Sparse GPs

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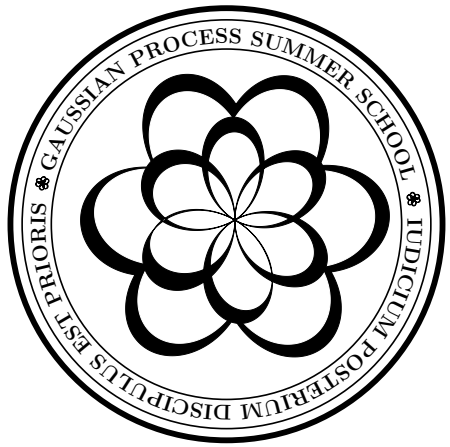

Overview

Motivation

Posteriors over function values

Posteriors over inducing points

Distributed Computation and Stochastic optimization

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Motivation

Inference in a GP has the following demands:

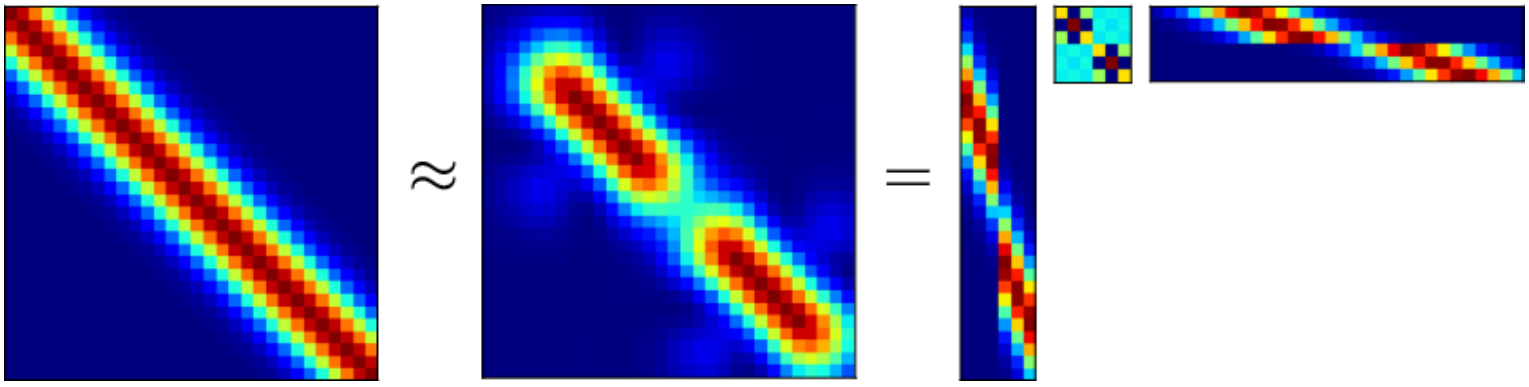
$$\begin{aligned} \text{Complexity:} \quad & \mathcal{O}(n^3) \\ \text{Storage:} \quad & \mathcal{O}(n^2) \end{aligned}$$

Inference in a *sparse* GP has the following demands:

$$\begin{aligned} \text{Complexity:} \quad & \mathcal{O}(nm^2) \\ \text{Storage:} \quad & \mathcal{O}(nm) \end{aligned}$$

where we get to pick m!

How to make computational savings



$$\mathbf{K}_{nn} \approx \mathbf{Q}_{nn} = \mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{K}_{mn}$$

Instead of inverting $\mathbf{K}_{nn}$, we make a low rank (or Nyström) approximation, and invert $\mathbf{K}_{mm}$ instead.

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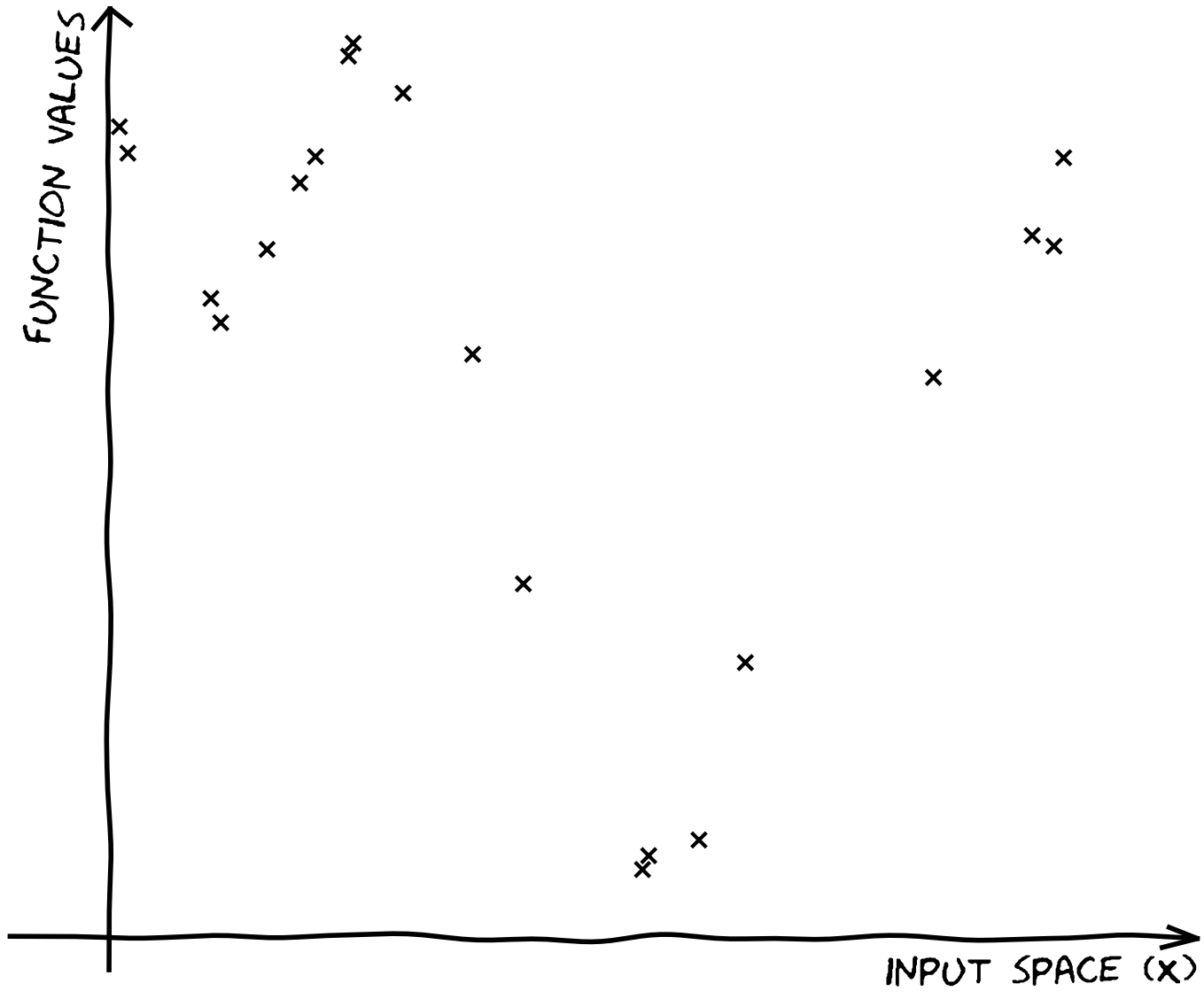
Posteriors over function values

