Variational inference for Gaussian processes

Mauricio A. Álvarez

Reasoning and Learning under Uncertainty
The University of Manchester

Contents

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?

- A successful approach uses 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 Quiñonero-Candela and Rasmussen (2005).
- However, if we couple this idea with a variational inference approach, we have a powerful tool to build complex GP models.

Contents

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

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

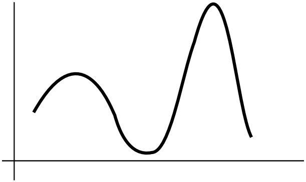
  where $p(\mathbf{u})$ and $p(\mathbf{f}, \mathbf{u})$ are both Gaussians.

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

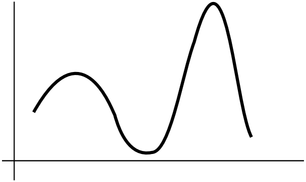
Auxiliary variables

A sample from $p(f)$

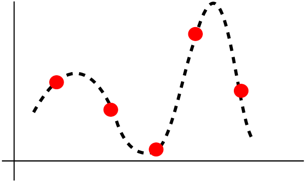


Auxiliary variables

A sample from $p(f)$

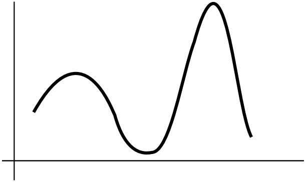


Inducing variables $\mathbf{u}$

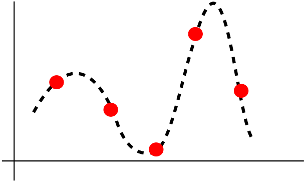


Auxiliary variables

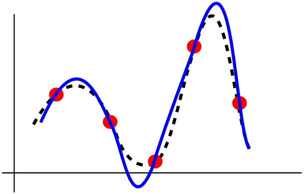
A sample from $p(f)$



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 $\mathrm{KL}(q(\mathbf{f}) \| p(\mathbf{f}|\mathbf{y})) > 0$ 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 (Hensman et al., 2013):
  - 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 (Titsias, 2009):
  - 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 (Hoffman et al., 2013) the use of stochastic gradients over variational lower bounds.

- Hensman et al. (2013) 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 first compute $q(\mathbf{f})$, which is given as

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

where

$$\begin{aligned} p(\mathbf{f}|\mathbf{u}) &= \mathcal{N}(\mathbf{f}|\mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{u}, \mathbf{K}(\mathbf{X},\mathbf{X}) - \mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{K}^{\top}(\mathbf{X},\mathbf{Z})) \\ q(\mathbf{u}) &= \mathcal{N}(\mathbf{u}|\boldsymbol{\mu}, \mathbf{S}). \end{aligned}$$

- Leading to

$$q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu}, \boldsymbol{\Lambda}),$$

with

$$\boldsymbol{\Lambda} = \mathbf{K}(\mathbf{X},\mathbf{X}) + \mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\left(\mathbf{S} - \mathbf{K}(\mathbf{Z},\mathbf{Z})\right)\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{K}^{\top}(\mathbf{X},\mathbf{Z}))$$

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

- The first term of the lower bound $\mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y}|\mathbf{f})]$ is then given as

$$\mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y}|\mathbf{f})] = \mathbb{E}_{q(\mathbf{f})}\left[-\frac{n}{2}\log 2\pi - \frac{n}{2}\log \sigma_n^2 - \frac{1}{2\sigma_n^2}(\mathbf{y}-\mathbf{f})^\top(\mathbf{y}-\mathbf{f})\right].$$

- We are only interested in the terms involving $\mathbf{f}$, then

$$\begin{aligned}
\mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y}|\mathbf{f})] &= \frac{1}{\sigma_n^2}\mathbf{y}^\top\mathbb{E}_{q(\mathbf{f})}(\mathbf{f}) - \frac{1}{2\sigma_n^2}\mathbb{E}_{q(\mathbf{f})}(\mathbf{f}^\top\mathbf{f}) + \text{const} \\
&= \frac{1}{\sigma_n^2}\mathbf{y}^\top\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} - \frac{1}{2\sigma_n^2}\mathbb{E}_{q(\mathbf{f})}[\text{tr}(\mathbf{f}\mathbf{f}^\top)] + \text{const} \\
&= \frac{1}{\sigma_n^2}\mathbf{y}^\top\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} - \frac{1}{2\sigma_n^2}\,\text{tr}(\mathbb{E}_{q(\mathbf{f})}[\mathbf{f}\mathbf{f}^\top]) + \text{const} \\
&= \frac{1}{\sigma_n^2}\mathbf{y}^\top\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} - \frac{1}{2\sigma_n^2}\,\text{tr}(\boldsymbol{\Lambda} + \\
&\quad \mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu}\boldsymbol{\mu}^\top[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\mathbf{K}(\mathbf{Z},\mathbf{X})) + \text{const.}
\end{aligned}$$

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

- The second term of the lower bound is $\mathrm{KL}(q(\mathbf{u}) \| p(\mathbf{u}))$.

