Deep Learning: Classics and Trends

Imperial College London

# Variational Gaussian Processes without Matrix Inverses

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# Work in progress

Ongoing work with some initial results presented in

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**Variational Gaussian Process Models without Matrix Inverses**

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# Motivation: Model selection

In deep learning, how to choose the hyperparameters like

- number of layers?
- number of hidden units?
- convolutional or fully connected layer?
- other invariances?
- parameters of data augmentation?
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Wouldn't it be great
if we could just find these by backprop?

# Bayesian model selection

Bayesian inference gives a solution

$$p(f, \theta \mid \mathbf{y}, X) = \frac{p(\mathbf{y}, f, \theta \mid X)}{p(\mathbf{y}|X)} = \frac{p(\mathbf{y} \mid f, X, \theta) p(f|\theta) p(\theta)}{p(\mathbf{y}|X)} \tag{1}$$

$$= \underbrace{\frac{p(\mathbf{y} \mid f, X, \theta) p(f|\theta)}{p(\mathbf{y} \mid X, \theta)}}_{p(f|\mathbf{y},X)} \underbrace{\frac{p(\mathbf{y} \mid X, \theta) p(\theta)}{p(\mathbf{y}|X)}}_{p(\theta \mid \mathbf{y},X)} \tag{2}$$

Posterior over $f$ and $\theta$ consists of two parts

1. The original posterior over $f$,
2. A posterior over $\theta$ using the **marginal likelihood**:

$$p(\mathbf{y}|X, \theta) = \int p(\mathbf{y}|f, X, \theta) p(f|\theta) \mathrm{d}\theta \tag{3}$$

# Bayesian Deep Learning

Bayesian deep learning has

- focussed strongly on getting uncertainty from the posterior $p(f \mid \mathbf{y}, X)$.
- **not** focussed on model selection, because it is **very hard** to find an approximation to the marginal likelihood $p(\mathbf{y}|X, \theta) = \int p(\mathbf{y}|f, X, \theta) p(f|\theta) \mathrm{d}\theta$.

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- *Learning Invariances using the Marginal Likelihood* (van der Wilk et al., 2018)
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- *Deep Gaussian Processes* (Damianou and Lawrence, 2013)
  How many hidden units to use? **Deep, but with marg. lik.!**

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So why aren't we using deep Gaussian processes everywhere?

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- Neural networks only rely on cheap matrix-vector products.
- As long as GPs rely on matrix decompositions in each iteration, they will be slower
- Want **computations** to be similar to deep learning. Doing things **through optimisation** seems key.

# Overview

Variational inference in Gaussian processes

An inverse-free approximate posterior

A general inverse-free variational bound

Recent progress

Conclusions

# A solution to many problems

Variational inference for GPs has been developed over a long period of time

1. Avoid large matrix inverse for regression (Titsias, 2009)
2. Allow big data through minibatching (Hensman et al., 2013)
3. Analytical intractability of non-Gaussian likelihoods (Hensman et al., 2015)
4. General models: Latent variables (Titsias and Lawrence, 2010), deep structure (Damianou and Lawrence, 2013), recurrent structure (Frigola et al., 2014), ...

