Inference in Stochastic Processes Reading Group

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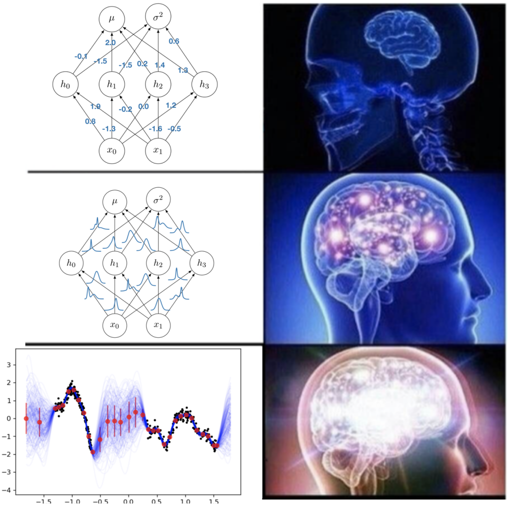
In the end we only care about functions

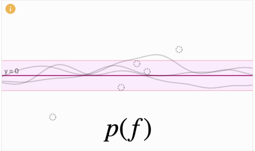
MAP Estimation

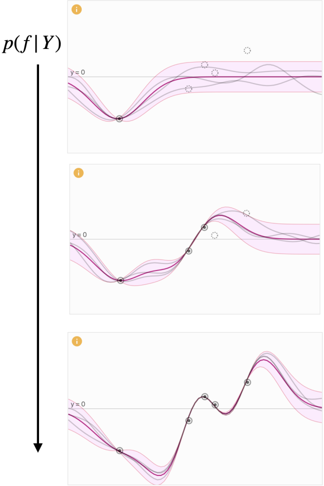
Parametric Inference

Functional Inference



Gaussian processes (GPs) as a motivating example





A Visual Exploration of Gaussian Processes

How to turn a collection of small building blocks into a versatile tool for solving regression problems.

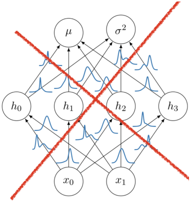
distill.pub/2019/visual-exploration-gaussian-processes/

Does functional inference mean non-parametrics?

NO!

Functional inference refers to performing probabilistic reasoning about functions $\mathbf{f}$ directly, as opposed to model parameters θ.

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$$

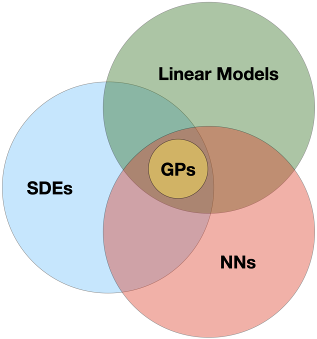


$$p(\mathbf{f}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{f})p(\mathbf{f})}{p(\mathcal{D})}$$

$\mathbf{f}$ could be the output of a parametric model.

Contents

1. Constructing (non-Gaussian) stochastic processes with linear combinations of basis functions
2. Functional inference in neural networks
3. Stochastic differential equations (SDE)



Relevant topics that will not be covered

- Rigorous measure theoretic background
- Approximate inference in Gaussian processes
- Infinite width limits of neural networks - NTK

Basis function view

$$f(\mathbf{x}) = \sum_{m=1}^{M} w_m \phi_m(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w}$$

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- Basis function $\phi(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}^M$.

e.g. $\phi(x) = [1, x, x^2, x^3, ..., x^{M-1}]^T$

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- Prior over $\mathbf{w} \implies$ prior over $f(\cdot)$.

$$p(f(\mathbf{X})) = \int \underbrace{\delta\left[f(\mathbf{X}) - \Phi(\mathbf{X})\mathbf{w}\right]}_{p(f(\mathbf{X})|\mathbf{w})} p(\mathbf{w}) d\mathbf{w}$$

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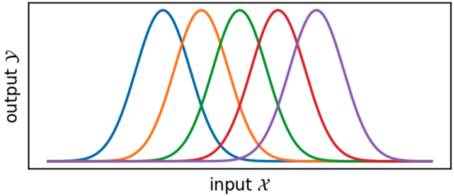

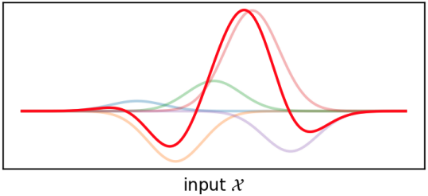

Left: $\{\phi_m(\mathbf{x})\}_{m=1}^{5}$. **Right**: $f(\mathbf{x}) = \sum_{m=1}^{M} w_m \phi_m(\mathbf{x})$.

Weight space view of Gaussian processes

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- Function-space prior:

$$p(f(\mathbf{X})) = \int \delta\left[f(\mathbf{X}) - \Phi(\mathbf{X})\mathbf{w}\right] p(\mathbf{w}) d\mathbf{w} = \mathcal{N}(\mathbf{f}; \boldsymbol{\mu}, \mathbf{K}_{\mathbf{ff}})$$

$$\boldsymbol{\mu} = \Phi(\mathbf{X})\mathbb{E}[\mathbf{w}] = \mathbf{0} \quad \mathbf{K}_{\mathbf{ff}} = \Phi(\mathbf{X})\Phi(\mathbf{X})^T$$

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- Equivalent to GP prior with kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = \left[\Phi(\mathbf{X})\Phi(\mathbf{X})^T\right]_{ij} = \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j) = \sum_{m=1}^{M} \phi_m(\mathbf{x}_i)\phi_m(\mathbf{x}_j)$$

Non-Gaussian priors?

