Sparse GP Approximations

An Introduction to Pseudo-Input Methods

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Agenda

1. Standard GP Recap
2. Model Augmentation
3. SPGP: More Hyperparameters
4. SGPR: A Variational Approach
5. SVGP: Stochastic Optimization

Standard GP Recap

Gaussian Processes

Definition

A **Gaussian Process (GP)** is a collection of random variables $\{F_x\}$, any finite subset of which has a joint Gaussian distribution.

- Extension of Gaussians to (infinite) function spaces
- F_x models the function value $f(x)$

Mean and Kernel Functions

A GP is completely determined by two functions.

Mean function $\mu_f(x) = \mathbb{E}[f(x)]$

Kernel function $\mathcal{K}(x, x') = \mathrm{cov}[f(x), f(x')]$

GP Posterior

GP predictive posterior

The predictive posterior for a function $f \sim \mathcal{GP}(\mathbf{0}, \mathcal{K})$ with observations $\boldsymbol{y} = f(\boldsymbol{X}) + \mathcal{N}(\mathbf{0}, \sigma_n^2 \mathbf{I})$ is

$$\mathrm{p}(\boldsymbol{f}_* \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{X}_*) = \mathcal{N}(\boldsymbol{f}_* \mid \boldsymbol{\mu}_*, \Sigma_*), \text{ with}$$

$$\boldsymbol{\mu}_* = \boldsymbol{K}_{*f} \left(\boldsymbol{K}_{ff} + \sigma_n^2 \mathbf{I}\right)^{-1} \boldsymbol{y}$$

$$\Sigma_* = \boldsymbol{K}_{**} - \boldsymbol{K}_{*f} \left(\boldsymbol{K}_{ff} + \sigma_n^2 \mathbf{I}\right)^{-1} \boldsymbol{K}_{f*}.$$

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- We always need to consider the **whole dataset**
- The matrix inversion is $\mathcal{O}(N^3)$ in time and $\mathcal{O}(N^2)$ in space
- With precomputation we still have to pay $\mathcal{O}(N^2)$ for Σ_*

GP Marginal Likelihood

GP marginal likelihood

We usually use the marginal likelihood $\mathcal{L}$ for model selection with maximum likelihood

$$
\begin{aligned}
\mathcal{L}^{\mathrm{GP}}(\boldsymbol{\theta}) &= -\log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}) \\
&= -\log \int \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f}, \boldsymbol{\theta})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{\theta})\, \mathrm{d}\boldsymbol{f} \\
&= -\log \int \mathcal{N}(\boldsymbol{y} \mid \boldsymbol{f}, \sigma_n^2 \mathbf{I})\, \mathcal{N}(\boldsymbol{f} \mid \mathbf{0}, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}})\, \mathrm{d}\boldsymbol{f} \\
&= -\log \mathcal{N}(\boldsymbol{y} \mid \mathbf{0}, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} + \sigma_n^2 \mathbf{I}) \\
&= \frac{1}{2} \boldsymbol{y}^{\mathsf{T}} \left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} + \sigma_n^2 \mathbf{I}\right)^{-1} \boldsymbol{y} + \frac{1}{2} \log \left| \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} + \sigma_n^2 \mathbf{I} \right| + \frac{N}{2} \log(2\pi).
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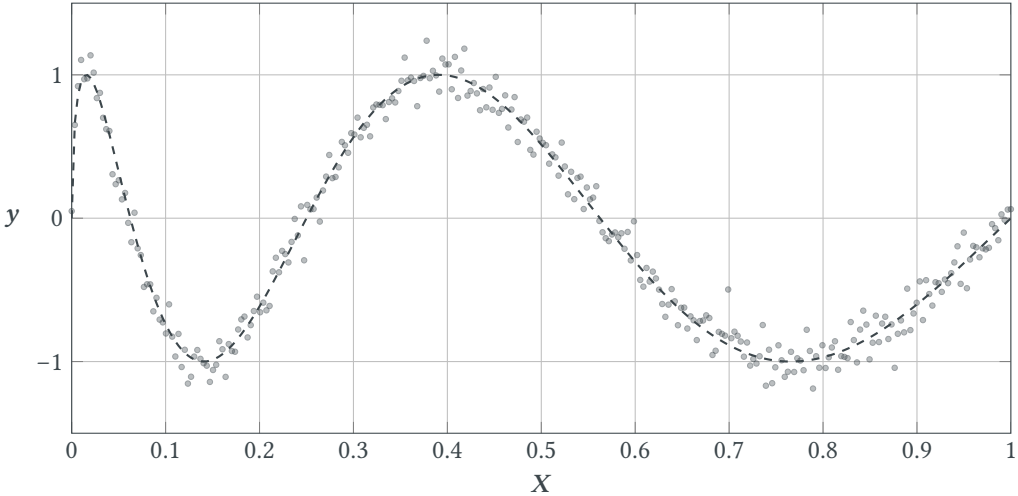
\end{aligned}
$$

- Choose $\boldsymbol{\theta}^* \in \operatorname{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta})$
- $\mathcal{L}$ is also $\mathcal{O}(N^3)$ in time and $\mathcal{O}(N^2)$ in space

Reducing the Data Set



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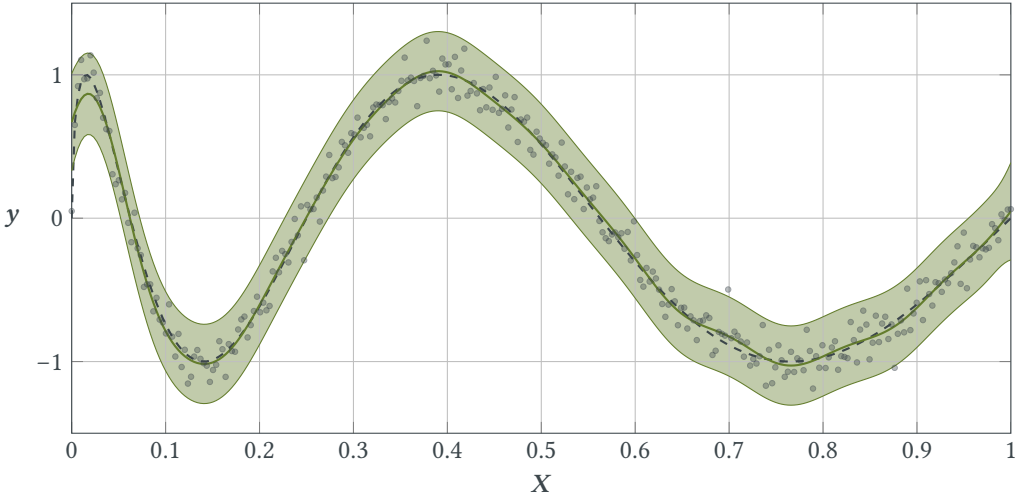

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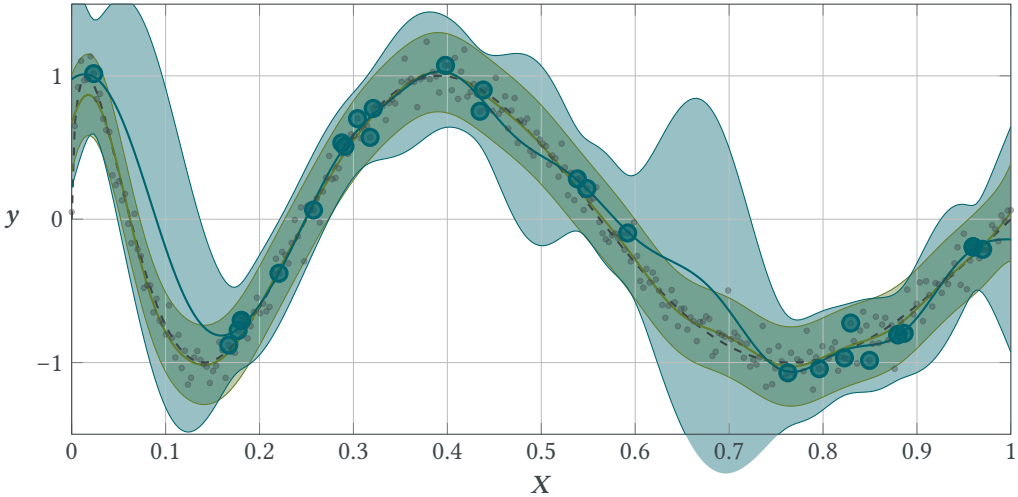