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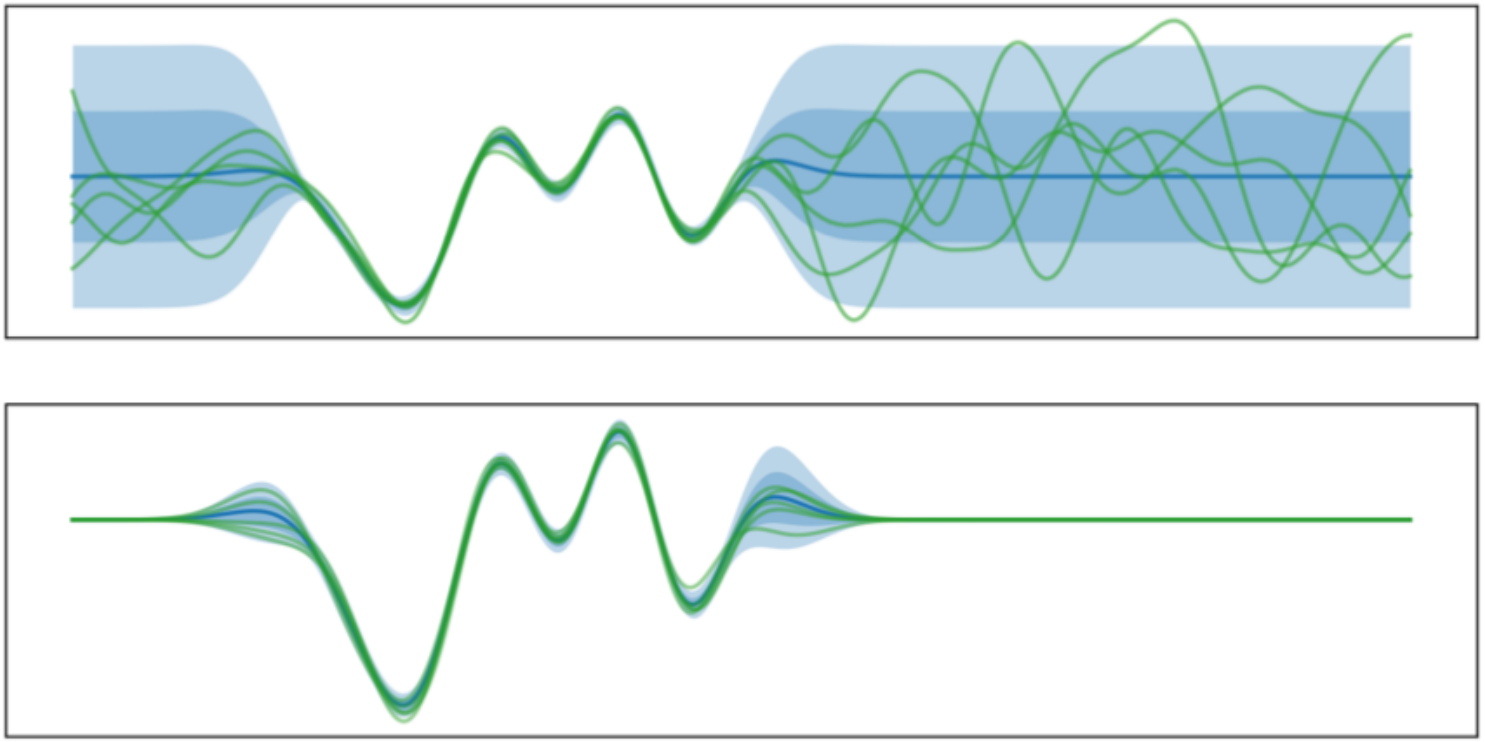
Currently it is **generally applicable** to a wide variety of models.

# Variational Inference in GPs

Crucial property that other approximations lack



Variational approx maintain properties of the non-parametric GP

- Predict with infinite basis functions (better uncertainty)
- Approximate marginal likelihood of non-parametric model

# Recap: Sparse Stochastic Variational Inference

In three simple steps.

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$$\mathcal{L} = \sum_n \mathbb{E}_{q(f(\mathbf{x}_n))}[\log p(y_n|f(\mathbf{x}_n))] - \mathrm{KL}[q(f(Z))||p(f(Z))] \tag{5}$$

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3. Maximise $\mathcal{L}$ to minimise $\mathrm{KL}[q(f)||p(f|\mathbf{y})]$

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1. Conditioning the prior on observations at **inducing input locations** $Z$. We sometimes denote $\mathbf{u} = f(Z)$ for brevity.

$$p(f(\cdot) \mid \mathbf{u}) = \mathcal{N}\left(f(\cdot); \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{u}, k_{\cdot\cdot} - \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot}\right) \tag{6}$$

