Variational inference for Gaussian processes

Mauricio A. Álvarez

Topics on Deep Probabilistic Models

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Posterior inference

- When using Bayesian inference, we need to compute the posterior distribution of $\mathbf{f}$ given the data.

- We then use that posterior distribution to compute the predictive distribution.

- Reasons as why computing the posterior distribution is an issue for GPs.
  - Computational complexity.
  - Non-Gaussian likelihood.
  - Both of the above.

Computational complexity

- To compute the predictive mean and the predictive covariance we need to compute $\left[\mathbf{K}(\mathbf{X},\mathbf{X}) + \sigma_n^2\mathbf{I}\right]^{-1}$
- The usual way to do this is using the Cholesky decomposition which costs $\mathcal{O}(n^3)$.
- If $n = 1000$, then we need to perform 10^9 operations.

Non-Gaussian likelihoods

- In Bayesian inference we want to compute

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

  where $p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f})d\mathbf{f}$.

- When $p(\mathbf{y}|\mathbf{f})$ is a Gaussian likelihood, then we can compute $p(\mathbf{y})$ and $p(\mathbf{f}|\mathbf{y})$ analytically.

- When $p(\mathbf{y}|\mathbf{f})$ is non-Gaussian (e.g. Bernoulli with a sigmoid link function) both $p(\mathbf{y})$ and $p(\mathbf{f}|\mathbf{y})$ are intractable.

How to address these issues?

- One successful approach is by using the idea of *inducing variables* or *pseudo-variables*.
- The idea in itself was quite well know in the GP literature. See for example Chapter 8 of the GPML book and in the paper **?**.
- However, if we couple this idea with a variational inference approach, we have a powerful tool to build complex GP models.

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Auxiliary variables

- We introduce a new set of M variables $\mathbf{u} = \{u(\mathbf{z}_m)\}_{m=1}^{M}$ that we refer to as inducing variables or pseudo-variables.

- The set of points $\mathbf{Z} = \{\mathbf{z}_m\}_{m=1}^{M}$ is usually known as inducing inputs.

- We augment the original prior $p(\mathbf{f})$ to $p(\mathbf{f}, \mathbf{u})$ such that

$$p(\mathbf{f}) = \int p(\mathbf{f}, \mathbf{u}) d\mathbf{u} = \int p(\mathbf{f}|\mathbf{u}) p(\mathbf{u}) d\mathbf{u},$$

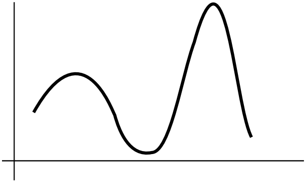
  where $p(\mathbf{u})$ and $p(\mathbf{f}, \mathbf{u})$ are both Gaussians.

- The auxiliary variables $\mathbf{u}$ can be part of the GP $f(\mathbf{x})$ or they can be linearly related to $f(\mathbf{x})$ (sometimes known as interdomain inducing variables).

- In the former case, $p(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\mathbf{0}, \mathbf{K}(\mathbf{Z}, \mathbf{Z}))$.

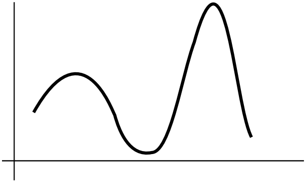
Auxiliary variables

A sample from $p(f)$

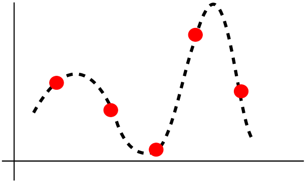


Auxiliary variables

A sample from $p(f)$



Inducing variables $\mathbf{u}$

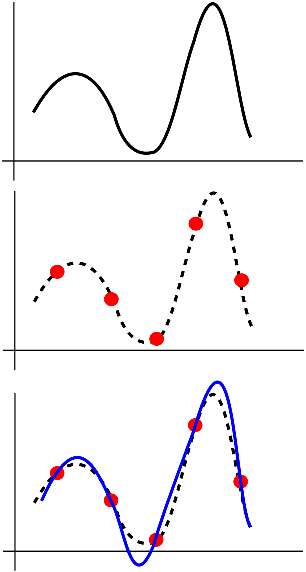


Auxiliary variables

A sample from $p(f)$

Inducing variables $\mathbf{u}$

A sample from $p(f|\mathbf{u})$



Variational lower-bound for the marginal likelihood (I)