Everything we want to do with a GP involves marginalising $\mathbf{f}$

- Predictions
- Marginal likelihood
- Estimating covariance parameters

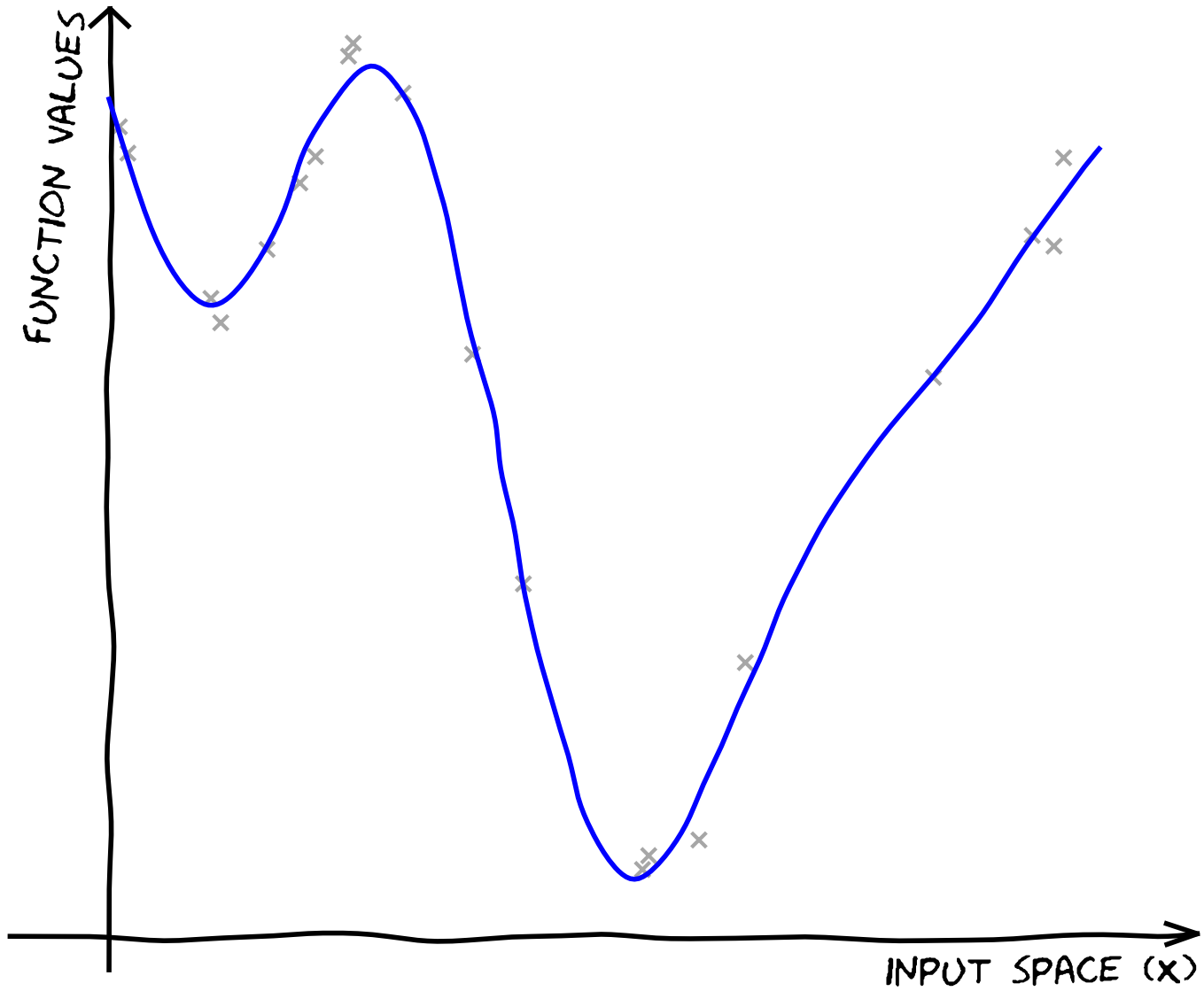
The posterior of $\mathbf{f}$ is the central object. This means inverting $\mathbf{K}_{nn}$.