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$$p(\mathbf{w}) \text{ non-Gaussian? } \implies \text{ non-Gaussian process } p(f(\cdot)).$$

Method for constructing non-Gaussian prior $p(\mathbf{w})$:

$$p_\theta(\mathbf{w}) = \int p_\theta(\mathbf{w}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

- $p(\mathbf{z})$ simple, i.e. $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})$
- $p(\mathbf{w})$ arbitrarily complex.

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How to learn $p_\theta(\mathrm{w}|\mathrm{z})$? From data (functions).

Learning non-Gaussian priors

Given K samples from N functions: $\left\{ \underbrace{\{\mathbf{x}_i^n, y_i^n\}_{i=1}^K}_{\text{samples from } f_n(\cdot)} \right\}_{n=1}^N$

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- ML learning of $\{\mathbf{w}^n\}_{n=1}^N$ and ϕ:

$$\arg\max_{\mathbf{w},\phi} \sum_{n=1}^N \log p(\mathbf{y}^n | \Phi(\mathbf{X}^n), \mathbf{w}^n)$$

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- Train generative model on $\{\mathbf{w}^n\}_{n=1}^N$ to learn $p_\theta(\mathbf{w}|\mathbf{z})$, i.e. VAE:

$$\arg\max_{\theta,\eta_e} \sum_{n=1}^N \mathbb{E}_{q_{\eta_e}(\mathbf{z}|\mathbf{w}^n)} \left[\log p_\theta(\mathbf{w}^n|\mathbf{z})\right] - \mathrm{KL}\left[q_{\eta_e}(\mathbf{z}|\mathbf{w}^n) || p(\mathbf{z})\right]$$

Efficient posterior inference

Given ϕ and $p_\theta(\mathbf{w}|\mathbf{z}) = \delta\left[d_\theta(\mathbf{z}) - \mathbf{w}\right]$

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$$\implies f^{(s)}(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w}^{(s)}$$

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- Sampling functions from **posterior**? Perform MCMC in latent space:

$$p(\mathbf{z}|\mathcal{D}_*, \phi) \propto p(\mathbf{y}_*|\Phi(\mathbf{X}_*), \mathbf{z})p(\mathbf{z})$$

$$\mathbf{z}^{(s)}|\mathcal{D} \sim p(\mathbf{z}|\mathcal{D}_*, \phi) \quad \mathbf{w}^{(s)} = d_\theta(\mathbf{z}^{(s)})$$

$$\implies f^{(s)}(\mathbf{x}) \mid \mathcal{D}_* = \phi(\mathbf{x})^T \mathbf{w}^{(s)}$$

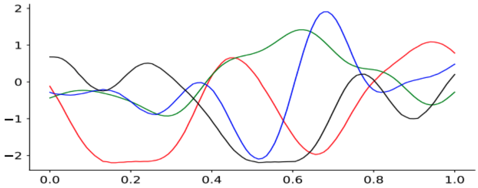
πVAE: end-to-end training (Mishra et al. 2020)

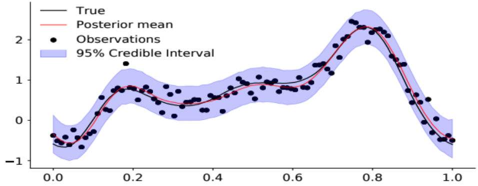
$$\mathcal{L} = \sum_{n=1}^{N} \log p(\mathbf{y}^n|\Phi(\mathbf{X}^n), \mathbf{w}^n) + \mathbb{E}_{q_{\eta_e}(\mathbf{z}|\mathbf{w}^n)p_\theta(\hat{\mathbf{w}}^n|\mathbf{z})}\left[\log p(\mathbf{y}^n|\Phi(\mathbf{X}^n), \hat{\mathbf{w}}^n)\right]$$
$$-\mathrm{KL}\left[q_{\eta_e}(\mathbf{z}|\mathbf{w}^n)||p(\mathbf{z})\right]$$

- $\log p(\mathbf{y}|\Phi(\mathbf{X}), \mathbf{w}) \implies \phi$ and $\mathbf{w}$ explain the data.
- $\mathbb{E}_{q_{\eta_e}(\mathbf{z}|\mathbf{w})}\left[\mathbb{E}_{p_\theta(\hat{\mathbf{w}}|\mathbf{z})}\left[\log p(\mathbf{y}|\Phi(\mathbf{X}), \hat{\mathbf{w}}\right]\right] \implies \phi$ and reconstructed $\mathbf{w}$ explain the data.
- $\mathrm{KL}\left[q_{\eta_e}(\mathbf{z}|\mathbf{w})||p(\mathbf{z})\right] \implies q_{\eta_e}(\mathbf{z}|\mathbf{w})$ close to the prior $p(\mathbf{z})$.