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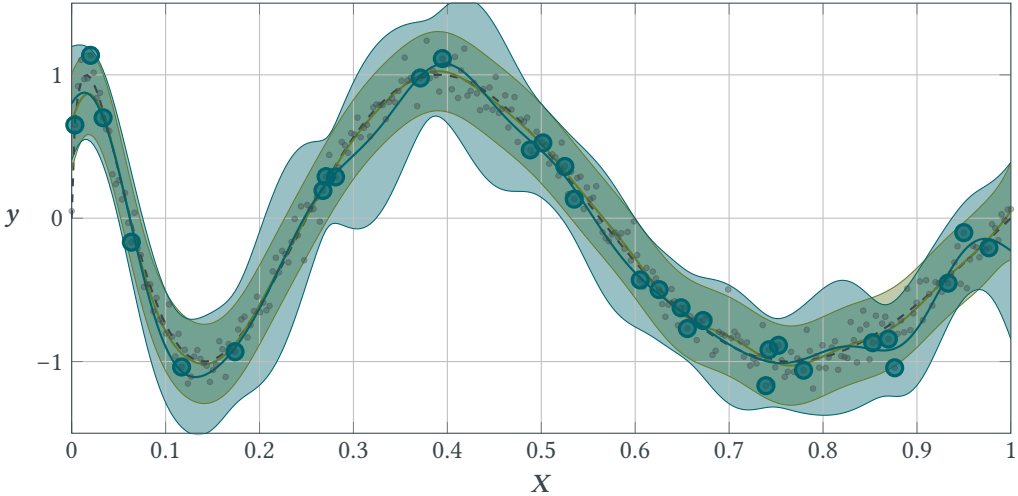

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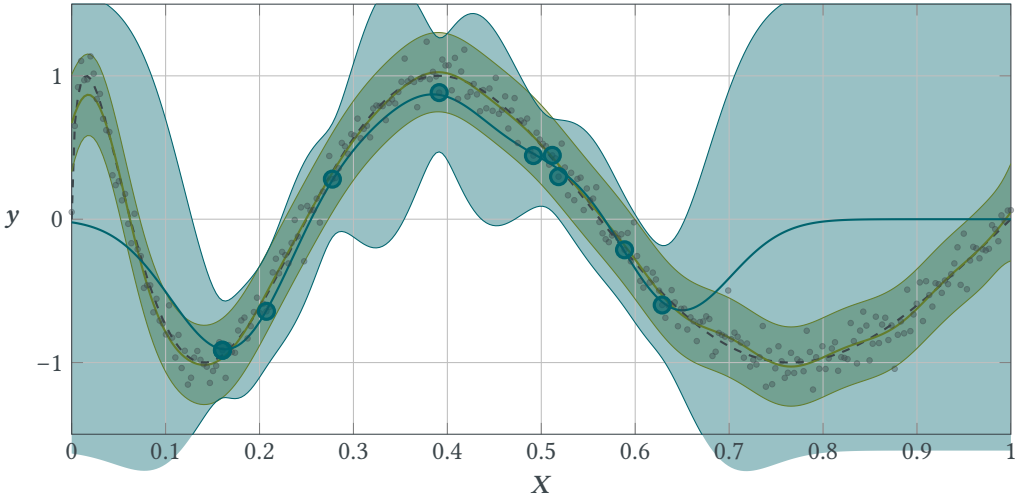

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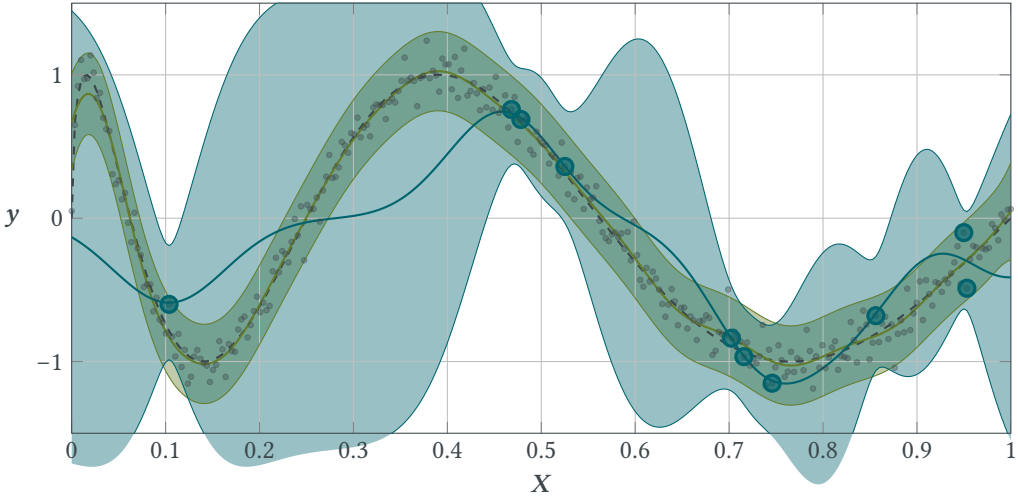

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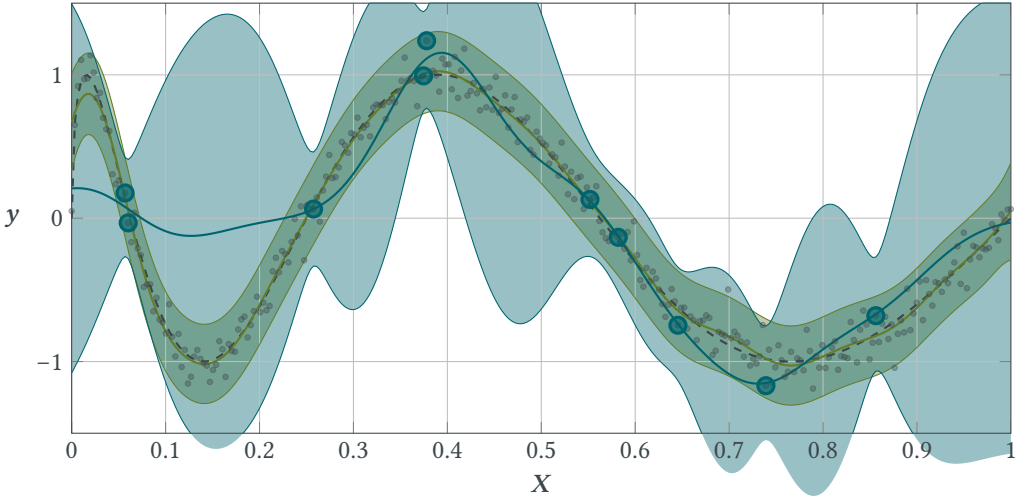

Can we somehow not ignore most of the data?