$\mathbf{X}$, $\mathbf{y}$



X, y

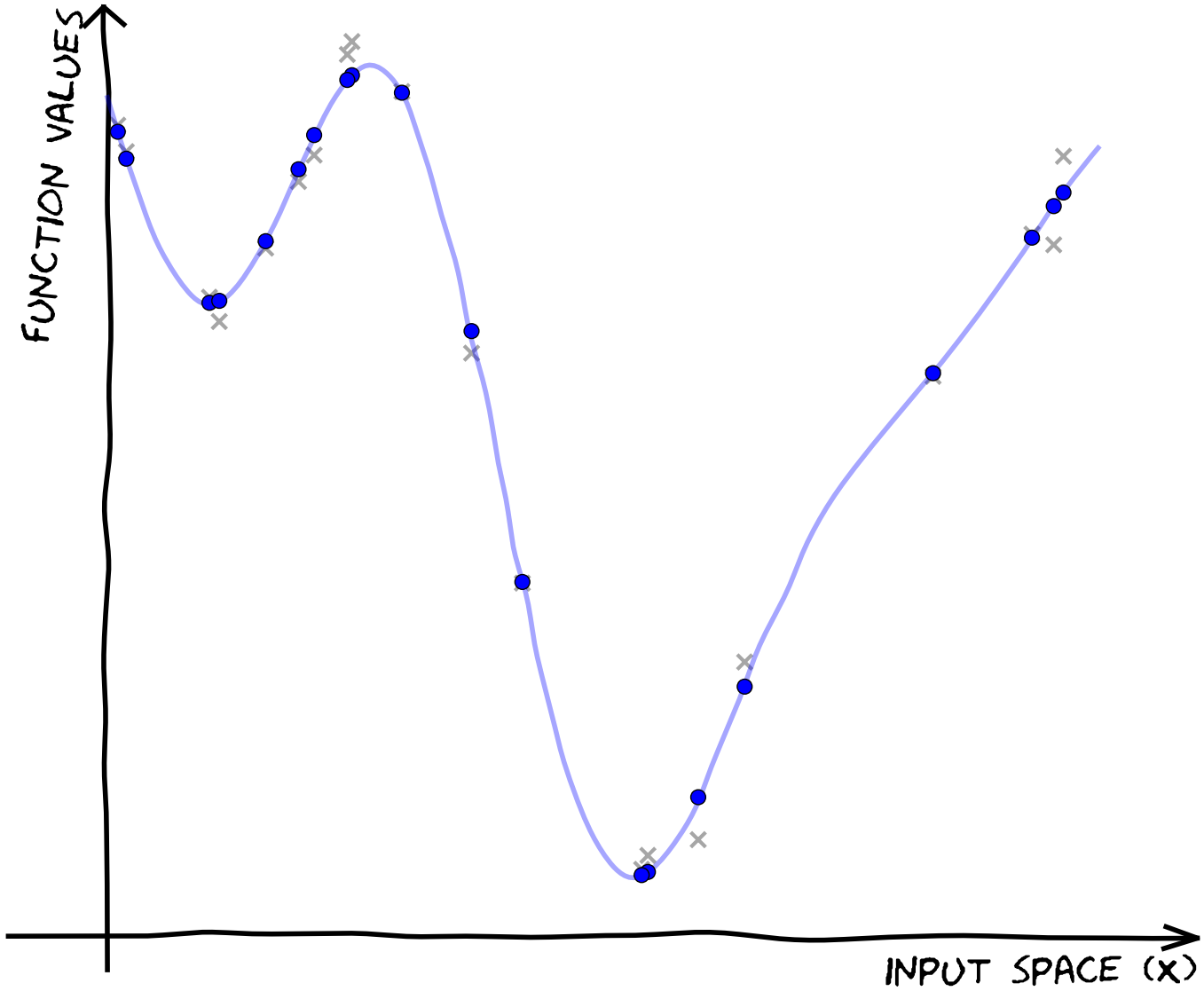
$f(\mathbf{x}) \sim \mathcal{GP}$



$\mathbf{X}$, $\mathbf{y}$

$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

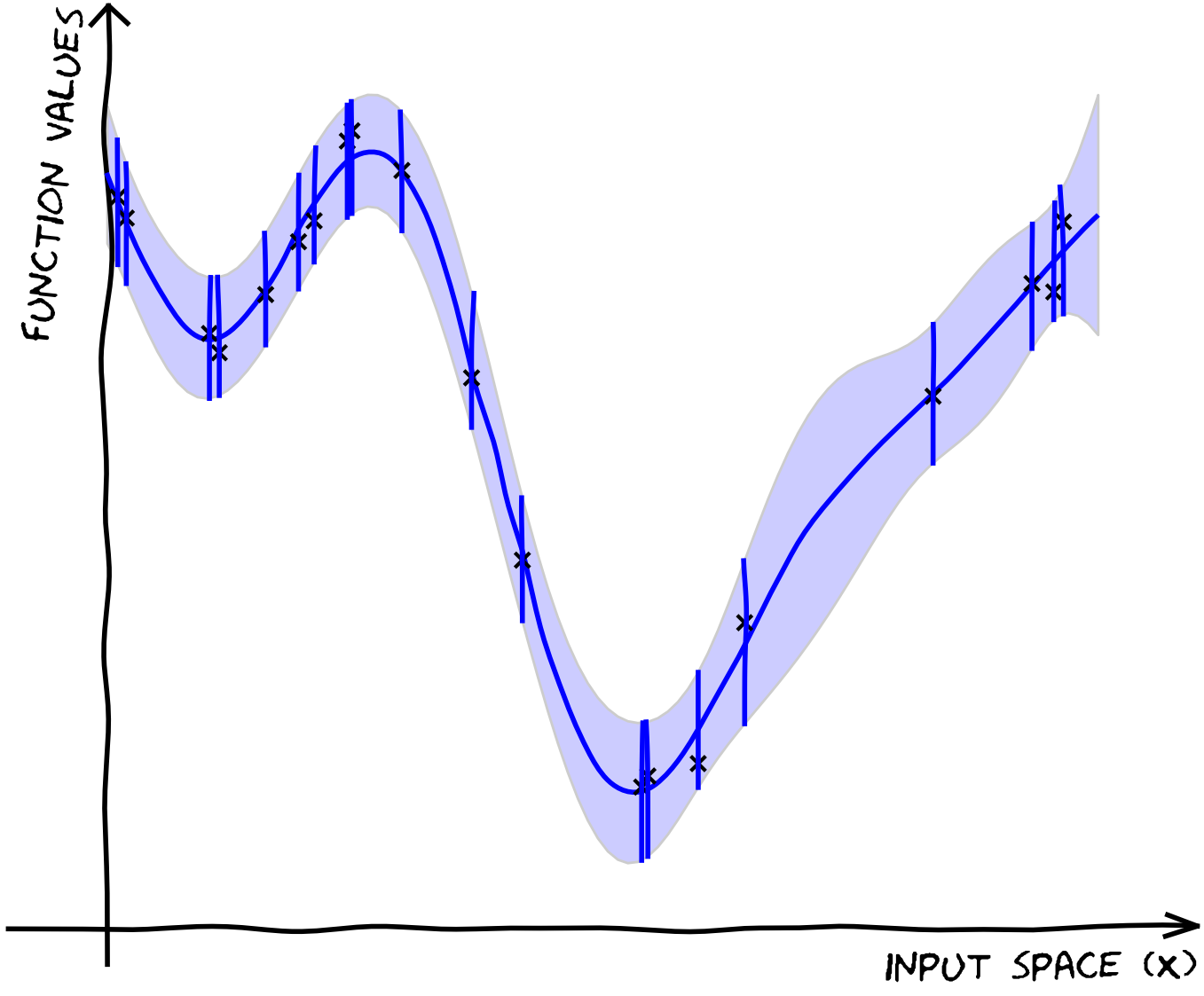