πVAE: learning a GP prior (Mishra et al. 2020)

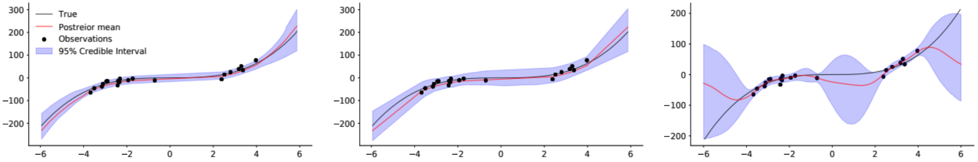
πVAE trained on Gaussian process samples





Left: prior samples. **Right**: posterior predictive distribution.

πVAE: posterior inference (Mishra et al. 2020)



Left: πVAE, samples from cubic functions. **Middle**: πVAE, samples from RBF kernel. **Right:** GP with RBF kernel

Stochastic process generator (Ma et al.)

Approximate stochastic process posterior

$$p(f|\mathcal{D}) = \frac{p(f)p(\mathcal{D}|f)}{p(\mathcal{D})} \approx q_{\mathsf{SPG}}(f)$$

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'Stochastic process generator' (SPG) family:

$$f_{\mathsf{SPG}}(\mathbf{x}) = \sum_{m=1} w_m \phi_m(\mathbf{x}), \quad q(\mathbf{w}) = \int p_\theta(\mathbf{w}|\mathbf{z}) q(\mathbf{z}) d\mathbf{z}$$

- Non-Gaussian $q(\mathbf{w}) \implies$ non-Gaussian process $q_{\mathsf{SPG}}(f)$.
- ϕ_m are a set of trainable basis functions.

Functional variational inference

Function space ELBO:

$$\mathcal{L} = \underbrace{\mathbb{E}_{q(f)}\left[\log p(\mathcal{D}|f)\right]}_{\text{nice}} - \underbrace{\mathrm{KL}\left[q(f)||p(f)\right]}_{\text{not nice}}$$

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KL between stochastic processes? Sun et al. (2019):

$$\mathrm{KL}\left[q(f)||p(f)\right] = \sup_{n\in\mathbb{N},\mathbf{X}\in\mathcal{X}^n} \mathrm{KL}\left[q(f(\mathbf{X}))||p(f(\mathbf{X}))\right]$$

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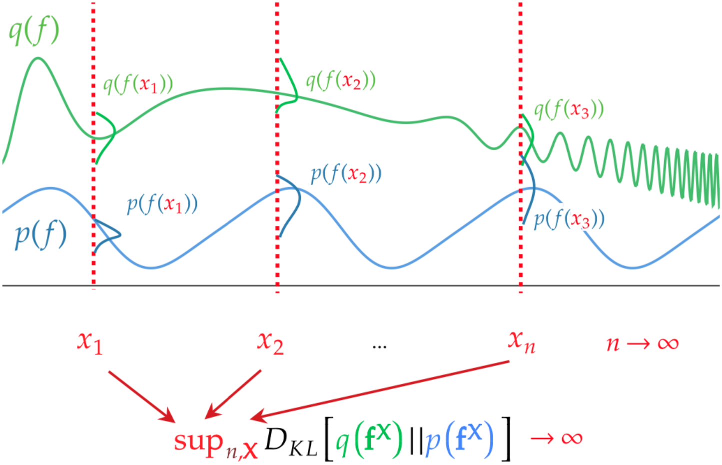
Can't compute supremum! $\implies$ **approximate with**

$$\mathrm{KL}\left[q(f)||p(f)\right] \geq \mathbb{E}_{\mathbf{X}_O\sim c}\left[\mathrm{KL}\left[q(f(\mathbf{X}_O))||p(f(\mathbf{X}_O))\right]\right]$$

(However, true KL may not be finite...)

Functional variational inference



FVI via SPGs (Ma et al.)

$$f_{\mathsf{SPG}}(\mathbf{x}) = \sum_{m=1} w_m \phi_m(\mathbf{x}), \quad q(\mathbf{w}) = \int p_\theta(\mathbf{w}|\mathbf{z}) q(\mathbf{z}) d\mathbf{z}$$

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- Approximate prior $p(f) \approx \tilde{p}_{\mathsf{SPG}}(f)$.

$\Longrightarrow$ Learns $\{\phi_m\}_{m=1}^M$, $p_\theta(\mathbf{w}|\mathbf{z})$ and $\tilde{q}(\mathbf{z}|f(\mathbf{X}_O)) \approx \tilde{p}_{\mathsf{SPG}}(\mathbf{z}|f(\mathbf{X}_O))$ through VAE-like ELBO.

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- Share $\{\phi_m\}_{m=1}^M$ and $p_\theta(\mathbf{w}|\mathbf{z})$ between $p_{\mathsf{SPG}}(f)$ and $q_{\mathsf{SPG}}(f)$.