- We can write the log marginal probability for $\mathbf{y}$ using

$$\log p(\mathbf{y}) = \mathcal{L}(q(\mathbf{f})) + \mathrm{KL}(q(\mathbf{f}) \| p(\mathbf{f}|\mathbf{y})),$$

  where

$$\mathcal{L}(q(\mathbf{f})) = \int q(\mathbf{f}) \log \left\{ \frac{p(\mathbf{y}, \mathbf{f})}{q(\mathbf{f})} \right\} d\mathbf{f},$$

$$\mathrm{KL}(q(\mathbf{f}) \| p(\mathbf{f}|\mathbf{y})) = -\int q(\mathbf{f}) \log \left\{ \frac{p(\mathbf{f}|\mathbf{y})}{q(\mathbf{f})} \right\} d\mathbf{f},$$

  with $q(\mathbf{f})$ the approximated posterior, $\mathrm{KL}(q||p)$ is the Kullback-Leibler divergence between q and p and $p(\mathbf{f}|\mathbf{y})$ is the true posterior.

- The KL divergence is zero when $q = p$. In that case, $\log p(\mathbf{y}) = \mathcal{L}(q(\mathbf{f}))$.

- If this is not the case $\mathrm{KL}(q(\mathbf{f}) \| p(\mathbf{f}|\mathbf{y}))$ and $\log p(\mathbf{y}) > \mathcal{L}(q(\mathbf{f}))$.

Variational lower-bound for the marginal likelihood (II)

- We have two ways to find the optimal $q(\mathbf{f})$
  1. We find $q(\mathbf{f})$ by minimising $\mathrm{KL}(q(\mathbf{f})||p(\mathbf{f}|\mathbf{y}))$.
  2. We find $q(\mathbf{f})$ by maximising $\mathcal{L}(q(\mathbf{f}))$.

- Option 1 is not possible since $p(\mathbf{f}|\mathbf{y})$ is unknown.

- So, in general, we appeal to option 2

$$\log p(\mathbf{y}) \geq \mathcal{L}(q(\mathbf{f})).$$

Lower-bound with inducing variables

- For our augmented model we want to find an approximated posterior $q(\mathbf{f}, \mathbf{u})$ by maximising

$$\mathcal{L}(q(\mathbf{f}, \mathbf{u})) = \int \int q(\mathbf{f}, \mathbf{u}) \log \left\{ \frac{p(\mathbf{y}, \mathbf{f}, \mathbf{u})}{q(\mathbf{f}, \mathbf{u})} \right\} d\mathbf{u} d\mathbf{f},$$

  where $p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})p(\mathbf{u})$ and we will approximate the posterior $q(\mathbf{f}, \mathbf{u})$ as $q(\mathbf{f}, \mathbf{u}) \approx p(\mathbf{f}|\mathbf{u})q(\mathbf{u})$.

- Since we know that $q(\mathbf{f}) = \int_{\mathbf{u}} p(\mathbf{f}|\mathbf{u})q(\mathbf{u})d\mathbf{u}$, the bound above really only depends on $q(\mathbf{u})$

$$\begin{aligned}\mathcal{L}(q(\mathbf{u})) &= \int \int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \log \left\{ \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})p(\mathbf{u})}{p(\mathbf{f}|\mathbf{u})q(\mathbf{u})} \right\} d\mathbf{u} d\mathbf{f}, \\ &= \int \int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \log \left\{ \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{u})}{q(\mathbf{u})} \right\} d\mathbf{u} d\mathbf{f}.\end{aligned}$$