$\mathbf{X}$, $\mathbf{y}$

$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$



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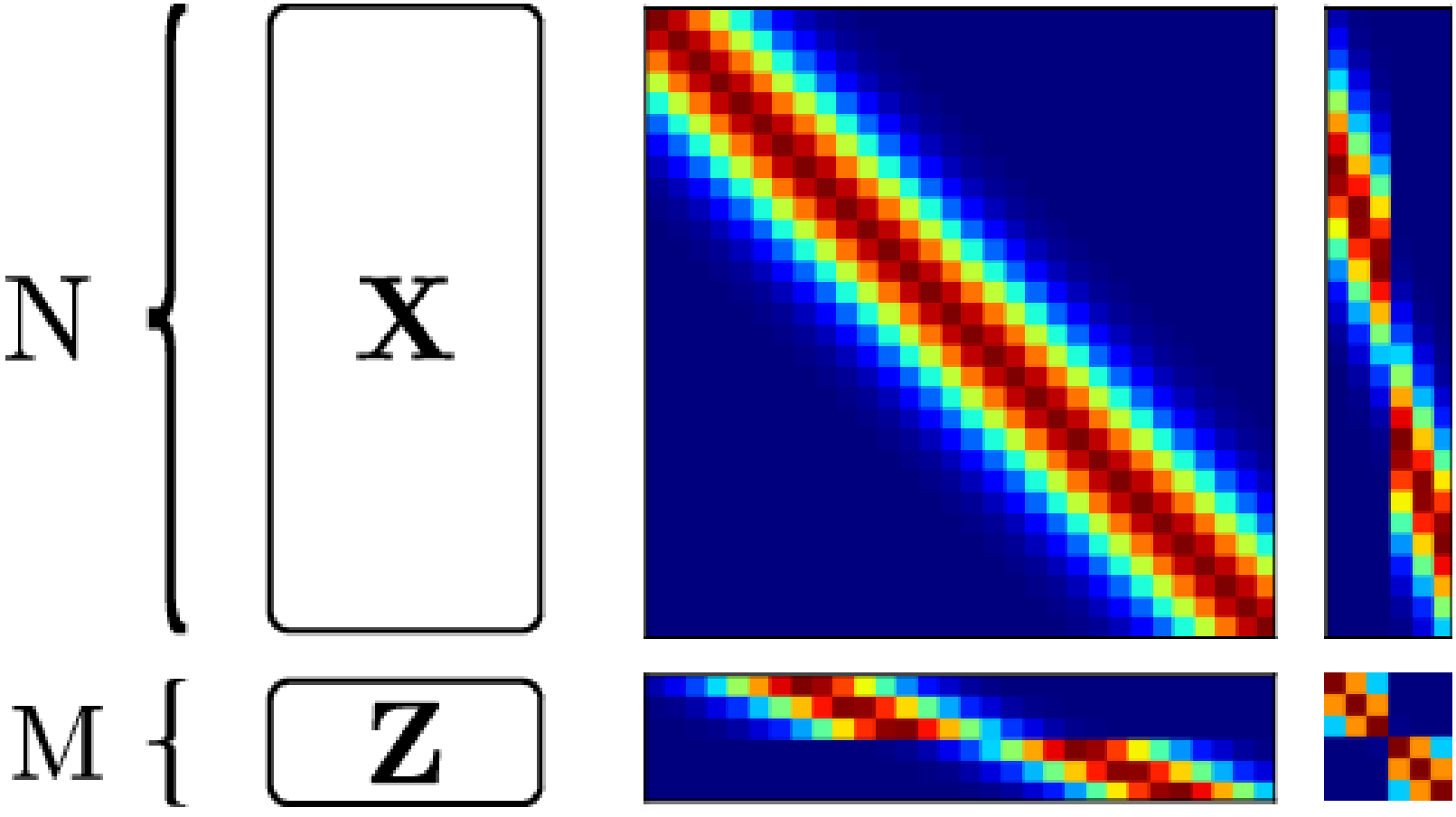
Introducing $\mathbf{u}$