  $\Longrightarrow$ Simplifies KL divergence:

$$\begin{aligned}&\mathrm{KL}\left[q_{\mathsf{SPG}}(f(\mathbf{X}_O)) || p_{\mathsf{SPG}}(f(\mathbf{X}_O))\right] \\ &\qquad \approx \mathbb{E}_{p_{\mathsf{SPG}}(f(\mathbf{X}_O))}\left[\int \tilde{q}(\mathbf{z}|f(\mathbf{X}_O)) \frac{q(\mathbf{z})}{p_0(\mathbf{z})}\right] d\mathbf{z}\end{aligned}$$

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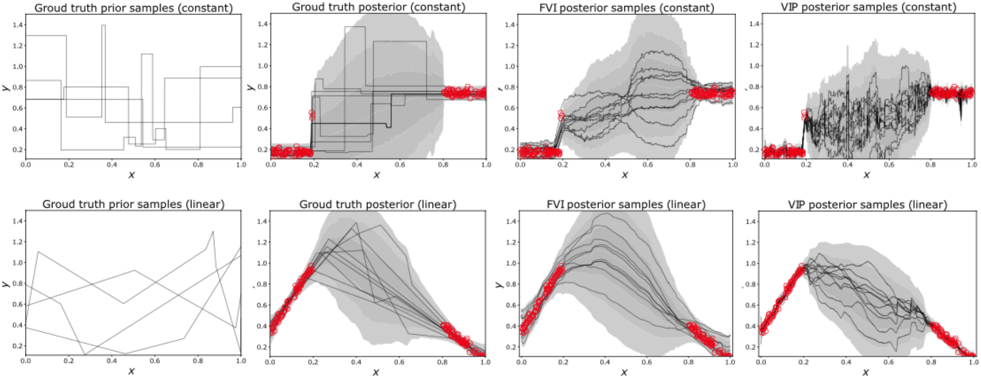
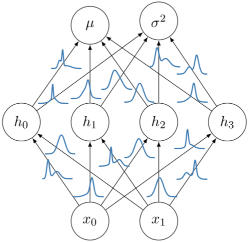


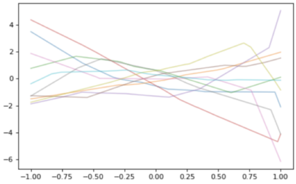
Neural Networks as Stochastic Processes

Functions sampled from NN prior:

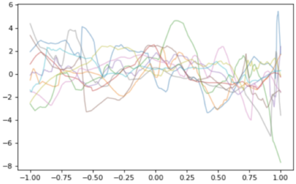


$$p(\theta) = \mathcal{N}(\theta; 0, I)$$

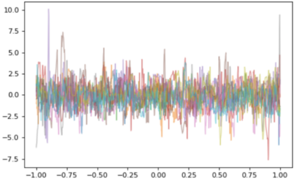
1 Hidden Layer



5 Hidden Layer



20 Hidden Layer



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- Lets define some NN $f_\theta(\cdot)$ and some weight setting θ^*:

$$f_\theta(x) \approx f_\theta^{\text{lin}}(x) = f_{\theta^*}(x) + \left(\frac{\partial f_{\theta^*}(x)}{\partial \theta^*}\right)^\mathsf{T} (\theta - \theta^*)$$

- $f_\theta^{\text{lin}}(x)$ is a linear model in θ with basis functions $\phi(x) = \frac{\partial f_{\theta^*}(x)}{\partial \theta^*}$ [7].
- This corresponds to a GP with $k(x_1, x_2) = \left(\frac{\partial f_{\theta^*}(x_1)}{\partial \theta^*}\right)^\mathsf{T} \left(\frac{\partial f_{\theta^*}(x_2)}{\partial \theta^*}\right)$!

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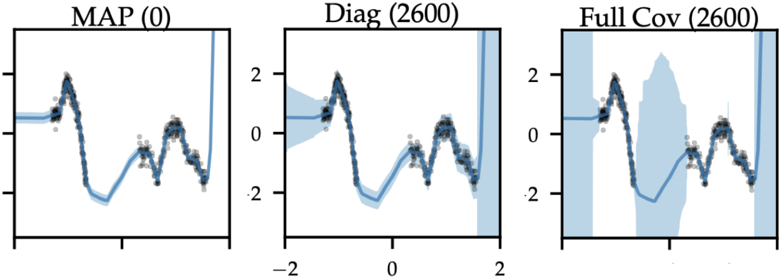
Could also make an argument about infinite width limits...

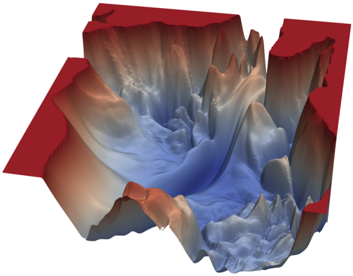
A Linearised NN-GP in action (Daxberger et. al.)

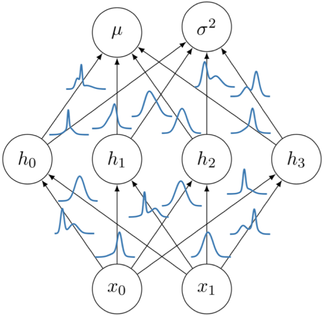


Inference in finite, non-Linearised NNs

- They are not GPs.

- Probabilistic inference over their weight space is intractable.

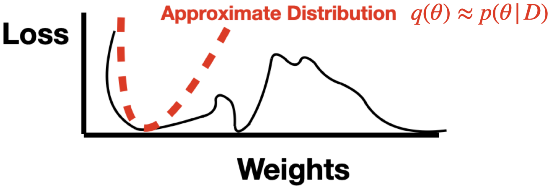


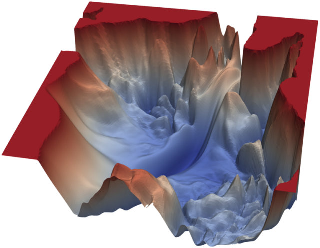


[Li et. al.]