Model Augmentation

Pseudo Data

- Keep N original observations $\mathcal{D} = (X, \boldsymbol{y})$
- Assume M different **pseudo data points** $\bar{\mathcal{D}} = (Z, \boldsymbol{u})$
- $\boldsymbol{u} = f(Z)$ are **observations of the latent function**
- The $\bar{\mathcal{D}}$ are also called **inducing points**

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Augmented GP Joint

Due to the consistency of GPs, the data and pseudo data are **jointly Gaussian**.

$$\mathrm{p}(\boldsymbol{f}, \boldsymbol{u}) = \mathcal{N}\left(\begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{u} \end{pmatrix} \middle| \, \boldsymbol{0}, \begin{pmatrix} \boldsymbol{K}_{\boldsymbol{ff}} & \boldsymbol{K}_{\boldsymbol{fu}} \\ \boldsymbol{K}_{\boldsymbol{uf}} & \boldsymbol{K}_{\boldsymbol{uu}} \end{pmatrix} \right)$$

- We usually drop the conditioning on $\boldsymbol{X}$, $\boldsymbol{Z}$ and $\boldsymbol{\theta}$

Conditioning on the Pseudo Data

Augmented GP conditional likelihood

Because $\mathrm{p}(\boldsymbol{f}, \boldsymbol{u})$ is Gaussian, we can calculate the conditional likelihood easily.

$$
\begin{aligned}
\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{u}) &= \int \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{d}\boldsymbol{f} \\
&= \int \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{f}, \sigma_n^2 \mathbf{I}\right) \mathcal{N}\left(\boldsymbol{f} \,\middle|\, \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{K}_{\boldsymbol{uf}}\right) \mathrm{d}\boldsymbol{f} \\
&= \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{K}_{\boldsymbol{uf}} + \sigma_n^2 \mathbf{I}\right) \\
&= \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}} + \sigma_n^2 \mathbf{I}\right)
\end{aligned}
$$

- We call $\boldsymbol{Q}_{\boldsymbol{ff}}$ the low rank covariance

Conditioning on the Pseudo Data

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&= \int \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{f}, \sigma_n^2 \mathbf{I}\right) \mathcal{N}\left(\boldsymbol{f} \,\middle|\, \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{K}_{\boldsymbol{uf}}\right) \mathrm{d}\boldsymbol{f} \\
&= \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{K}_{\boldsymbol{uf}} + \sigma_n^2 \mathbf{I}\right) \\
&= \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{fu}} \boldsymbol{K}_{\boldsymbol{uu}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}} + \sigma_n^2 \mathbf{I}\right)
\end{aligned}
$$

- We call $\boldsymbol{Q}_{\boldsymbol{ff}}$ the low rank covariance
- This is just the predictive distribution again
- Assuming iid data, we can calculate the likelihood in (at most) $\mathcal{O}(N^2)$

But what use is it if we have no idea about $\tilde{D}$?

SPGP: More Hyperparameters

SPGP

Sparse Pseudo-input Gaussian Process (SPGP)

We interpret the augmented model as a new regression problem arising from $\tilde{\mathcal{D}}$.

- Assume **conditional independence of f (and y) given $\boldsymbol{u}$**
- We can choose Z and only have to handle $\boldsymbol{u}$

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- We can choose Z and only have to handle $\boldsymbol{u}$

$$
\begin{aligned}
\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{u}) &= \prod_n \mathrm{p}(y_n \mid \boldsymbol{u}) \\
&= \mathcal{N}\left(\boldsymbol{y} \,\middle|\, K_{fu} K_{uu}^{-1} \boldsymbol{u}, \operatorname{diag}(K_{ff} - Q_{ff}) + \sigma_n^2 \mathbf{I}\right)
\end{aligned}
$$

Using the low rank covariance

$$
Q_{ab} := K_{au} K_{uu}^{-1} K_{ub}
$$

SPGP Marginal Likelihood

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$$
\begin{aligned}
\mathcal{L}^{\text{SPGP}}(\boldsymbol{\theta}) &= -\log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}) \\
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&= -\log \int \mathcal{N}\left(\boldsymbol{y} \,\middle|\, K_{fu} K_{uu}^{-1} \boldsymbol{u}, \operatorname{diag}(K_{ff} - Q_{ff}) + \sigma_n^2 \mathbf{I}\right) \mathcal{N}(\boldsymbol{u} \mid \mathbf{0}, K_{uu})\, \mathrm{d}\boldsymbol{u} \\
&= -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, Q_{ff} + \operatorname{diag}(K_{ff} - Q_{ff}) + \sigma_n^2 \mathbf{I}\right)
\end{aligned}
$$

- We do not know $\boldsymbol{u} = f(Z)$, so we **marginalize**
- Use the original **GP prior** $\mathrm{p}(\boldsymbol{u} \mid \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{u} \mid \mathbf{0}, K_{uu})$
- **Joint optimization of Z** with other hyperparameters
- Time-complexity is $\mathcal{O}(NM^2)$, **linear** in the data

Interpretation of the SPGP

$$\mathcal{L}^{\text{GP}}(\boldsymbol{\theta}) = -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{K}_{ff} + \sigma_n^2 \mathbf{I}\right)$$

$$\mathcal{L}^{\text{SPGP}}(\boldsymbol{\theta}) = -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{Q}_{ff} + \operatorname{diag}(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}) + \sigma_n^2 \mathbf{I}\right)$$

SPGP kernel

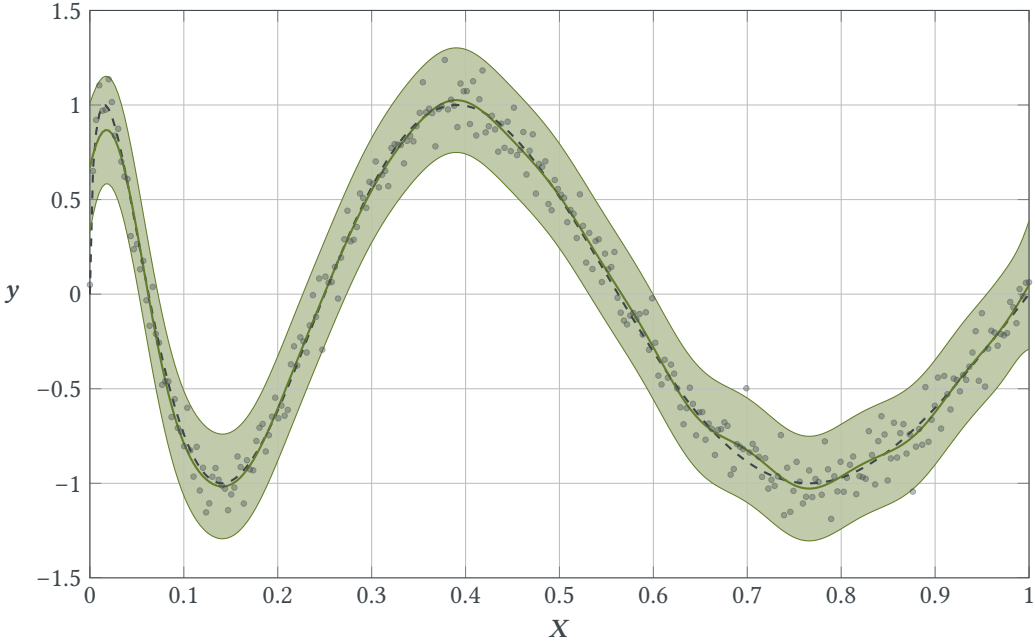
The SPGP derived from $\mathcal{GP}(\mathbf{0}, \mathcal{K})$ is a **new Gaussian Process $\mathcal{GP}(\mathbf{0}, \mathcal{K}^{\text{SPGP}})$** with

$$\mathcal{K}^{\text{SPGP}}(\boldsymbol{x}, \boldsymbol{x}') = \mathcal{Q}(\boldsymbol{x}, \boldsymbol{x}') + \delta_{\boldsymbol{x}\boldsymbol{x}'} \left(\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') - \mathcal{Q}(\boldsymbol{x}, \boldsymbol{x}')\right)$$

$$\mathcal{Q}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{K}_{\boldsymbol{x}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{x}'}$$

- $\mathcal{K}^{\text{SPGP}}$ is heavily dependent on $\boldsymbol{Z}$ and no longer interpretable
- It has a potentially **huge number of (hyper-)parameters**...
- ...which makes the model prone to **overfitting**