Take and extra M points on the function, $\mathbf{u} = f(\mathbf{Z})$.

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}) p(\mathbf{u})$$

Introducing **u**



Introducing $\mathbf{u}$

Take and extra M points on the function, $\mathbf{u} = f(\mathbf{Z})$.

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}) p(\mathbf{u})$$

$$\begin{aligned} p(\mathbf{y} \mid \mathbf{f}) &= \mathcal{N}\left(\mathbf{y} | \mathbf{f}, \sigma^2 \mathbf{I}\right) \\ p(\mathbf{f} \mid \mathbf{u}) &= \mathcal{N}\left(\mathbf{f} | \mathbf{K}_{nm} \mathbf{K}_{mm1} \mathbf{u}, \widetilde{\mathbf{K}}\right) \\ p(\mathbf{u}) &= \mathcal{N}\left(\mathbf{u} | \mathbf{0}, \mathbf{K}_{mm}\right) \end{aligned}$$

$\mathbf{X}$, $\mathbf{y}$

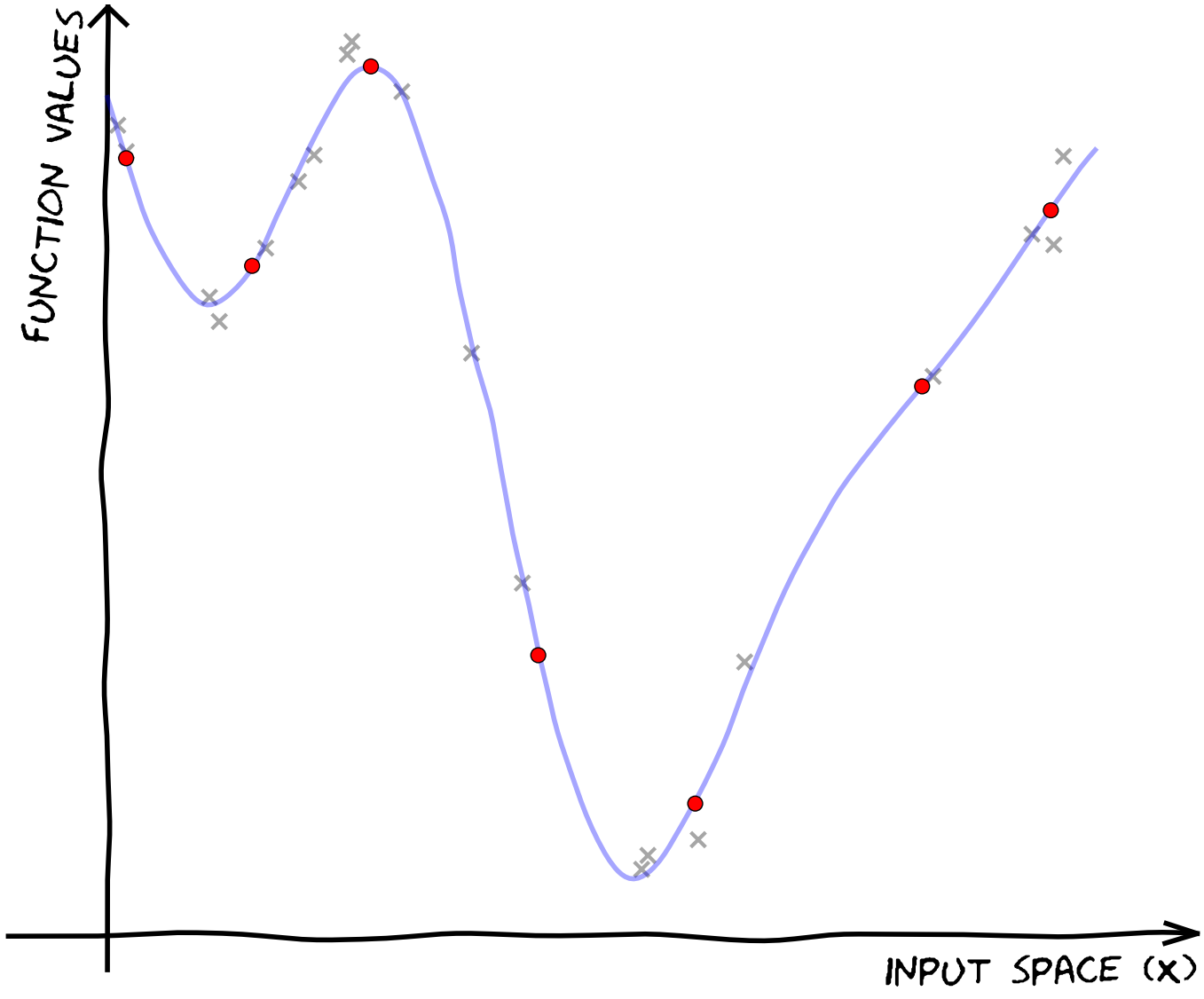
$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