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3. Marginalise $\mathbf{u}$ to find approximate posterior:

$$\begin{aligned} q(f(\cdot)) &= \int p(f(\cdot) \mid \mathbf{u}) q(\mathbf{u}) \mathrm{d}\mathbf{u} \\ &= \mathcal{N}\left(f(\cdot); \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{m}, k_{\cdot\cdot} - \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot} + \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{S}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot}\right) \end{aligned} \tag{8}$$

Variational parameters: $\{Z, \mathbf{m}, \mathbf{S}\}$

# Predictions and bound

Remember the ELBO:

$$\mathcal{L} = \sum_n \mathbb{E}_{q(f(\mathbf{x}_n))}[\log p(y_n|f(\mathbf{x}_n))] - \mathrm{KL}[q(f(Z))||p(f(Z))] \tag{9}$$

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$$\mathbb{E}_{q(f(\mathbf{x}_n))}[\log p(y_n|f(\mathbf{x}_n))] = -\frac{1}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}(y_n - \mu_n)^2 - \frac{\sigma_n^2}{2\sigma^2} \tag{10}$$

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We require computation of matrix inverse $\mathbf{K}_{ZZ}^{-1}$

# Removing matrix inverses

Can we reparameterise the approximate posterior to remove the matrix inverses?

$$q(f(\cdot)) = \mathcal{N}\left(f(\cdot); \mu_n, \sigma_n^2\right) \tag{11}$$

$$\mu_n = \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{m} = \mathbf{k}_{\cdot Z}\mathbf{m}' \tag{12}$$

$$\begin{aligned}\sigma_n^2 &= k_{\cdot\cdot} - \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot} + \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{S}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot} \\ &= k_{\cdot\cdot} - \mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot} + \mathbf{k}_{\cdot Z}\mathbf{S}'\mathbf{k}_{Z\cdot}\end{aligned} \tag{13}$$

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Some progress, but $\mathbf{k}_{\cdot Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\cdot}$ is the difficult term.

# Upper bounding the predictive variance

Looking back at the expected log likelihood term

$$\mathbb{E}_{q(f(\mathbf{x}_n))}[\log p(y_n|f(\mathbf{x}_n))] = -\frac{1}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}(y_n - \mu_n)^2 - \frac{\sigma_n^2}{2\sigma^2} \quad (14)$$

$$\sigma_n^2 = k_{..} - \mathbf{k}_{.Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n} + \mathbf{k}_{.Z}\mathbf{S}'\mathbf{k}_{Z\mathbf{x}_n} \quad (15)$$

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Observation: An upper bound on $\sigma_n^2$ gives a lower bound to the ELBO. I.e. for $\bar{\sigma}_n^2 \geqslant \sigma_n^2$,

$$\mathcal{L}' = \mathbb{E}_{\mathcal{N}\left(f(\mathbf{x}_n);\mu_n,\bar{\sigma}_n^2\right)}[\log p(y_n|f(\mathbf{x}_n))] - \mathrm{KL} \leqslant \mathcal{L} \leqslant p(\mathbf{y}) \quad (16)$$

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Can we find an upper bound to the predictive variance?

$$\sigma_n^2 = k_{\mathbf{x}_n\mathbf{x}_n} - \mathbf{k}_{\mathbf{x}_n Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}\mathbf{S}'\mathbf{k}_{Z\mathbf{x}_n} \tag{17}$$

Observation: $-\mathbf{k}_{\mathbf{x}_n Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n}$ is the minimum of a quadratic.

$$-\mathbf{k}_{\mathbf{x}_n Z}\mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n} = \min_{\mathbf{v}} \quad \mathbf{v}^\top\mathbf{K}_{ZZ}\mathbf{v} - 2\mathbf{k}_{\mathbf{x}_n Z}^\top\mathbf{v} \tag{18}$$

$$\mathbf{v}_n^* = \mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n} = \operatorname*{argmin}_{\mathbf{v}} \quad \mathbf{v}^\top\mathbf{K}_{ZZ}\mathbf{v} - 2\mathbf{k}_{\mathbf{x}_n Z}^\top\mathbf{v} \tag{19}$$