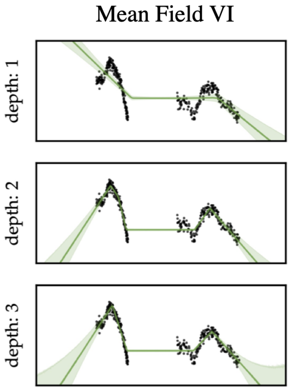
Lets try weight Space VI

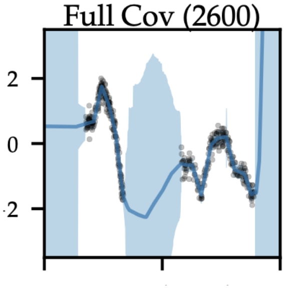
$$p(\theta|\mathcal{D}) \geq \mathsf{ELBO}_{q(\theta)} = E_{q(\theta)}[\log p(\mathcal{D}|\theta)] - KL(q(\theta)\,||\,p(\theta))$$





Empirical Underperformance





We know Mean Field distributions are flexible enough to do better [5]. It looks like the problem is the inference!

We resort to functional variational inference!

The functional posterior is intractable for NNs so we again resort to **functional VI** [12].

$$p(\theta|\mathcal{D}) \geq \mathsf{ELBO}_{q(f)} = E_{q(f))}[\log p(\mathcal{D}|f)] - KL(q\,||\,p);$$

$$KL(q\,||\,p) = \sup_{n\in\mathbb{N}, X\in\mathcal{X}^n} D_{\mathsf{KL}}(q(f(X))\,||\,p(f(X)))$$

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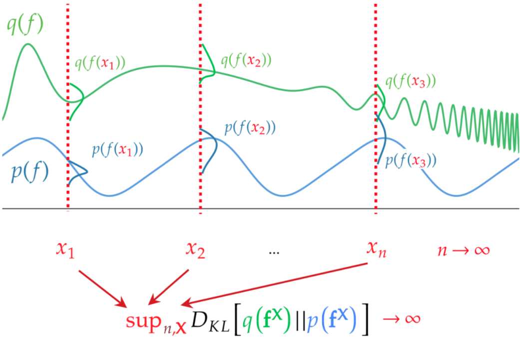
By the information processing inequality, this should yield a tighter ELBO than weight space VI [2].

$$\log p(\mathcal{D}) \geq \mathsf{ELBO}_{q(f)} \geq \mathsf{ELBO}_{q(\theta)} \tag{1}$$

Intuition: Different parameter settings induce different functions which explain the data.

$$\theta \to f \to y; \quad I(y:f) \geq I(y:\theta) \tag{2}$$

The functional KL, again



- Supremum over all input sets is intractable to compute!
- Functional KL between GP and parametric models or between different parametric models may not even be finite [2].

Approximations used by Sun et. al.

- Supremum formulation of functional KL suggests an **adversarial learning scheme**: One player chooses approximate process q and the other chooses the measurement set X.

$$\max_{q} \min_{X \in \mathcal{X}^n} E_{q(f))}[\log p(\mathcal{D}|f)] - D_{\mathsf{KL}}(q(f(X)) \,||\, p(f(X)))$$

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- **Sampling-based measurement sets**: Define a sampling distribution c from which to draw X.

$$\max_{q} E_{q(f)}[\log p(\mathcal{D}|f)] - \mathbb{E}_{X\sim c}[D_{\mathsf{KL}}(q(f(X)) \,||\, p(f(X)))]$$

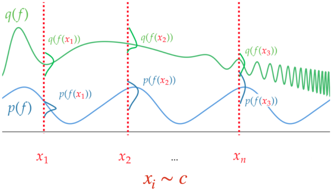
A remaining issue might be estimating $q(f(X))$...

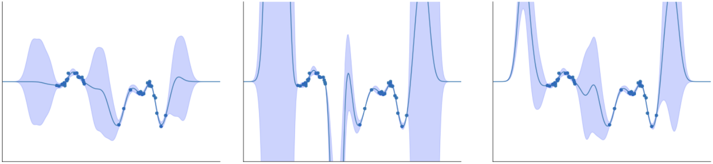
Choosing measurement points

Sun et. al. show that the resulting objective is still a lower bound on $\log p(\mathcal{D})$ as long as $X_{\mathcal{D}} \subset X$.

Burt et. al. compare approaches on linear models:

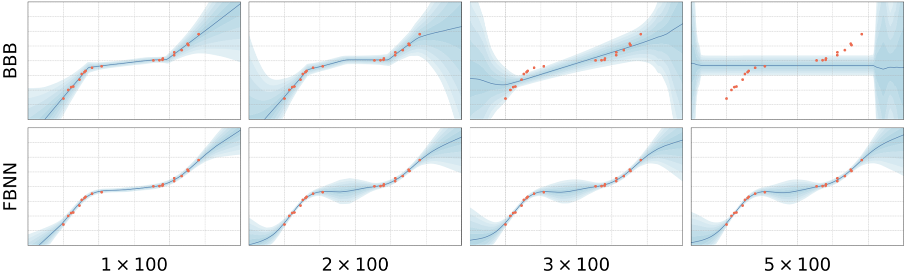
- Randomly sample X once and leave it **fixed**.
- Resample $X \sim c$ in every iteration (**random**.)