$\mathbf{Z}$, $\mathbf{u}$

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



$\mathbf{X}$, $\mathbf{y}$

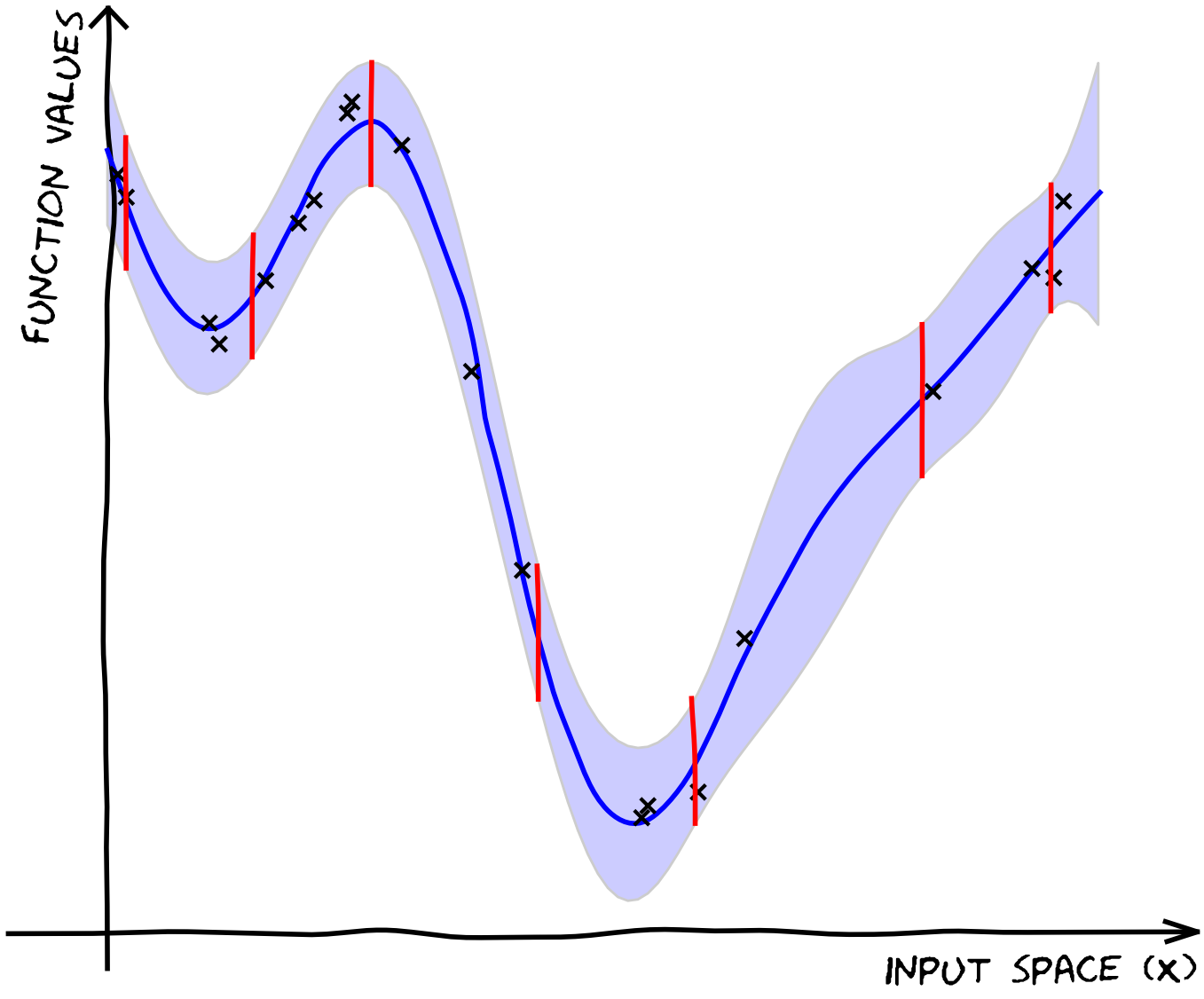
$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

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

$\tilde{p}(\mathbf{u} \mid \mathbf{y}, \mathbf{X})$



The alternative posterior

Instead of doing

$$p(\mathbf{f}\,|\,\mathbf{y},\mathbf{X}) = \frac{p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{X})}{\int p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{X})\mathrm{d}\mathbf{f}}$$

We'll do

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

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but $p(\mathbf{y}\,|\,\mathbf{u})$ involves inverting $\mathbf{K}_{nn}$

Variational marginalisation of $\mathbf{f}$

$$p(\mathbf{y} \mid \mathbf{u}) = \frac{p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u})}{p(\mathbf{f} \mid \mathbf{y}, \mathbf{u})}$$

Variational marginalisation of $\mathbf{f}$

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$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln p(\mathbf{y} \mid \mathbf{f}) + \ln \frac{p(\mathbf{f} \mid \mathbf{u})}{p(\mathbf{f} \mid \mathbf{y}, \mathbf{u})}$$