Two approaches for optimising $\mathcal{L}(q(\mathbf{u}))$

- There are two approaches for optimising $q(\mathbf{u})$ in $\mathcal{L}(q(\mathbf{u}))$.
- First approach (**?**):
  - We assume a multi-variate Gaussian form for $q(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\boldsymbol{\mu}, \mathbf{S})$ with $\boldsymbol{\mu} \in \mathbb{R}^{M\times 1}$ and $\mathbf{S} \in \mathbb{R}^{M\times M}$.
  - We then find $\boldsymbol{\mu}$ and $\mathbf{S}$ by numerically optimising $\mathcal{L}(q(\mathbf{u}))$.
- Second approach (**?**):
  - We marginalise $q(\mathbf{u})$ from the bound and then compute it by using Jensen's inequality.
  - We then find $\boldsymbol{\mu}$ and $\mathbf{S}$ by using the rules of probability.

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Stochastic variational inference

- Stochastic variational inference (SVI) allows (**?**) the use of stochastic gradients over variational lower bounds.

- **?** proposed the use of SVI for sparse GPs.

- The idea is to use stochastic gradients for optimising $\mathcal{L}(q(\mathbf{u}))$ with respect to $q(\mathbf{u})$, this is, $\boldsymbol{\mu}$ and $\mathbf{S}$.

Lower bound $\mathcal{L}(q(\mathbf{u}))$ (I)

- From a previous slide,

$$\mathcal{L}(q(\mathbf{u})) = \int\int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \log\left\{\frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{u})}{q(\mathbf{u})}\right\} d\mathbf{u}d\mathbf{f}.$$

- We can re-arrange the expression above using

$$\begin{aligned}
\mathcal{L}(q(\mathbf{u})) &= \int\int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \log\left\{\frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{u})}{q(\mathbf{u})}\right\} d\mathbf{u}d\mathbf{f}, \\
&= \int\int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \left[\log p(\mathbf{y}|\mathbf{f}) + \log\frac{p(\mathbf{u})}{q(\mathbf{u})}\right] d\mathbf{u}d\mathbf{f}, \\
&= \int\int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \log p(\mathbf{y}|\mathbf{f}) d\mathbf{u}d\mathbf{f} + \int q(\mathbf{u}) \log\frac{p(\mathbf{u})}{q(\mathbf{u})} d\mathbf{u}, \\
&= \int \log p(\mathbf{y}|\mathbf{f}) \int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) d\mathbf{u}d\mathbf{f} + \int q(\mathbf{u}) \log\frac{p(\mathbf{u})}{q(\mathbf{u})} d\mathbf{u}, \\
&= \int \log p(\mathbf{y}|\mathbf{f}) q(\mathbf{f}) d\mathbf{f} - \mathrm{KL}(q(\mathbf{u})\|p(\mathbf{u})) d\mathbf{u}, \\
&= \mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y}|\mathbf{f})] - \mathrm{KL}(q(\mathbf{u})\|p(\mathbf{u})).
\end{aligned}$$

Lower bound $\mathcal{L}(q(\mathbf{u}))$ (II)

- The lower bound is

$$\mathcal{L}(q(\mathbf{u})) = \mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y}|\mathbf{f})] - \mathrm{KL}(q(\mathbf{u})\|p(\mathbf{u})).$$

- We can find an estimate for $\boldsymbol{\mu}$ and $\mathbf{S}$ by maximising $\mathcal{L}(q(\mathbf{u}))$ using numerical optimisation.

- We need to compute the gradients

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}}, \ \frac{\partial \mathcal{L}}{\partial \mathbf{S}}$$

Exercises

- Recall that $q(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\boldsymbol{\mu}, \mathbf{S})$ and $p(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\mathbf{0}, \mathbf{K}(\mathbf{Z}, \mathbf{Z}))$. Now, for the regression case,

$$p(\mathbf{y}|\mathbf{f}) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma_n^2\mathbf{I}).$$

  1. Write the expression for the bound in terms of $\boldsymbol{\mu}, \mathbf{S}$ and σ_n^2.
  2. Compute $\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}}$ and $\frac{\partial \mathcal{L}}{\partial \mathbf{S}}$.

- For the case above, what is the computational complexity of this method?