SPGP Showcase



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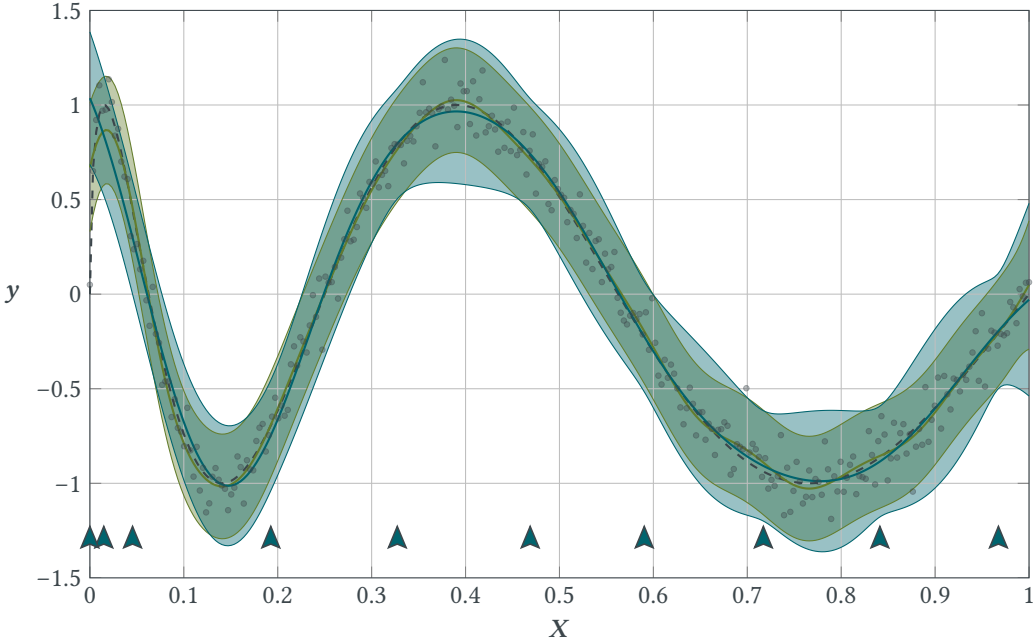

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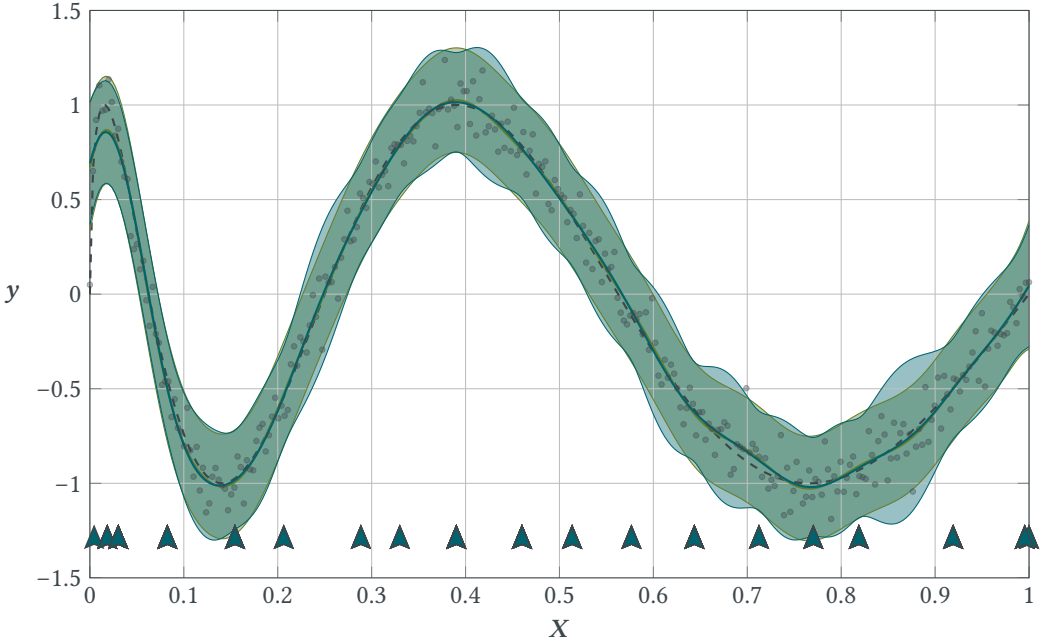

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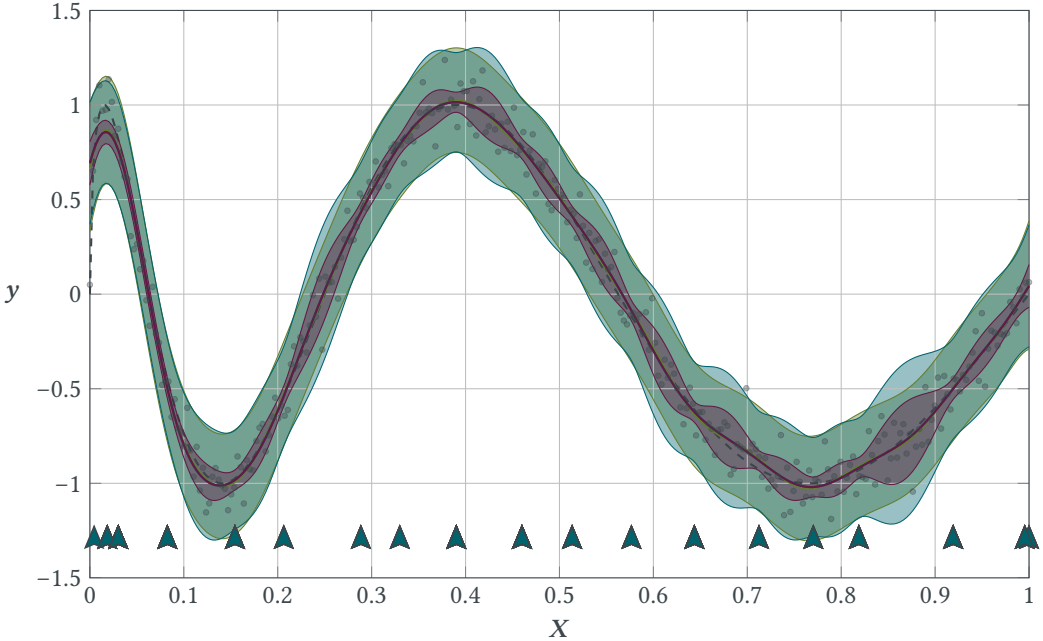

SGPR: A Variational Approach

SGPR

Sparse Gaussian Process Regression (SGPR)

We want to variationally approximate the original Gaussian Process.

- Derive a variational lower bound on the original marginal likelihood $\mathcal{L}^{\mathrm{GP}}$
- Consider a custom variational scheme $\mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) = \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})$

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- Inspect the augmented predictive posterior

$$\mathrm{p}(\boldsymbol{f}^* \mid \boldsymbol{y}) = \int \mathrm{p}(\boldsymbol{f}^* \mid \boldsymbol{f}, \boldsymbol{u})\, \mathrm{p}(\boldsymbol{f}, \boldsymbol{u} \mid \boldsymbol{y})\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u}$$

- **$\boldsymbol{u}$ is optimal** if $\boldsymbol{f}^*$ and $\boldsymbol{f}$ are **independent given $\boldsymbol{u}$**

$$\mathrm{p}(\boldsymbol{f}^* \mid \boldsymbol{f}, \boldsymbol{u}) = \mathrm{p}(\boldsymbol{f}^* \mid \boldsymbol{u})$$

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

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- We will approximate this situation with

$$\mathrm{q}(\boldsymbol{f}^*) = \int \mathrm{p}(\boldsymbol{f}^* \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} = \int \mathrm{p}(\boldsymbol{f}^* \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{u}$$