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Both follow from

$$(\mathbf{v}_n - \mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n})^\top\mathbf{K}_{ZZ}(\mathbf{v}_n - \mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n}) \geqslant 0 \tag{20}$$

Also noted by Gibbs and MacKay (1997) and discussed in Davies (2015) for Conjugate Gradient implementations of GPs

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Since solution $\mathbf{v}_n^* = \mathbf{K}_{ZZ}^{-1}\mathbf{k}_{Z\mathbf{x}_n}$, we can alternatively parameterise

$$\bar{\sigma}_n^2 = k_{\mathbf{x}_n\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}\mathbf{T}\mathbf{K}_{ZZ}\mathbf{T}\mathbf{v}_n - 2\mathbf{k}_{\mathbf{x}_n Z}\mathbf{T}\mathbf{k}_{Z\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}\mathbf{S}'\mathbf{k}_{Z\mathbf{x}_n} \tag{21}$$

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- Optimise over $\mathbf{T} \in \mathbb{R}^{M\times M}$ instead of $N$ times $\mathbf{v}_n \in \mathbb{R}^M$.
- Recovers original bound at $\mathbf{T} = \mathbf{K}_{ZZ}^{-1}$

# Log-concave bound

Using the upper bound on the predictive variance

$$\bar{\sigma}_n^2 = k_{\mathbf{x}_n\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}^\top \mathbf{T}\mathbf{K}_{ZZ}\mathbf{T}\mathbf{k}_{Z\mathbf{x}_n} - 2\mathbf{k}_{\mathbf{x}_n Z}\mathbf{T}\mathbf{k}_{Z\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}\mathbf{S}'\mathbf{k}_{Z\mathbf{x}_n} \geqslant \sigma_n^2\,, \quad (22)$$

we get a lower bound on the ELBO

$$\mathcal{L}_{\mathrm{lc}} = \mathbb{E}_{\mathcal{N}\left(f(\mathbf{x}_n);\mu_n,\bar{\sigma}_n^2\right)}[\log p(y_n|f(\mathbf{x}_n))] - \mathrm{KL} \quad (23)$$

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- Recovers the original bound when $\mathbf{T} = \mathbf{K}_{ZZ}^{-1}$

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- Contains no matrix inverses ($O(M^2)$ instead of $O(M^3)$)
- Valid for all **log-concave** likelihoods
- Recovers the original bound when $\mathbf{T} = \mathbf{K}_{ZZ}^{-1}$
- Is it a **variational** bound?

# Log-concave bound

Using the upper bound on the predictive variance

$$\bar{\sigma}_n^2 = k_{\mathbf{x}_n\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}^\top \mathbf{T}\mathbf{K}_{ZZ}\mathbf{T}\mathbf{k}_{Z\mathbf{x}_n} - 2\mathbf{k}_{\mathbf{x}_n Z}\mathbf{T}\mathbf{k}_{Z\mathbf{x}_n} + \mathbf{k}_{\mathbf{x}_n Z}\mathbf{S}'\mathbf{k}_{Z\mathbf{x}_n} \geqslant \sigma_n^2\,, \quad (22)$$

we get a lower bound on the ELBO

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- Recovers the original bound when $\mathbf{T} = \mathbf{K}_{ZZ}^{-1}$
- Is it a **variational** bound? No! $\log p(\mathbf{y}) - \mathcal{L}_{\text{lc}} \neq \text{KL}[q||p(f\,|\,\mathbf{y})]$

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$$\mathrm{KL}[q(\mathbf{u})||p(\mathbf{u})] = \frac{1}{2}[\mathrm{Tr}[\mathbf{K}_{ZZ}\mathbf{S}'] + \mathbf{m}^\top \mathbf{K}_{ZZ}\mathbf{m} - M - \log|\mathbf{K}_{ZZ}| - \log|\mathbf{S}'|]\,.$$