Stochastic gradient descend

- It can be shown that the lower bound can be written as

$$\mathcal{L}(q(\mathbf{u})) = \sum_{i=1}^{n} \ell(y_i, \mathbf{x}_i, \boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{u}) \| p(\mathbf{u})),$$

  where $\ell(y_i, \mathbf{x}_i, \boldsymbol{\theta})$ is a function that depends on the data, the variational parameters $\boldsymbol{\mu}$, $\mathbf{S}$, and any other (hyper) parameters in the model (e.g. the hyperparameters of the kernel).

- For n large, we could only use a subset of the data to compute the gradients to be used in numerical optimisation.

- This is usually known as *stochastic gradient descend*.

- The computational complexity is this model is $\mathcal{O}(nM^2)$, where M is the number of inducing points.

Example SVI for Sparse GPs

Lab SVI for Sparse GPs (GPFlow)

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Marginalising $q(\mathbf{u})$ from the bound (I)

- Instead of finding particular parameters $\boldsymbol{\mu}$ and $\mathbf{S}$ as before, we can marginalise $q(\mathbf{u})$ from the lower bound and then use probability rules to compute $q(\mathbf{u})$.

- Let us go back to the general expression for the bound

$$\mathcal{L}(q(\mathbf{u})) = \int \int p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \log \left\{ \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{u})}{q(\mathbf{u})} \right\} d\mathbf{u} d\mathbf{f}.$$

- Let us assume that $q(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\boldsymbol{\mu}, \mathbf{S})$ and find expressions for $\mathbf{u}$ and $\mathbf{S}$.

- We first integrate over $\mathbf{f}$.

Marginalising $q(\mathbf{u})$ from the bound (II)

- The bound can be expressed as

$$\mathcal{L}(q(\mathbf{u})) = \int \int p(\mathbf{f}|\mathbf{u}) q(\mathbf{u}) \log \left\{ \frac{p(\mathbf{y}|\mathbf{f}) p(\mathbf{u})}{q(\mathbf{u})} \right\} d\mathbf{u} d\mathbf{f}$$
$$= \int q(\mathbf{u}) \int p(\mathbf{f}|\mathbf{u}) \left\{ \log p(\mathbf{y}|\mathbf{f}) + \log \left[\frac{p(\mathbf{u})}{q(\mathbf{u})} \right] \right\} d\mathbf{f} d\mathbf{u}.$$

- Let us focus on the integral over $\mathbf{f}$

$$\log T(\mathbf{y}, \mathbf{u}) = \int \log p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}|\mathbf{u}) d\mathbf{f}.$$

Exercise

- $p(\mathbf{f}|\mathbf{u})$ is a conditional Gaussian distribution given as,

$$\mathcal{N}(\mathbf{f}|\mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{u},\mathbf{K}(\mathbf{X},\mathbf{X})-\mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{K}(\mathbf{X},\mathbf{Z})^{\top}),$$

  and $p(\mathbf{y}|\mathbf{f})$ is again a Gaussian given as $\mathcal{N}(\mathbf{y}|\mathbf{f},\sigma_n^2\mathbf{I})$.

- Compute the expression $\log T(\mathbf{y},\mathbf{u})$

Marginalising $q(\mathbf{u})$ from the bound (III)

- The bound can now be expressed as

$$\mathcal{L}(q(\mathbf{u})) = \int q(\mathbf{u}) \left\{ \log \mathcal{N}(\mathbf{y}|\boldsymbol{\alpha}, \sigma_n^2 \mathbf{I}) - \frac{1}{2} \operatorname{trace}(\sigma_n^{-2} \widetilde{\mathbf{K}}) + \log \left[\frac{p(\mathbf{u})}{q(\mathbf{u})} \right] \right\} d\mathbf{u},$$

where

$$\begin{aligned} \boldsymbol{\alpha} &= \mathbf{K}(\mathbf{X}, \mathbf{Z}) \mathbf{K}^{-1}(\mathbf{Z}, \mathbf{Z}) \mathbf{u} \\ \widetilde{\mathbf{K}} &= \mathbf{K}(\mathbf{X}, \mathbf{X}) - \mathbf{K}(\mathbf{X}, \mathbf{Z}) \mathbf{K}^{-1}(\mathbf{Z}, \mathbf{Z}) \mathbf{K}(\mathbf{X}, \mathbf{Z})^{\top}. \end{aligned}$$