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= -\log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}, Z, \boldsymbol{u}) \\
&= -\log \int \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\log \int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&\geq -\int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
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&= -\log \int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&\geq -\int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u}
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= -\log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}, Z, \boldsymbol{u}) \\
&= -\log \int \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\log \int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&\geq -\int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u}
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= -\log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}, Z, \boldsymbol{u}) \\
&= -\log \int \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\log \int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&\geq -\int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u}
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= -\log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}, Z, \boldsymbol{u}) \\
&= -\log \int \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\log \int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&\geq -\int \mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{f}, \boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u}) \log \frac{\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\, \mathrm{d}\boldsymbol{f}\, \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f})\, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u}
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathbb{E}_{\mathrm{p}(\boldsymbol{f}|\boldsymbol{u})}[\log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})] &= \int \mathrm{p}(\boldsymbol{f}\,|\,\boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})\,\mathrm{d}\boldsymbol{f} \\
&= \int \log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{f}, \sigma_n^2 \mathbf{I}\right) \mathcal{N}\left(\boldsymbol{f} \,\middle|\, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}}\right) \mathrm{d}\boldsymbol{f} \\
&= \log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{u}, \sigma_n^2 \mathbf{I}\right) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}}\right) \\
&= \log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}}\right)
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathbb{E}_{\mathrm{p}(\boldsymbol{f}|\boldsymbol{u})}[\log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})] &= \int \mathrm{p}(\boldsymbol{f}\,|\,\boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})\,\mathrm{d}\boldsymbol{f} \\
&= \int \log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{f}, \sigma_n^2 \mathbf{I}\right) \mathcal{N}\left(\boldsymbol{f} \,\middle|\, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}}\right) \mathrm{d}\boldsymbol{f} \\
&= \log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{u}, \sigma_n^2 \mathbf{I}\right) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}}\right) \\
&= \log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}}\right)
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathbb{E}_{\mathrm{p}(\boldsymbol{f}|\boldsymbol{u})}[\log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})] &= \int \mathrm{p}(\boldsymbol{f}\mid\boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})\,\mathrm{d}\boldsymbol{f} \\
&= \int \log \mathcal{N}\left(\boldsymbol{y}\,\middle|\,\boldsymbol{f}, \sigma_n^2\mathbf{I}\right) \mathcal{N}\left(\boldsymbol{f}\,\middle|\,\boldsymbol{K}_{\boldsymbol{fu}}\boldsymbol{K}_{\boldsymbol{uu}}^{-1}\boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}}\right) \mathrm{d}\boldsymbol{f} \\
&= \log \mathcal{N}\left(\boldsymbol{y}\,\middle|\,\boldsymbol{K}_{\boldsymbol{fu}}\boldsymbol{K}_{\boldsymbol{uu}}^{-1}\boldsymbol{u}, \sigma_n^2\mathbf{I}\right) - \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}}\right) \\
&= \log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}}\right)
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathbb{E}_{\mathrm{p}(\boldsymbol{f}|\boldsymbol{u})}[\log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})] &= \int \mathrm{p}(\boldsymbol{f}\mid\boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y}\,|\,\boldsymbol{f})\,\mathrm{d}\boldsymbol{f} \\
&= \int \log \mathcal{N}\left(\boldsymbol{y}\,\middle|\,\boldsymbol{f}, \sigma_n^2\mathbf{I}\right) \mathcal{N}\left(\boldsymbol{f}\,\middle|\,\boldsymbol{K}_{\boldsymbol{fu}}\boldsymbol{K}_{\boldsymbol{uu}}^{-1}\boldsymbol{u}, \boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}}\right) \mathrm{d}\boldsymbol{f} \\
&= \log \mathcal{N}\left(\boldsymbol{y}\,\middle|\,\boldsymbol{K}_{\boldsymbol{fu}}\boldsymbol{K}_{\boldsymbol{uu}}^{-1}\boldsymbol{u}, \sigma_n^2\mathbf{I}\right) - \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}}\right) \\
&= \log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{ff}} - \boldsymbol{Q}_{\boldsymbol{ff}}\right)
\end{aligned}
$$

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, \boldsymbol{Z}, \mathrm{q}(\boldsymbol{u})) &= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f}) \, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}} \right) + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u}) \, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \, \mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{f}} - \boldsymbol{Q}_{\boldsymbol{f}\boldsymbol{f}} \right)
\end{aligned}
$$

- Phew!
- We have not specified $\mathrm{q}(\boldsymbol{u})$. How should we choose it?

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, \boldsymbol{Z}, \mathrm{q}(\boldsymbol{u})) &= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f}) \, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff} \right) + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u}) \, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \, \mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff} \right)
\end{aligned}
$$

- Phew!
- We have not specified $\mathrm{q}(\boldsymbol{u})$. How should we choose it?

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, \boldsymbol{Z}, \mathrm{q}(\boldsymbol{u})) &= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f}) \, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff} \right) + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u}) \, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \, \mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff} \right)
\end{aligned}
$$

- Phew!
- We have not specified $\mathrm{q}(\boldsymbol{u})$. How should we choose it?

SGPR variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, \boldsymbol{Z}, \mathrm{q}(\boldsymbol{u})) &= -\int \mathrm{q}(\boldsymbol{u}) \left(\int \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u}) \log \mathrm{p}(\boldsymbol{y} \mid \boldsymbol{f}) \, \mathrm{d}\boldsymbol{f} + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \left(\log G(\boldsymbol{u}) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff} \right) + \log \frac{\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \right) \mathrm{d}\boldsymbol{u} \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u}) \, \mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})} \, \mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff} \right)
\end{aligned}
$$

- Phew!
- We have not specified $\mathrm{q}(\boldsymbol{u})$. How should we choose it?

The optimal $\mathrm{q}(\boldsymbol{u})$

$$
\begin{aligned}
\min_{\mathrm{q}(\boldsymbol{u})} \mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= \min_{\mathrm{q}(\boldsymbol{u})} - \int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= \min_{\mathrm{q}(\boldsymbol{u})} - \int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} \\
&= \min_{\mathrm{q}(\boldsymbol{u})} \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \,\|\, G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u}))
\end{aligned}
$$

The optimal $\mathrm{q}(\boldsymbol{u})$

$$
\begin{aligned}
\min_{\mathrm{q}(\boldsymbol{u})} \mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= \min_{\mathrm{q}(\boldsymbol{u})} - \int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= \min_{\mathrm{q}(\boldsymbol{u})} - \int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} \\
&= \min_{\mathrm{q}(\boldsymbol{u})} \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \,\|\, G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u}))
\end{aligned}
$$

- Minimize the divergence by choosing

$$
\mathrm{q}^*(\boldsymbol{u}) \propto G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u}) = \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{fu}\boldsymbol{K}_{uu}^{-1}\boldsymbol{u}, \sigma_n^2\mathrm{I}\right)\mathcal{N}(\boldsymbol{u} \mid \boldsymbol{0}, \boldsymbol{K}_{uu})
$$

The optimal $\mathrm{q}(\boldsymbol{u})$

$$
\begin{aligned}
\min_{\mathrm{q}(\boldsymbol{u})} \mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}(\boldsymbol{u})) &= \min_{\mathrm{q}(\boldsymbol{u})} - \int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= \min_{\mathrm{q}(\boldsymbol{u})} - \int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} \\
&= \min_{\mathrm{q}(\boldsymbol{u})} \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \,\|\, G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u}))
\end{aligned}
$$

- Minimize the divergence by choosing

$$
\mathrm{q}^*(\boldsymbol{u}) \propto G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u}) = \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{fu}\boldsymbol{K}_{uu}^{-1}\boldsymbol{u}, \sigma_n^2\mathrm{I}\right)\mathcal{N}(\boldsymbol{u} \mid \boldsymbol{0}, \boldsymbol{K}_{uu})
$$