(a) Exact $\quad$ (b) FixedA $\quad$ (c) RandA

Results: BNNs with Random sampling (Sun et. al.)



- Approximate functional VI is more flexible than weight space VI.
- In agreement with [5], at least 2 hidden layers are needed to capture in between uncertainty with mean field weight parametrisation.
- Is functional VI a practical approach?

Stochastic Differential Equations

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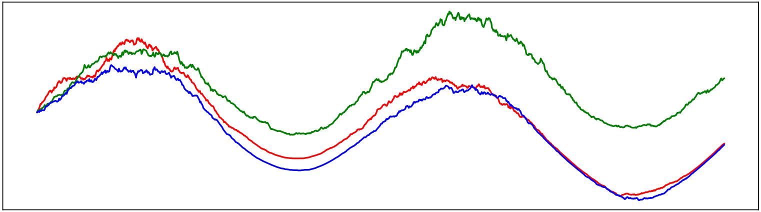

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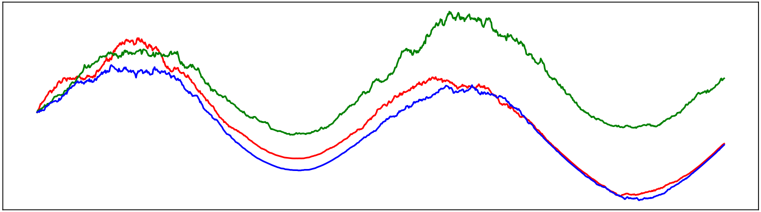

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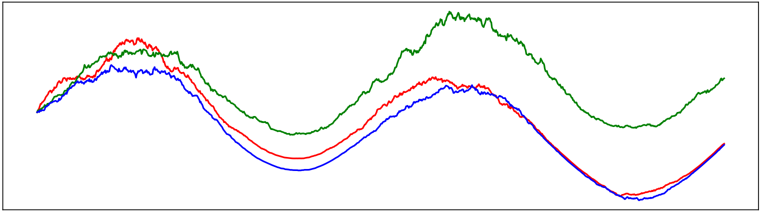

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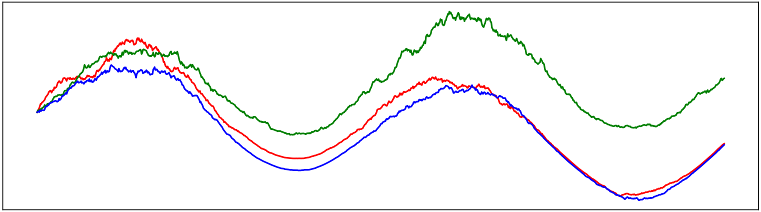

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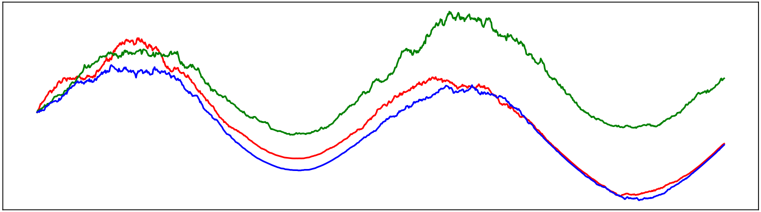

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3. Physical models, e.g. weather and climate

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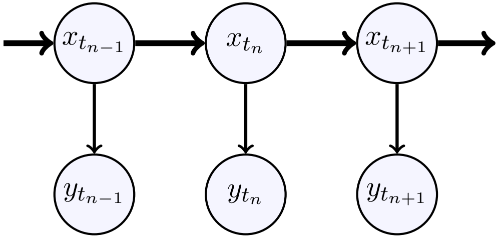

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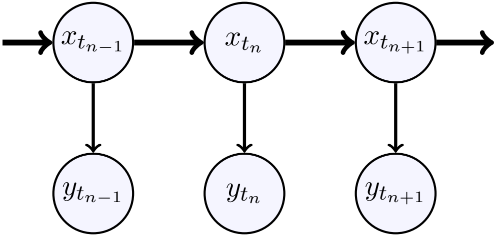

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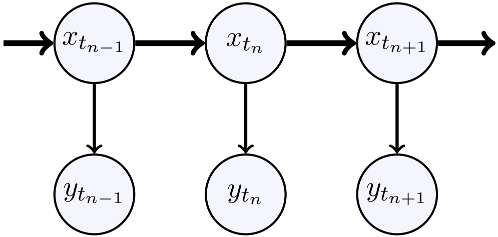

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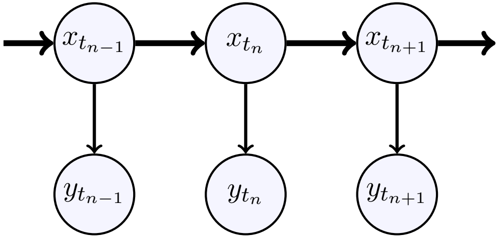

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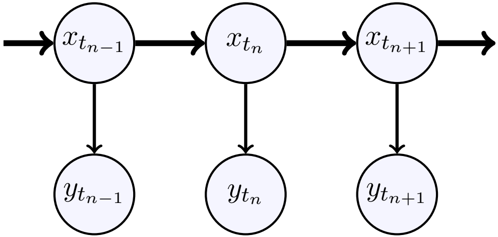