- It follows that

$$\mathcal{L}(q(\mathbf{u})) = \int q(\mathbf{u}) \left\{ \log \left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha}, \sigma_n^2 \mathbf{I}) p(\mathbf{u})}{q(\mathbf{u})} \right] \right\} d\mathbf{u} - \frac{1}{2} \operatorname{trace}(\sigma_n^{-2} \widetilde{\mathbf{K}})$$

Jensen's inequality

- A function φ is *convex* if
$$\varphi(\lambda a + (1-\lambda)b) \leq \lambda\varphi(a) + (1-\lambda)\varphi(b).$$
- A function φ is *concave* if
$$\varphi(\lambda a + (1-\lambda)b) \geq \lambda\varphi(a) + (1-\lambda)\varphi(b).$$
- Let φ be a convex function. It can be shown that
$$\varphi(\mathbb{E}(\mathbf{x})) \leq \mathbb{E}(\varphi(\mathbf{x}))$$
$$\varphi\left(\int \mathbf{x}p(\mathbf{x})d\mathbf{x}\right) \leq \int \varphi(\mathbf{x})p(\mathbf{x})d\mathbf{x}.$$
This inequality is known as the *Jensen's inequality*.
- If φ is a concave function then
$$\varphi(\mathbb{E}(\mathbf{x})) \geq \mathbb{E}(\varphi(\mathbf{x}))$$
$$\varphi\left(\int \mathbf{x}p(\mathbf{x})d\mathbf{x}\right) \geq \int \varphi(\mathbf{x})p(\mathbf{x})d\mathbf{x}.$$

Jensen's inequality applied to $\mathcal{L}(q(\mathbf{u}))$

- Reversing Jensen's inequality, we can write

$$\log\left[\int q(\mathbf{u})\left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})}{q(\mathbf{u})}\right]d\mathbf{u}\right] \geq$$
$$\int q(\mathbf{u})\left\{\log\left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})}{q(\mathbf{u})}\right]\right\}d\mathbf{u}$$

- The expression above can be simplified as

$$\log\left[\int \mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})d\mathbf{u}\right] \geq \int q(\mathbf{u})\left\{\log\left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})}{q(\mathbf{u})}\right]\right\}d\mathbf{u}$$

A tighter bound $\mathcal{L}(q(\mathbf{u}))$

- Reversing Jensen's inequality, we can write

$$\log\left[\int q(\mathbf{u})\left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})}{q(\mathbf{u})}\right]d\mathbf{u}\right] \geq \int q(\mathbf{u})\left\{\log\left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})}{q(\mathbf{u})}\right]\right\}d\mathbf{u}$$

- The expression above can be simplified as

$$\log\left[\int \mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})d\mathbf{u}\right] \geq \int q(\mathbf{u})\left\{\log\left[\frac{\mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})}{q(\mathbf{u})}\right]\right\}d\mathbf{u}$$

- If we define

$$\mathcal{L}_2 = \log\left[\int \mathcal{N}(\mathbf{y}|\boldsymbol{\alpha},\sigma_n^2\mathbf{I})p(\mathbf{u})d\mathbf{u}\right] - \frac{1}{2}\operatorname{trace}(\sigma_n^{-2}\widetilde{\mathbf{K}}),$$

then

$$\mathcal{L}_2 \geq \mathcal{L}(q(\mathbf{u})).$$

And $\mathcal{L}_2$ is closer to $\log p(\mathbf{y})$ than $\mathcal{L}(q(\mathbf{u}))$.

Exercise

- Show that $\mathcal{L}_2$ can be written as

$$\mathcal{L}_2 = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}(\mathbf{X}, \mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z}, \mathbf{Z})\mathbf{K}^{\top}(\mathbf{X}, \mathbf{Z}) + \sigma_n^2 \mathbf{I}) - \frac{1}{2}\,\mathrm{trace}(\sigma_n^{-2}\widetilde{\mathbf{K}}).$$

References I