- This is Gaussian again

$$
\mathrm{q}^*(\boldsymbol{u}) = \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}} = \mathcal{N}(\boldsymbol{u} \mid \boldsymbol{\mu}_u, \Sigma_u)
$$

$$
\boldsymbol{\mu}_u = \sigma_n^{-2}\boldsymbol{K}_{mm}\boldsymbol{B}^{-1}\boldsymbol{K}_{mn}\boldsymbol{y} \qquad \Sigma_u = \boldsymbol{K}_{mm}\boldsymbol{B}^{-1}\boldsymbol{K}_{mm} \qquad \boldsymbol{B} = \boldsymbol{K}_{mm} + \sigma_n^{-2}\boldsymbol{K}_{mn}\boldsymbol{K}_{nm}
$$

(Slight abuse of notation)

SGPR variational bound

- Resubstituting q^* into $\mathcal{L}^{\mathsf{SGPR}}$ yields the final bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z) &\geq \mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}^*(\boldsymbol{u})) \\
&= -\int \mathrm{q}^*(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}^*(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\int \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}} \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}}}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{0}, \boldsymbol{Q}_{ff} + \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)
\end{aligned}
$$

SGPR variational bound

- Resubstituting q^* into $\mathcal{L}^{\mathrm{SGPR}}$ yields the final bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z) &\geq \mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}^*(\boldsymbol{u})) \\
&= -\int \mathrm{q}^*(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}^*(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\int \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}} \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}}}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{0}, \boldsymbol{Q}_{ff} + \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)
\end{aligned}
$$

SGPR variational bound

- Resubstituting q^* into $\mathcal{L}^{\mathrm{SGPR}}$ yields the final bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z) &\geq \mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}^*(\boldsymbol{u})) \\
&= -\int \mathrm{q}^*(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}^*(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\int \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}} \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}}}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{0}, \boldsymbol{Q}_{ff} + \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)
\end{aligned}
$$

SGPR variational bound

- Resubstituting q^* into $\mathcal{L}^{\mathrm{SGPR}}$ yields the final bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z) &\geq \mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z, \mathrm{q}^*(\boldsymbol{u})) \\
&= -\int \mathrm{q}^*(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}^*(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\int \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}} \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}}}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \int G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{0}, \boldsymbol{Q}_{ff} + \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)
\end{aligned}
$$

Interpretation of SGPR

$$\mathcal{L}^{\mathrm{GP}}(\boldsymbol{\theta}) = -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{K}_{ff} + \sigma_n^2 \mathbf{I}\right)$$

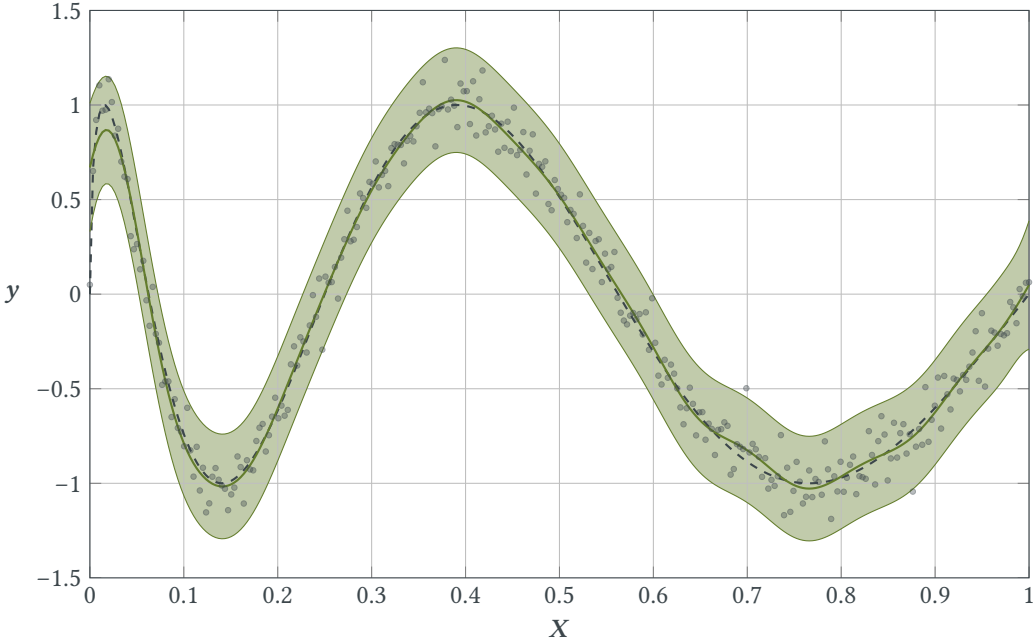
$$\mathcal{L}^{\mathrm{SPGP}}(\boldsymbol{\theta}) = -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{Q}_{ff} + \mathrm{diag}(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}) + \sigma_n^2 \mathbf{I}\right)$$

SGPR variational bound

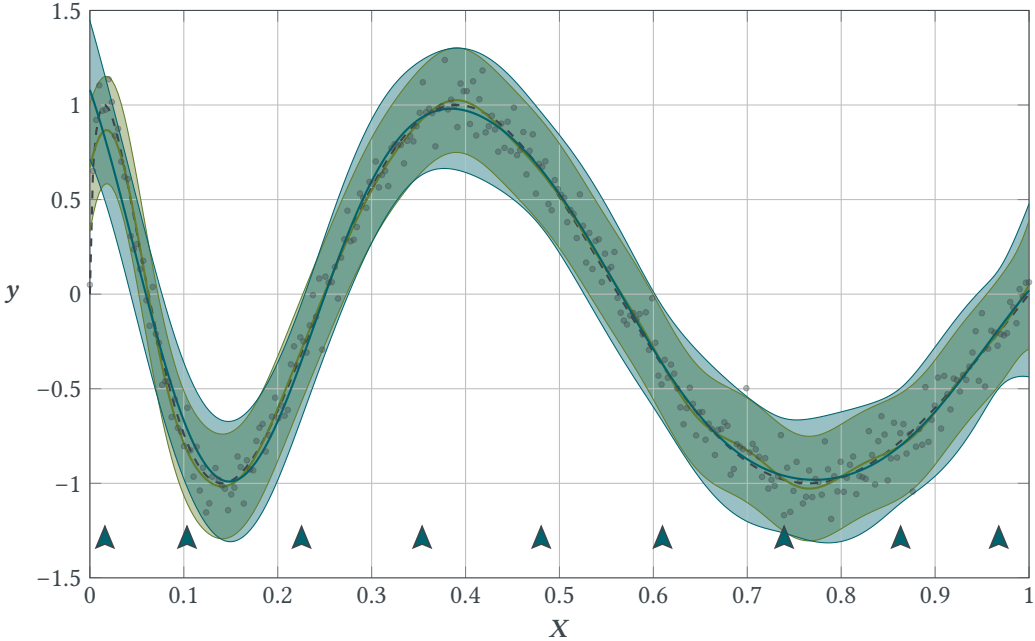
$$\mathcal{L}^{\mathrm{SGPR}}(\boldsymbol{\theta}, Z) \geq -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{Q}_{ff} + \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2} \mathrm{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)$$

- This likelihood is $\mathcal{O}(NM^2)$, same with approximate predictions
- It does **not factorize** along the data, which makes stochastic optimization impossible
- The bound is tight if $\bar{\mathcal{D}} = \mathcal{D}$
- Choosing good $\bar{\mathcal{D}}$ does only make the bound tighter and cannot lead to overfitting