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- Logdet is a bit harder

# Logdet estimator

We only need **gradient** of $\log|\mathbf{K}_{ZZ}|$ to train.

$$\begin{aligned}\frac{\partial \log|\mathbf{K}_{ZZ}|}{\partial \mathbf{K}_{ZZ}} &= \mathbf{K}_{ZZ}^{-1} = \mathbb{E}_{\mathbf{r}}\left[\mathbf{K}_{ZZ}^{-1}\mathbf{r}\mathbf{r}^{\top}\right] \\ &\approx \mathbf{K}_{ZZ}^{-1}\mathbf{r}\mathbf{r}^{\top} \end{aligned} \tag{26}$$

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Use **Conjugate Gradient** to estimate $\mathbf{K}_{ZZ}^{-1}\mathbf{r}$:

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- CG is iterative, and in worst case costs $O(M^3)$ to find the inverse-vector product.
- If we use $\mathbf{T}$ as a preconditioner: At the optimum it will converge in a **single iteration** since $\mathbf{K}_{ZZ}\mathbf{T}^* = \mathbf{I}$!

# Log-concave bound: overview

$$\mathcal{L}' = \mathbb{E}_{\mathcal{N}\left(f(\mathbf{x}_n);\mu_n,\bar{\sigma}_n^2\right)}[\log p(y_n|f(\mathbf{x}_n))] - \mathrm{KL} \tag{28}$$

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Log-concave bound has limitations. Can we find a "proper" variational bound?

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- Only KL term changes, can be dealt with in similar way

# Fully variational bound: overview

$$\mathcal{L} = \sum_n \mathbb{E}_{q(f(\mathbf{x}_n))}[\log p(y_n|f(\mathbf{x}_n))] - \mathrm{KL}[q(f(Z))||p(f(Z))] \tag{31}$$

- Identical to Hensman et al. (2013) bound with substitution $\mathbf{S} = \mathbf{K}_{ZZ} + \mathbf{K}_{ZZ}\mathbf{T}\mathbf{K}_{ZZ}\mathbf{T}\mathbf{K}_{ZZ} - 2\mathbf{K}_{ZZ}\mathbf{T}\mathbf{K}_{ZZ} + \mathbf{K}_{ZZ}\mathbf{S}'\mathbf{K}_{ZZ}$

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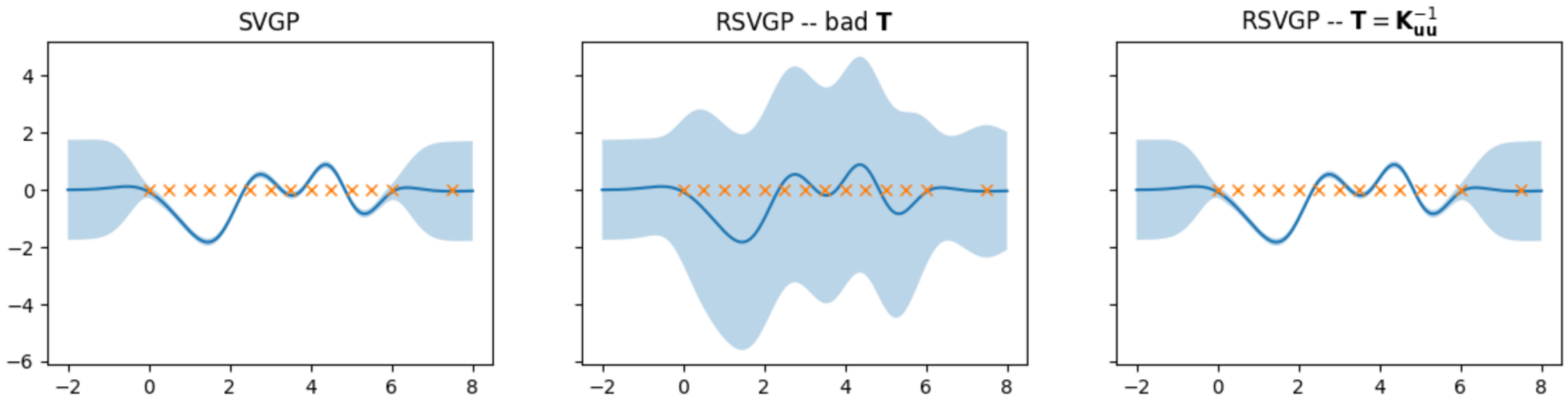
- Only requires matrix-vector multiplies, $O(M^2)$ cost when $\mathbf{T} \approx \mathbf{K}_{ZZ}^{-1}$.
- No additional gap when $\mathbf{T} = \mathbf{K}_{ZZ}^{-1}$.