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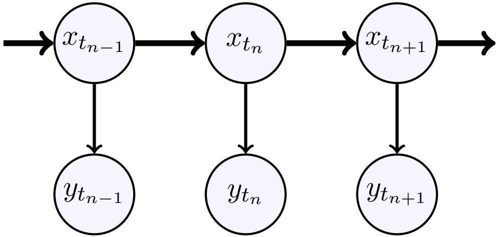

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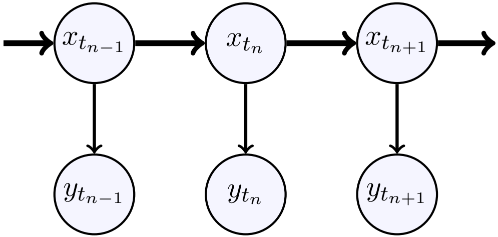

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We call x_t the solution to an SDE with drift f and diffusion g if

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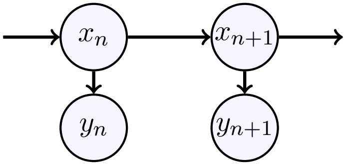

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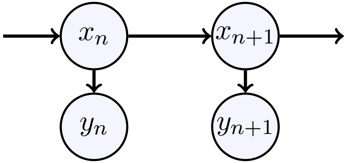

Compute posterior in $\mathcal{O}(T)$ time. (Kalman filtering/smoothing) [3, 10]

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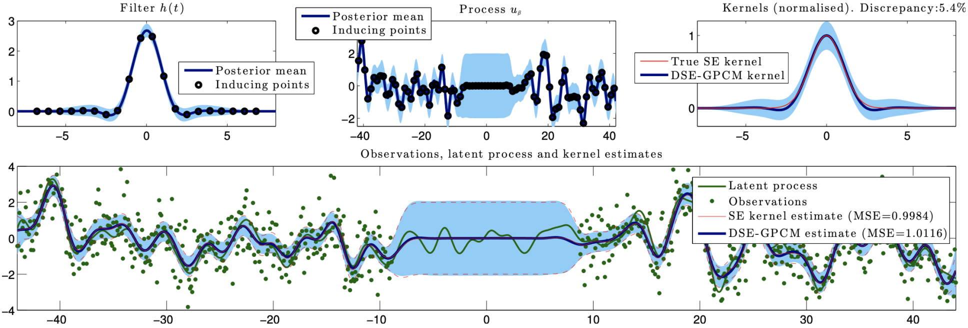

Figure 1: Posterior inference in GPCM from [14] (edited).

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Given an SDE and observation model

$$dx_t = f(x_t, t)dt + \Sigma^{1/2} d\beta_t \qquad \text{(prior SDE, p)}$$

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write $q(x_t)$ for its marginal distribution. KL between the exact SDE prior and the approximating SDE [1] is

$$\begin{aligned} KL\left[q || p\right] &= KL\left[q(x_0) || p(x_0)\right] + \\ &+ \frac{1}{2} \int_{t_0}^{t_1} \int (f(x, \tau) - g(x, \tau))^\top \Sigma^{-1} (f(x, \tau) - g(x, \tau)) q(x_n) dx_n d\tau. \end{aligned}$$

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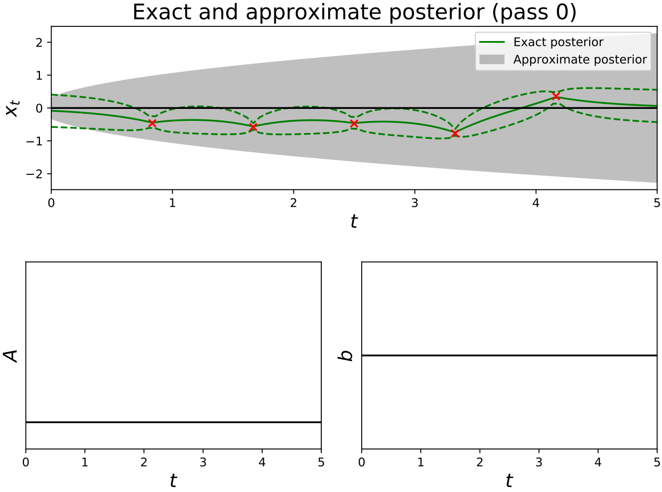

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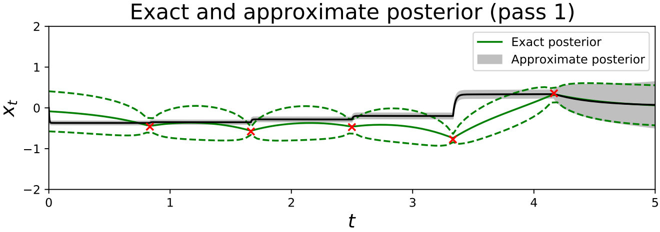