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$$\ln p(\mathbf{y} \mid \mathbf{u}) = \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u})}\Big[\ln p(\mathbf{y} \mid \mathbf{f}) \Big] + \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u})}\Big[\ln \frac{p(\mathbf{f} \mid \mathbf{u})}{p(\mathbf{f} \mid \mathbf{y}, \mathbf{u})} \Big]$$

Variational marginalisation of $\mathbf{f}$

$$p(\mathbf{y}\,|\,\mathbf{u}) = \frac{p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{u})}{p(\mathbf{f}\,|\,\mathbf{y},\mathbf{u})}$$

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$$\ln p(\mathbf{y}\,|\,\mathbf{u}) = \mathbb{E}_{p(\mathbf{f}\,|\,\mathbf{u})}\Big[\ln p(\mathbf{y}\,|\,\mathbf{f})\Big] + \mathbb{E}_{p(\mathbf{f}\,|\,\mathbf{u})}\Big[\ln \frac{p(\mathbf{f}\,|\,\mathbf{u})}{p(\mathbf{f}\,|\,\mathbf{y},\mathbf{u})}\Big]$$

$$\ln p(\mathbf{y}\,|\,\mathbf{u}) = \tilde{p}(\mathbf{y}\,|\,\mathbf{u}) + \mathrm{KL}[p(\mathbf{f}|\mathbf{u})\|p(\mathbf{f}\,|\,\mathbf{y},\mathbf{u})]$$

No inversion of $\mathbf{K}_{nn}$ required

Variational marginalisation of $\mathbf{f}$ (another way)

$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln \int p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}) \mathrm{d}\mathbf{f}$$

Variational marginalisation of $\mathbf{f}$ (another way)

$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln \int p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}) \mathrm{d}\mathbf{f}$$

$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X})} \left[p(\mathbf{y} \mid \mathbf{f}) \right]$$

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$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln \int p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}) \mathrm{d}\mathbf{f}$$

$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X})} \left[p(\mathbf{y} \mid \mathbf{f}) \right]$$

$$\ln p(\mathbf{y} \mid \mathbf{u}) \geq \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X})} \left[\ln p(\mathbf{y} \mid \mathbf{f}) \right] \triangleq \ln \tilde{p}(\mathbf{y} \mid \mathbf{u})$$

Variational marginalisation of $\mathbf{f}$ (another way)

$$\ln p(\mathbf{y} \mid \mathbf{u}) = \ln \int p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}) \mathrm{d}\mathbf{f}$$

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No inversion of $\mathbf{K}_{nn}$ required

An approximate likelihood

$$\tilde{p}(\mathbf{y}\,|\,\mathbf{u}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_i|\mathbf{k}_{mn}^\top \mathbf{K}_{mm}^{-1}\mathbf{u}, \sigma^2\right) \exp\left\{-\frac{1}{2\sigma^2}\left(k_{nn} - \mathbf{k}_{mn}^\top \mathbf{K}_{mm}^{-1}\mathbf{k}_{mn}\right)\right\}$$

A straightforward likelihood approximation, and a penalty term

Now we can marginalise $\mathbf{u}$

$$\tilde{p}(\mathbf{u} \mid \mathbf{y}, \mathbf{Z}) = \frac{\tilde{p}(\mathbf{y} \mid \mathbf{u}) p(\mathbf{u} \mid \mathbf{Z})}{\int \tilde{p}(\mathbf{y} \mid \mathbf{u}) p(\mathbf{u} \mid \mathbf{Z}) \mathrm{d}\mathbf{u}}$$

- Computing the (approximate) posterior costs $O(nm^2)$
- We also get a lower bound of the marginal likelihood
- This is the standard variational sparse GP (**?**).

The marginal likelihood lower bound

$$\begin{aligned}\tilde{p}(\mathbf{y}) &= \int \tilde{p}(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})\mathrm{d}\mathbf{u} \\ &= \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{K}_{mn} + \sigma^2\mathbf{I}\right) \exp \sum_i \left\{ -\tfrac{1}{2\sigma^2}\left(k_{nn} - \mathbf{k}_{mn}^\top \mathbf{K}_{mm}^{-1}\mathbf{k}_{mn}\right)\right\}\end{aligned}$$

Optimisation

The variational objective $\ln \tilde{p}(\mathbf{y})$ is a function of

- the parameters of the covariance function $\boldsymbol{\theta}$
- the inducing inputs, $\mathbf{Z}$

Strategy: jointly optimize $\boldsymbol{\theta}$ and $\mathbf{Z}$.

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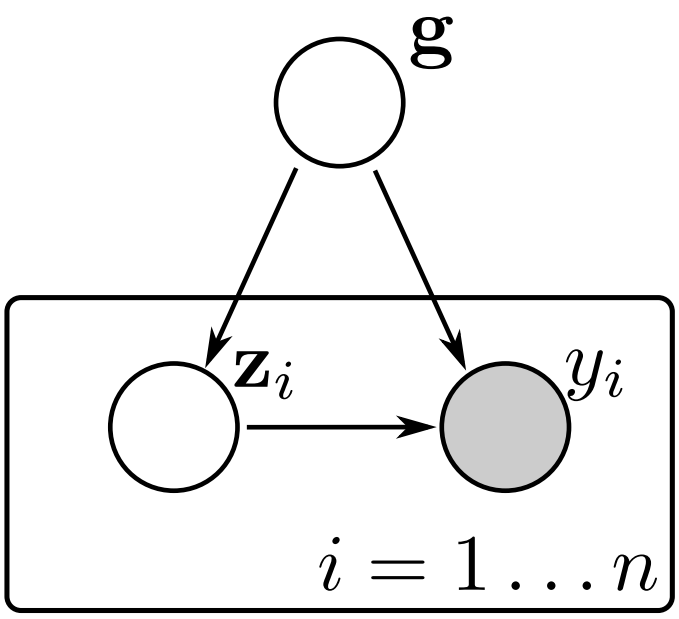
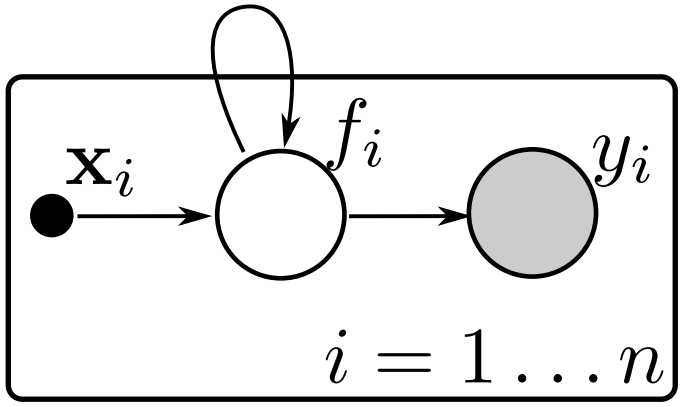
Variational Bayes