# Toy 1D dataset




- Left: SVGP fit to data
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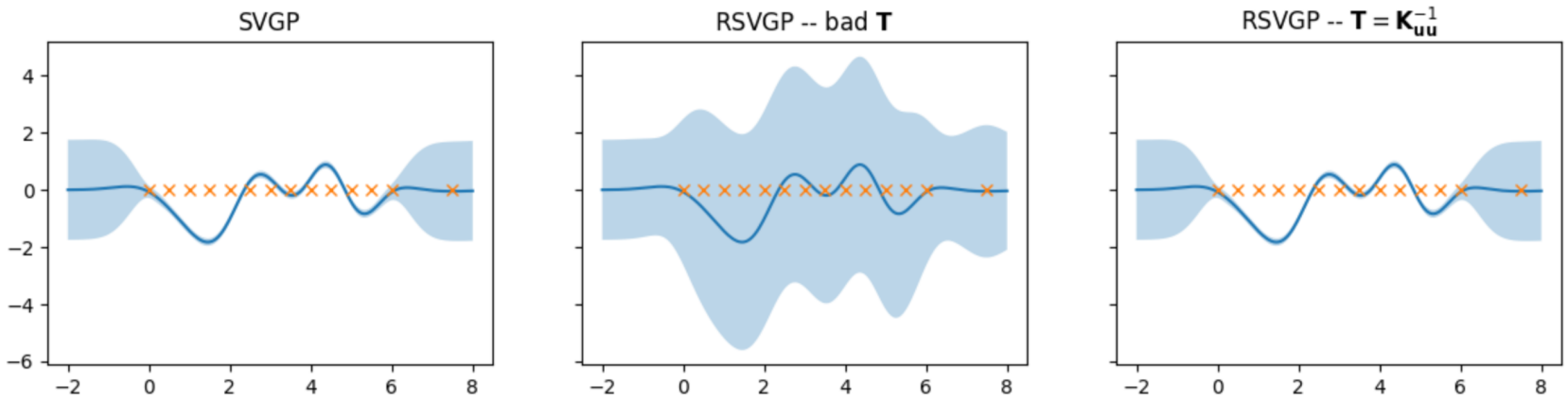