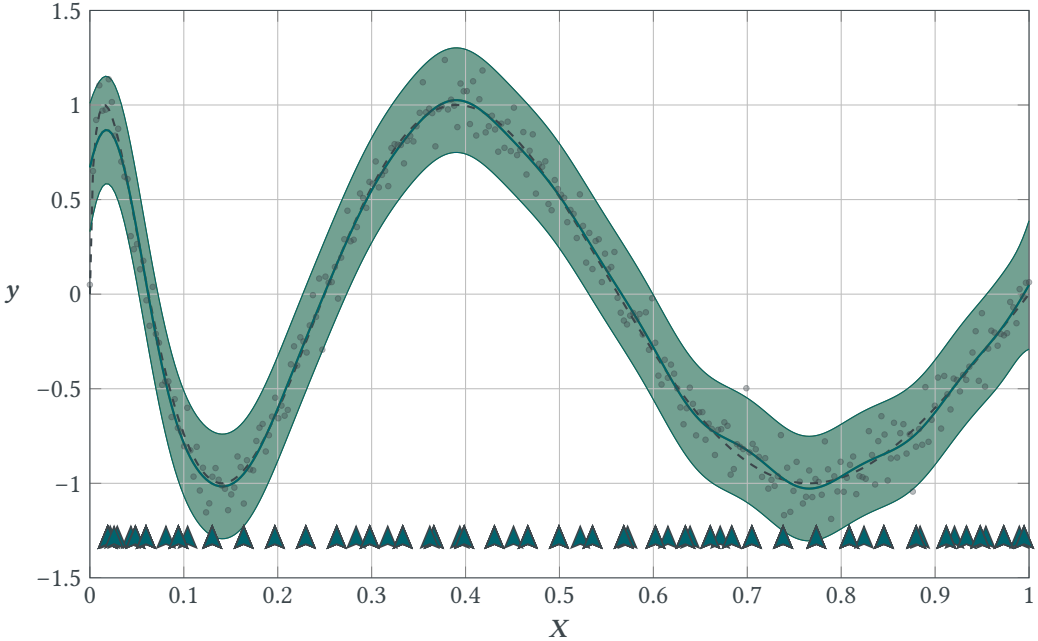
SGPR Showcase



SGPR Showcase



SGPR Showcase



SVGP: Stochastic Optimization

SVGP

Scalable Variational Gaussian Process (SVGP)

We want to variationally approximate the original Gaussian Process.

- Use the same strategy for the variational lower bound as SGPR
- Consider a custom variational scheme $\mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) = \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})$
- Instead of choosing $\mathrm{q}^*(\boldsymbol{u})$, optimize $\mathrm{q}(\boldsymbol{u}) = \mathcal{N}(\boldsymbol{u} \mid \boldsymbol{m}, \boldsymbol{S})$

SVGP

Scalable Variational Gaussian Process (SVGP)

We want to variationally approximate the original Gaussian Process.

- Use the same strategy for the **variational lower bound** as SGPR
- Consider a **custom variational scheme** $\mathrm{q}(\boldsymbol{f}, \boldsymbol{u}) = \mathrm{p}(\boldsymbol{f} \mid \boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})$
- Instead of choosing $\mathrm{q}^*(\boldsymbol{u})$, optimize $\mathrm{q}(\boldsymbol{u}) = \mathcal{N}(\boldsymbol{u} \mid \boldsymbol{m}, \boldsymbol{S})$

- q^* is optimal but expensive to evaluate
- Instead we find a cheaper but worse approximation via optimization
- This hurts the bound, but does not alter the model
- $\boldsymbol{S}$ has **quadratically many parameters**

SVGP variational bound

$$\mathcal{L}^{\mathsf{SVGP}}(\boldsymbol{\theta}, Z, \boldsymbol{m}, S) \geq -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)$$

$$= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)$$

$$= -\int \log G(\boldsymbol{u})\,\mathrm{q}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)$$

$$= -\,\mathbb{E}_{\mathrm{q}(\boldsymbol{u})}[\log G(\boldsymbol{u})] + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)$$

SVGP variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SVGP}}(\boldsymbol{\theta}, Z, \boldsymbol{m}, S) &\geq -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\int \log G(\boldsymbol{u})\,\mathrm{q}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\,\mathbb{E}_{\mathrm{q}(\boldsymbol{u})}[\log G(\boldsymbol{u})] + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\,\mathrm{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)
\end{aligned}
$$

SVGP variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SVGP}}(\boldsymbol{\theta}, \boldsymbol{Z}, \boldsymbol{m}, \boldsymbol{S}) &\geq -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\int \log G(\boldsymbol{u})\,\mathrm{q}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\mathbb{E}_{\mathrm{q}(\boldsymbol{u})}[\log G(\boldsymbol{u})] + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)
\end{aligned}
$$

SVGP variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathsf{SVGP}}(\boldsymbol{\theta}, Z, \boldsymbol{m}, S) &\geq -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\int \mathrm{q}(\boldsymbol{u}) \log \frac{G(\boldsymbol{u})\,\mathrm{p}(\boldsymbol{u})}{\mathrm{q}(\boldsymbol{u})}\,\mathrm{d}\boldsymbol{u} + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\int \log G(\boldsymbol{u})\,\mathrm{q}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big) \\
&= -\mathbb{E}_{\mathrm{q}(\boldsymbol{u})}[\log G(\boldsymbol{u})] + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\operatorname{tr}\big(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\big)
\end{aligned}
$$

SVGP variational bound

$$
\begin{aligned}
\mathbb{E}_{\mathrm{q}(\boldsymbol{u})}[\log G(\boldsymbol{u})] &= \int \log G(\boldsymbol{u})\, \mathrm{q}(\boldsymbol{u})\, \mathrm{d}\boldsymbol{u} \\
&= \int \log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{u}, \sigma_n^2 \mathrm{I}\right) \mathcal{N}(\boldsymbol{u} \mid \boldsymbol{m}, S)\, \mathrm{d}\boldsymbol{u} \\
&= \log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{m}, \sigma_n^2 \mathrm{I}\right) - \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{\boldsymbol{f}\boldsymbol{u}} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} S \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{u}}^{-1} \boldsymbol{K}_{\boldsymbol{u}\boldsymbol{f}}\right)
\end{aligned}
$$

SVGP variational bound

$$
\begin{aligned}
\mathcal{L}^{\mathrm{SVGP}}(\boldsymbol{\theta}, Z, \boldsymbol{m}, S) &\geq -\mathbb{E}_{\mathrm{q}(\boldsymbol{u})}[\log G(\boldsymbol{u})] + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) \\
&= -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{fu}\boldsymbol{K}_{uu}^{-1}\boldsymbol{m}, \sigma_n^2 \mathrm{I}\right) + \mathrm{KL}(\mathrm{q}(\boldsymbol{u}) \parallel \mathrm{p}(\boldsymbol{u})) \\
&\quad + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right) + \frac{1}{2\sigma_n^2}\operatorname{tr}\left(\boldsymbol{K}_{fu}\boldsymbol{K}_{uu}^{-1}\boldsymbol{S}\boldsymbol{K}_{uu}^{-1}\boldsymbol{K}_{uf}\right)
\end{aligned}
$$

SVGP interpretation

$$\mathcal{L}^{\mathsf{GP}}(\boldsymbol{\theta}) = -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{K}_{ff} + \sigma_n^2 \mathbf{I}\right)$$

$$\mathcal{L}^{\mathsf{SPGP}}(\boldsymbol{\theta}) = -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{Q}_{ff} + \operatorname{diag}(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}) + \sigma_n^2 \mathbf{I}\right)$$

$$\mathcal{L}^{\mathsf{SGPR}}(\boldsymbol{\theta}, Z) \geq -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \mathbf{0}, \boldsymbol{Q}_{ff} + \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)$$