- Approximate the true posterior distribution with a simpler one.
- Usually assume factorisation in the approximation
- Iterative 'update' procedure (like EM)
- Can be seen as a coordinate-wise steepest ascent method

Stochastic Variational Inference

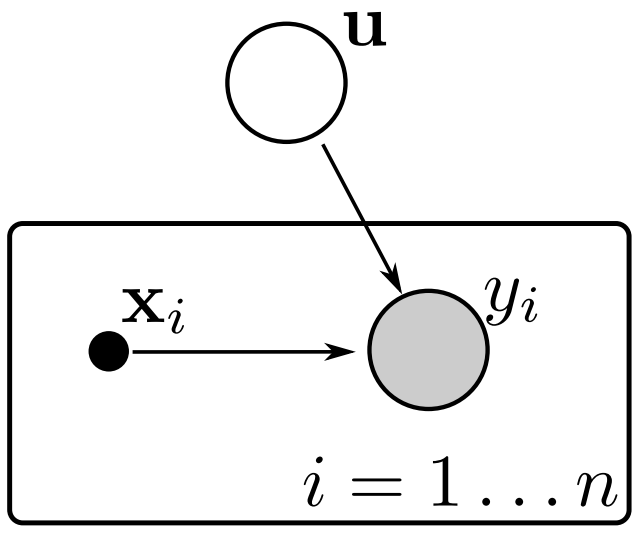
- Combine the ideas of stochastic optimisation with Variational inference
- example: apply Latent Dirichlet allocation to project Gutenberg
- Can apply variational techniques to Big Data
- How could this work in GPs?





Maintain the factorisation!

- The variational marginalisation of $\mathbf{f}$ introduced factorisation across the datapoints (conditioned on $\mathbf{u}$)
- Marginalising $\mathbf{u}$ re-introdcuced dependencies between the data
- Solution: a variational treatment of $\mathbf{u}$



$$\log p(\mathbf{y}\,|\,\mathbf{X}) \geq \left\langle \log \tilde{p}(\mathbf{y}\,|\,\mathbf{u}) + \log p(\mathbf{u}) - \log q(\mathbf{u}) \right\rangle_{q(\mathbf{u})} \triangleq \mathcal{L}. \tag{1}$$

$$\begin{aligned} \mathcal{L} = \sum_{i=1}^{n} \Bigg\{ & \log \mathcal{N}\left(y_i | \mathbf{k}_{mn}^{\top} \mathbf{K}_{mm}^{-1} \mathbf{m}, \beta^{-1}\right) \\ & - \frac{1}{2}\beta \tilde{k}_{i,i} - \frac{1}{2}\mathrm{tr}\left(\mathbf{S}\mathbf{\Lambda}_i\right) \Bigg\} \\ & - \mathrm{KL}\left(q(\mathbf{u}) \,\|\, p(\mathbf{u})\right) \end{aligned} \tag{2}$$

Optimisation

The variational objective $\mathcal{L}$ is a function of

- the parameters of the covariance function
- the parameters of $q(\mathbf{u})$
- the inducing inputs, $\mathbf{Z}$

Strategy: set $\mathbf{Z}$. Take the data in small minibatches, take stochastic gradient steps in the covariance function parameters, stochastic *natural* gradient steps in the parameters of $q(\mathbf{u})$.

Natural Gradients

$$\tilde{\mathbf{g}}(\boldsymbol{\theta}) = G(\boldsymbol{\theta})^{-1}\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\eta}}.$$

$$\begin{aligned}
\boldsymbol{\theta}_{2(t+1)} &= -\frac{1}{2}\mathbf{S}\mathbf{1}_{(t+1)} \\
&= -\frac{1}{2}\mathbf{S}\mathbf{1}_{(t)} + \ell\left(-\frac{1}{2}\boldsymbol{\Lambda} + \frac{1}{2}\mathbf{S}\mathbf{1}_{(t)}\right), \\
\boldsymbol{\theta}_{1(t+1)} &= \mathbf{S}\mathbf{1}_{(t+1)}\mathbf{m}_{(t+1)} \\
&= \mathbf{S}\mathbf{1}_{(t)}\mathbf{m}_{(t)} + \ell\left(\beta\mathbf{K}_{mm}\mathbf{1}\mathbf{K}_{mn}\mathbf{y} - \mathbf{S}\mathbf{1}_{(t)}\mathbf{m}_{(t)}\right),
\end{aligned}$$