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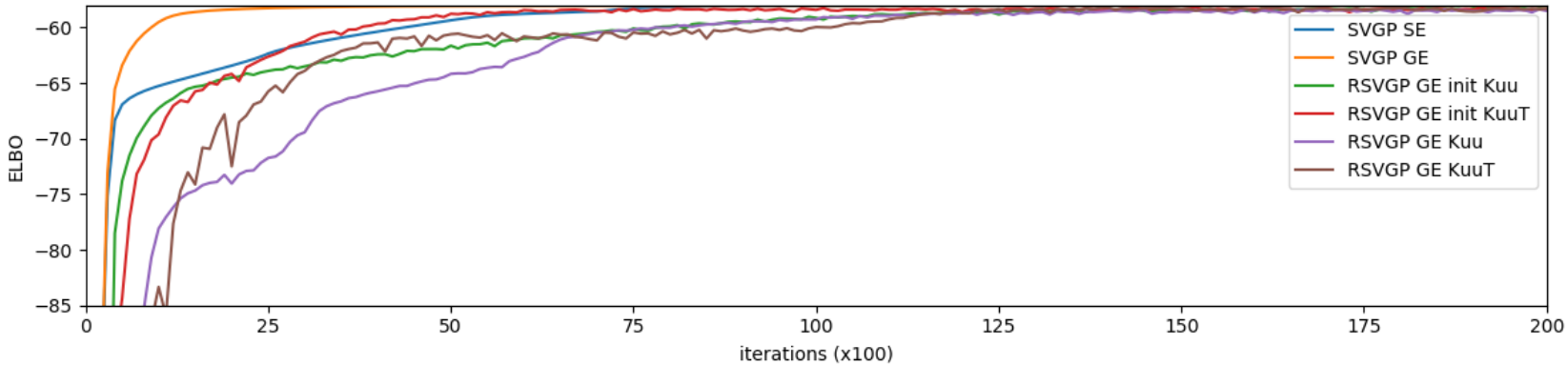
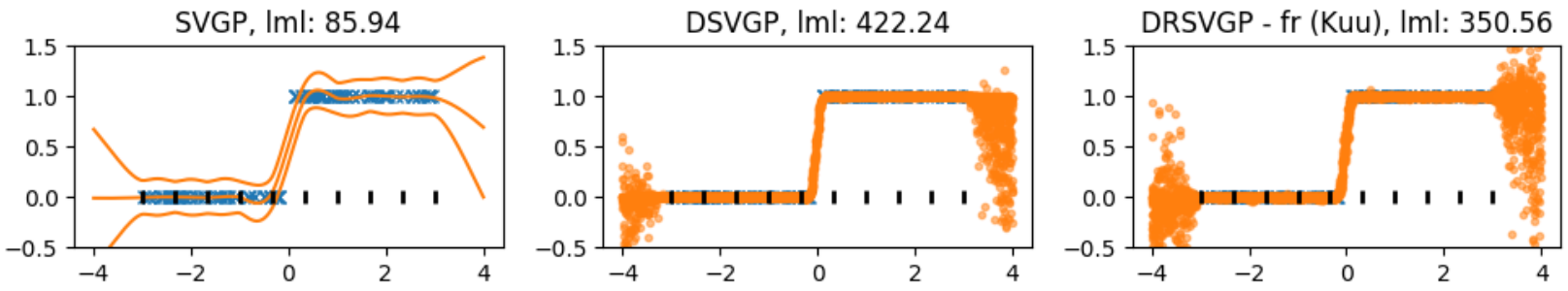
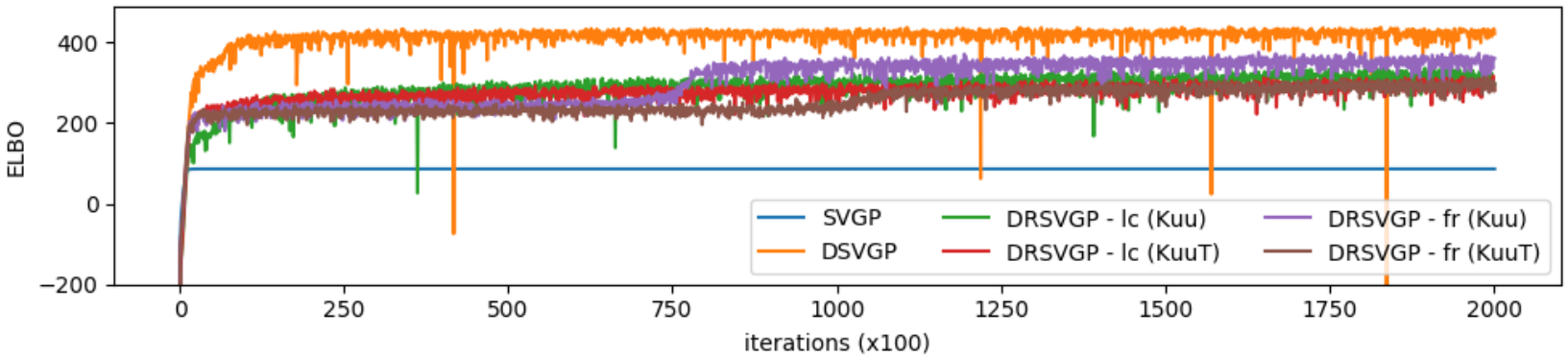