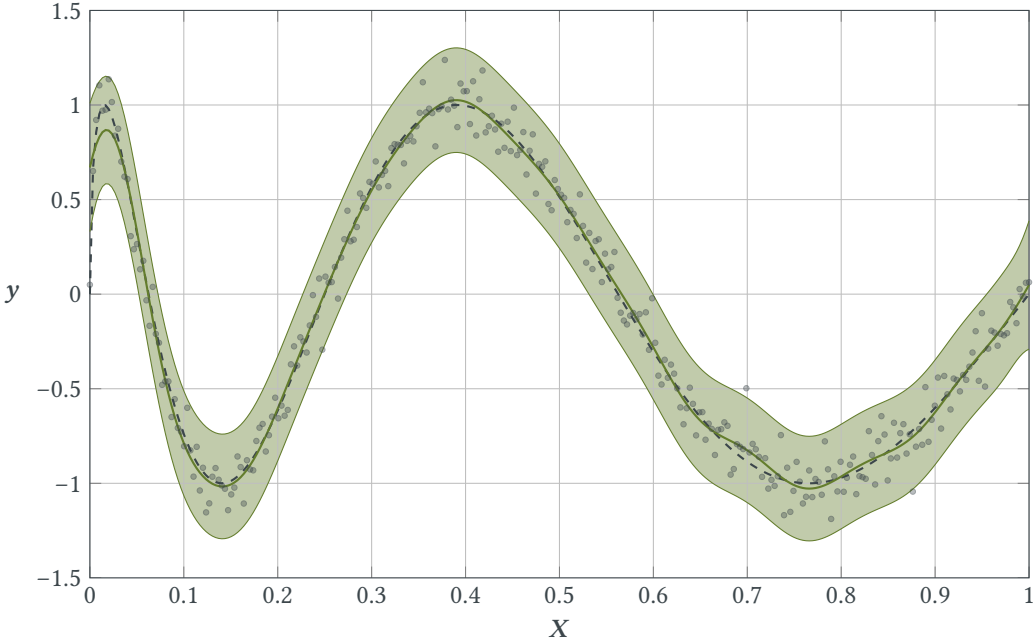
SVGP variational bound

$$\mathcal{L}^{\mathsf{SVGP}}(\boldsymbol{\theta}, Z, \boldsymbol{m}, S) \geq -\log \mathcal{N}\left(\boldsymbol{y} \,\middle|\, \boldsymbol{K}_{fu}\boldsymbol{K}_{uu}^{-1}\boldsymbol{m}, \sigma_n^2 \mathbf{I}\right) + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{ff} - \boldsymbol{Q}_{ff}\right)$$

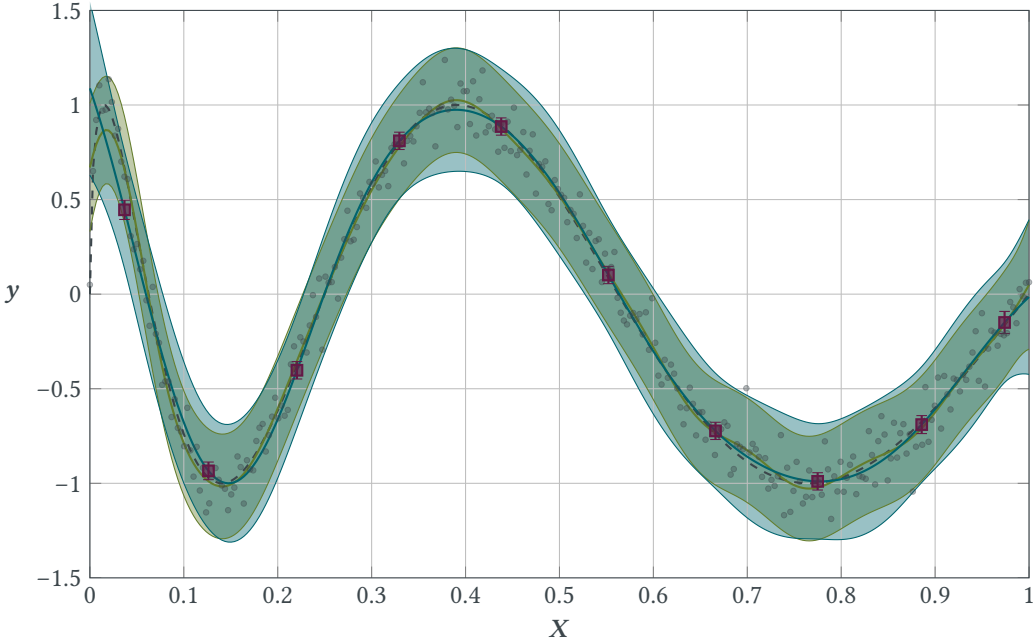
$$+ \operatorname{KL}(\mathrm{q}(\boldsymbol{u}) \,\|\, \mathrm{p}(\boldsymbol{u})) + \frac{1}{2\sigma_n^2} \operatorname{tr}\left(\boldsymbol{K}_{fu}\boldsymbol{K}_{uu}^{-1}\boldsymbol{S}\boldsymbol{K}_{uu}^{-1}\boldsymbol{K}_{uf}\right)$$

- The complete likelihood is still $\mathcal{O}(NM^2)$
- But it **factorizes** along the data - we can do stochastic optimization!
- A single prediction is only $\mathcal{O}(M^2)$ **and we do not need the data**

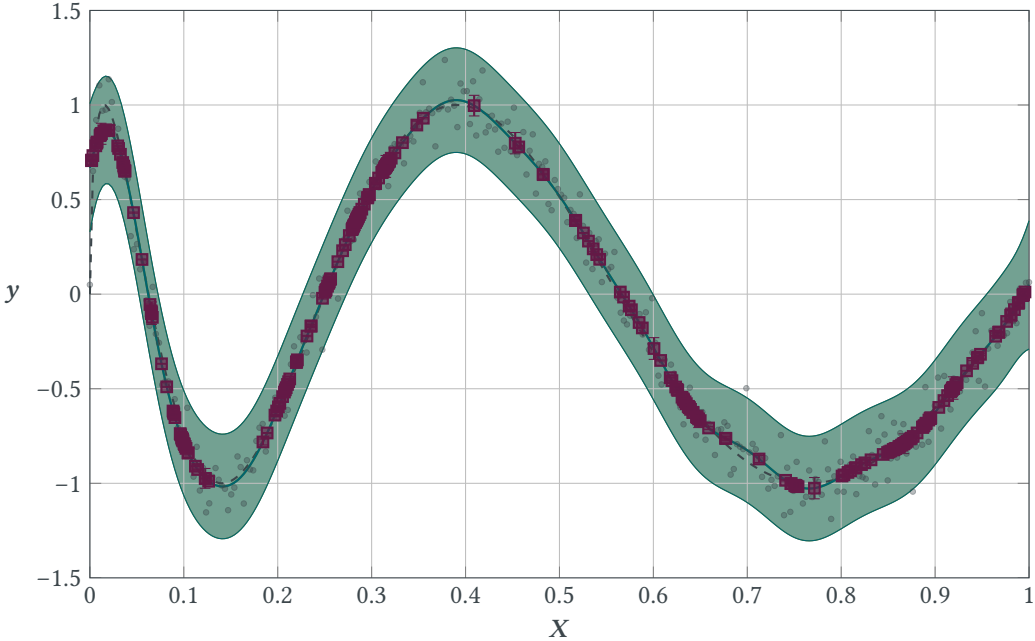
SVGP Showcase



SVGP Showcase



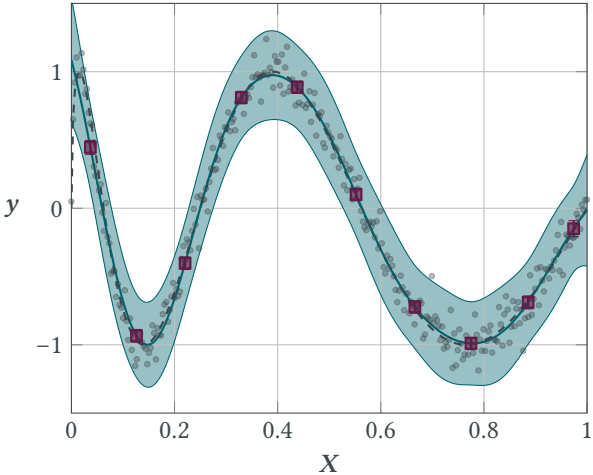
SVGP Showcase



Summary

We have made progress on seemingly fundamental restrictions of GPs:

- Scale to large data sets
- Scale to high dimensions (ish)
- Compact representations
- Acceptable speeds



Next time: Propagation of uncertainties?