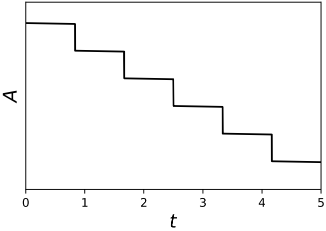

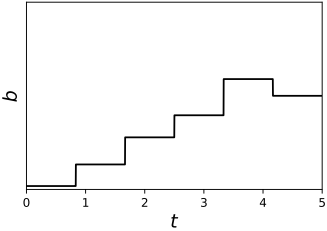

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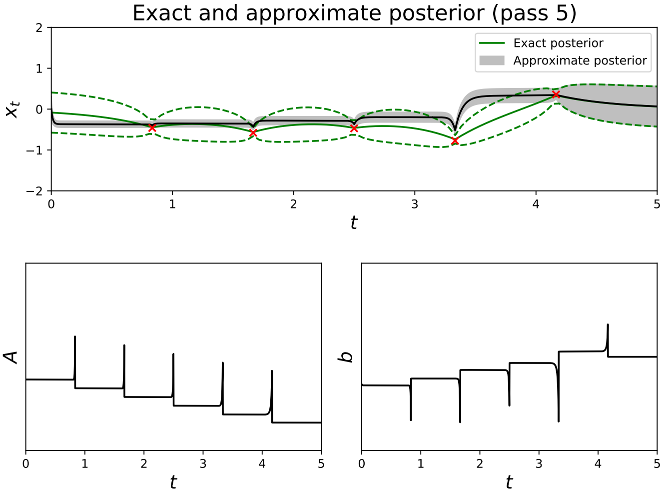

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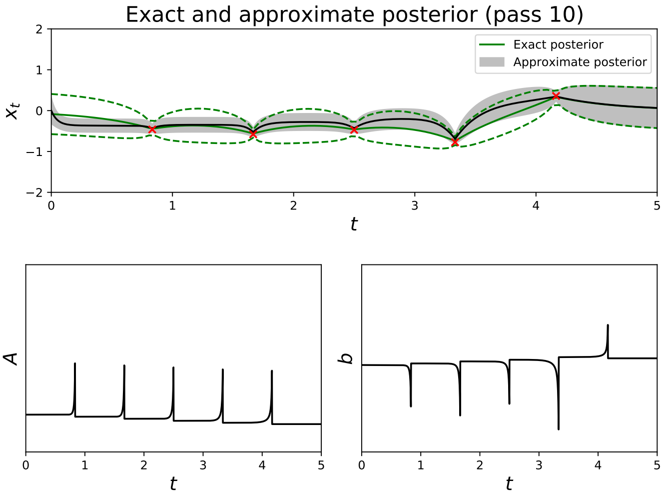

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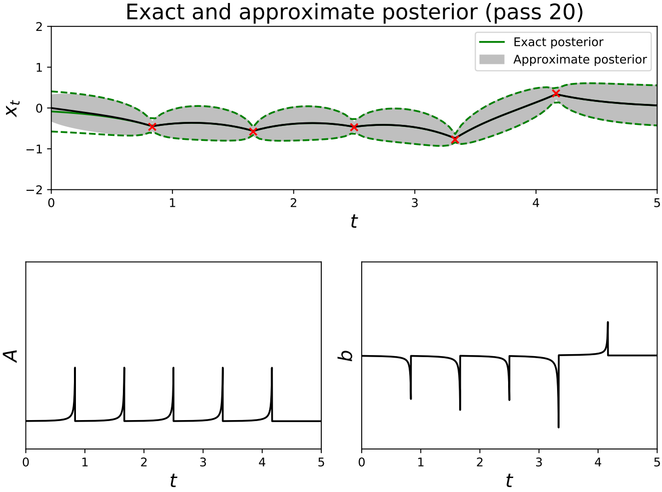

Stochastic integrals

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In regular calculus, these are equivalent. In stochastic calculus they are not – they give different answers!

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Stratonovich calculus [11]

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Scalable gradients for nonlinear SDEs [8]

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Uses KL between SDEs [1] and Stratonovich calculus [11] to train SDEs.

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Consider prior and approximating SDEs sharing the same noise model

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Train by optimising the ELBO

$$p(y_1, ..., y_n|\theta, \phi) \geq \mathbb{E}_q\left[\sum_{n=1}^{N} p(y_n|x_{t_n}) - \frac{1}{2}\int_0^T \left|\frac{f_\theta(x_\tau, \tau) - f_\phi(x_\tau, \tau)}{g(x_\tau, \tau)}\right|^2 d\tau\right],$$

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Stratonovich yields simplified equations for the dynamics of adjoint SDE.

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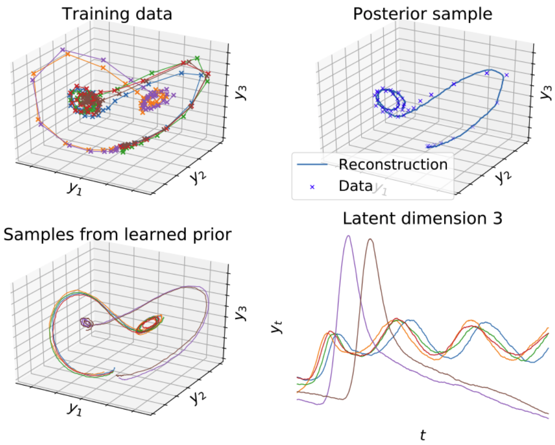

Figure 2: Training data, approximate q, learned p and latent dynamics. [8]

Thank you

Thank you for your attention!

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