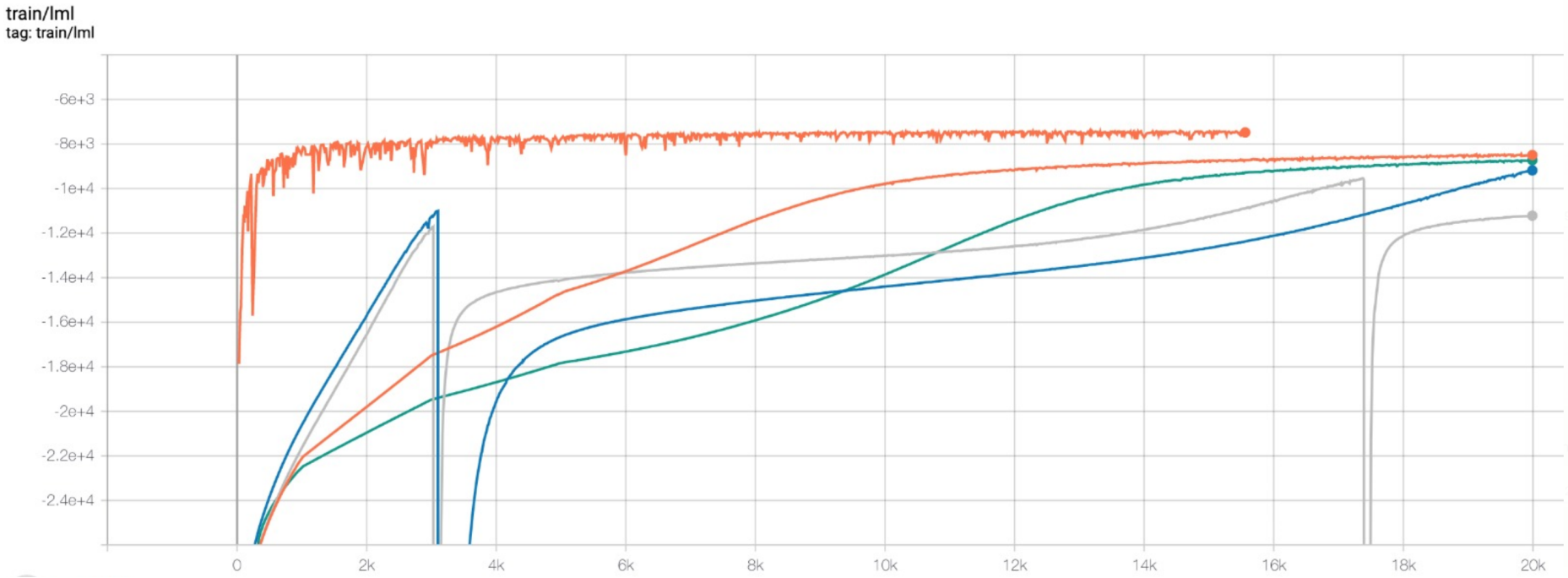
# Deep Gaussian process

## Fully variational bound



# The bad news




Orange: SVGP, Others: Inverse-free

Procedure: Optimise everything with Adam, including $\mathbf{T}$

- Less time per iteration
- Slower convergence
- Strange divergence behaviour

# Discussion

Work in progress because of the difficult optimisation behaviour.

Developments since AABI:

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Developments since AABI:

- Improved logdet estimators (no more CG inner loops)
- Analysis of curvature of objective function gives hints into what causes behaviour

# Conclusions

- We have introduced inverse-free variational bounds to GP models
- We prove properties about their optima, and validate those experimentally
- However, a wall-clock speed-up in training is still elusive

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**Thanks for your attention!**

I'm curious about your thoughts!

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