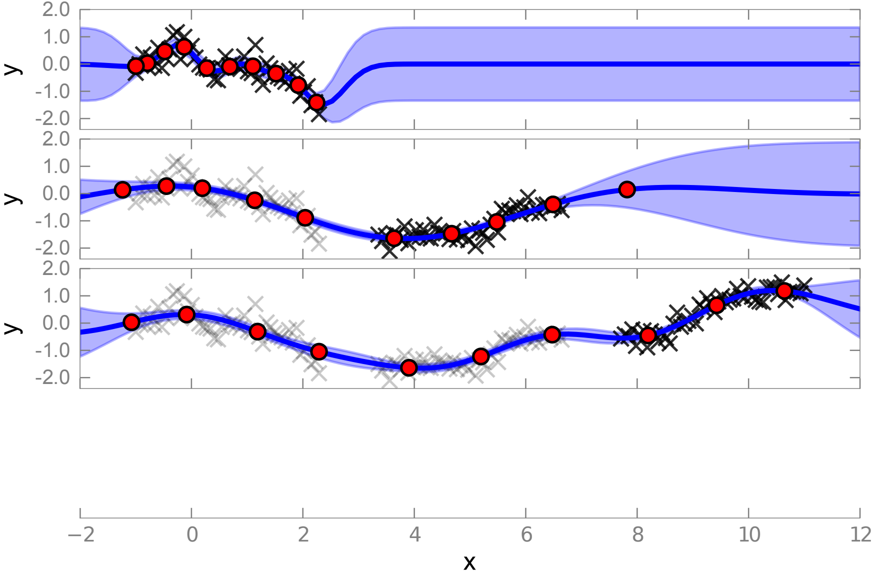
Online Sparse GP Approximations: Regression



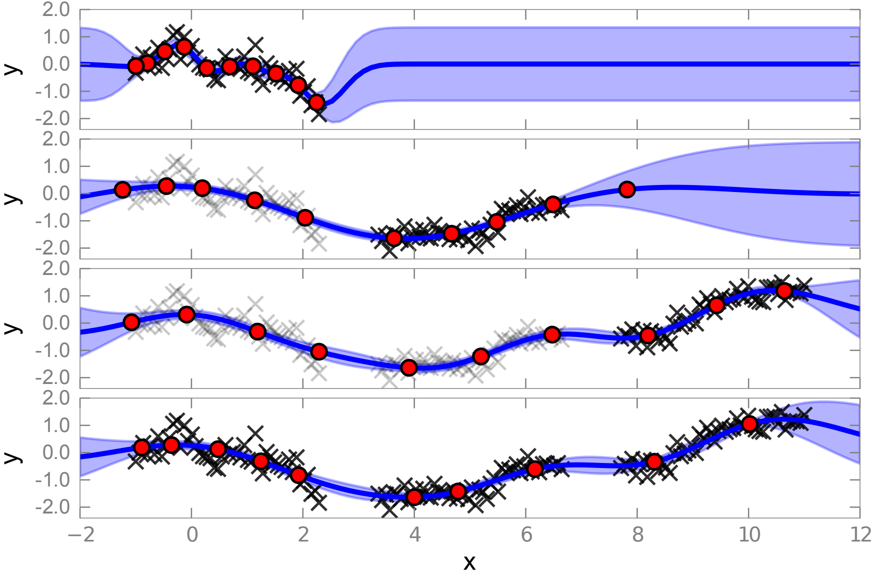
Online Sparse GP Approximations: Regression



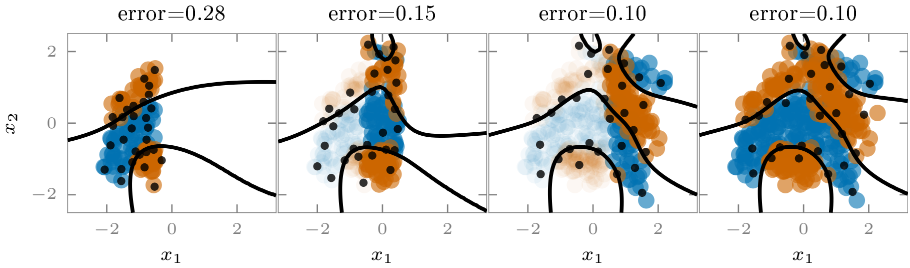
Online Sparse GP Approximations: Regression



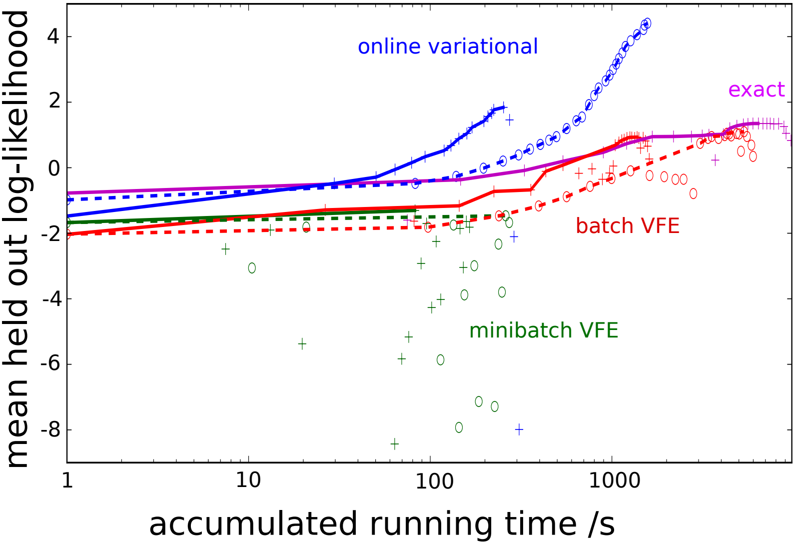
Online Sparse GP Approximations: Regression



Online Sparse GP Approximations: Classification



Streaming / Online Sparse Approximations: Time-series Regression



Summary

- Provided a unifying framework for Gaussian Process Approximation methods using pseudo-points via PEP
- FITC and PITC are EP in disguise and they use the same approximating distribution as VFE
- Intermediate powers in PEP perform best on average in batch setting (more theory and empirical work needed)
- VFE methods perform best in the online setting

Core material:

- A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation, arXiv preprint 2016
- Streaming Sparse Gaussian Process Approximations, arXiv preprint 2017

VFE is best for online inference and learning