- The KL divergence between two multivariate Gaussians $\mathcal{N}_0(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ and $\mathcal{N}_1(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$, $\mathrm{KL}(\mathcal{N}_0 \| \mathcal{N}_1)$ is given as

$$\frac{1}{2}\left[\mathrm{tr}(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^\top \boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - k + \log \frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|}\right].$$

- In this case, $q(\mathbf{u}) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{S})$ and $p(\mathbf{u}) \sim \mathcal{N}(\mathbf{0}, \mathbf{K}(\mathbf{Z}, \mathbf{Z}))$, and $\mathrm{KL}(q(\mathbf{u}) \| p(\mathbf{u}))$ is then given as

$$\frac{1}{2}\left[\mathrm{tr}(\mathbf{K}^{-1}(\mathbf{Z}, \mathbf{Z})\mathbf{S}) + \boldsymbol{\mu}^\top \mathbf{K}^{-1}(\mathbf{Z}, \mathbf{Z})\boldsymbol{\mu} - M + \log \frac{|\mathbf{K}(\mathbf{Z}, \mathbf{Z})|}{|\mathbf{S}|}\right]$$

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

- Putting both terms together, we get the following expression for the lower bound $\mathcal{L}(q(\mathbf{u}))$,

$$
\begin{aligned}
&\frac{1}{\sigma_n^2}\mathbf{y}^\top \mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} \\
&-\frac{1}{2\sigma_n^2}\operatorname{tr}(\mathbf{K}(\mathbf{X},\mathbf{X})+\mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\left(\mathbf{S}-\mathbf{K}(\mathbf{Z},\mathbf{Z})\right)\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{K}^\top(\mathbf{X},\mathbf{Z}))) \\
&+\frac{1}{2\sigma_n^2}\operatorname{tr}(\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu}\boldsymbol{\mu}^\top[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\mathbf{K}(\mathbf{Z},\mathbf{X})) \\
&-\frac{1}{2}\operatorname{tr}(\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{S})-\frac{1}{2}\boldsymbol{\mu}^\top\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\boldsymbol{\mu}-\frac{1}{2}\log\frac{|\mathbf{K}(\mathbf{Z},\mathbf{Z})|}{|\mathbf{S}|}+\text{const.}
\end{aligned}
$$

- 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

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

Partial derivative $\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}}$

- The terms in $\mathcal{L}(q(\mathbf{u}))$ that depend on $\boldsymbol{\mu}$ are

$$\begin{aligned}
&\frac{1}{\sigma_n^2}\mathbf{y}^\top \mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} \\
&+ \frac{1}{2\sigma_n^2}\boldsymbol{\mu}^\top [\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\mathbf{K}(\mathbf{Z},\mathbf{X})\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} \\
&- \frac{1}{2}\boldsymbol{\mu}^\top \mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\boldsymbol{\mu}.
\end{aligned}$$

- Taking the derivative with respect to $\boldsymbol{\mu}$ leads to

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}} &= \frac{1}{\sigma_n^2}\mathbf{K}(\mathbf{Z},\mathbf{Z})^{-1}\mathbf{K}(\mathbf{Z},\mathbf{X})\mathbf{y} \\
&+ \frac{1}{\sigma_n^2}[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\mathbf{K}(\mathbf{Z},\mathbf{X})\mathbf{K}(\mathbf{X},\mathbf{Z})[\mathbf{K}(\mathbf{Z},\mathbf{Z})]^{-1}\boldsymbol{\mu} - \mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\boldsymbol{\mu}.
\end{aligned}$$

Partial derivative $\frac{\partial \mathcal{L}}{\partial \mathbf{S}}$

- The terms in $\mathcal{L}(q(\mathbf{u}))$ that depend on $\mathbf{S}$ are

$$
\begin{aligned}
&-\frac{1}{2\sigma_n^2}\operatorname{tr}(\mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{S}\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{K}^{\top}(\mathbf{X},\mathbf{Z}))) \\
&-\frac{1}{2}\operatorname{tr}(\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{S}) + \frac{1}{2}\log|\mathbf{S}|.
\end{aligned}
$$

- Taking the derivative with respect to $\mathbf{S}$ leads to

$$
\frac{\partial \mathcal{L}}{\partial \mathbf{S}} = -\frac{1}{2\sigma_n^2}\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z})\mathbf{K}(\mathbf{Z},\mathbf{X})\mathbf{K}(\mathbf{X},\mathbf{Z})\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z}) - \frac{1}{2}\mathbf{K}^{-1}(\mathbf{Z},\mathbf{Z}) + \frac{1}{2}\mathbf{S}^{-1}.
$$

Stochastic gradient descent

- 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 descent*.

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

Contents

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

- Instead of finding particular parameters μ 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 $q(\mathbf{u}) = \mathcal{N}(\mathbf{u}|\mu, \mathbf{S})$ 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 $\mathbf{f}$

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

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

Expression for $q(\mathbf{u})$

- We can compute $q(\mathbf{u})$ using Bayes theorem and the properties of Gaussians.

- Starting with $p(\mathbf{y}|\mathbf{u})$ and $p(\mathbf{u})$, we use Bayes theorem to compute $q(\mathbf{u})$

$$q(\mathbf{u}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{u})p(\mathbf{u}).$$

- Using the properties of the Gaussian distribution, we get

$$q(\mathbf{u}|\mathbf{y}) = \mathcal{N}(\mathbf{u}|\sigma_n^{-2}\mathbf{K}(\mathbf{Z},\mathbf{Z})\mathbf{A}^{-1}\mathbf{K}(\mathbf{Z},\mathbf{X})\mathbf{y}, \mathbf{K}(\mathbf{Z},\mathbf{Z})\mathbf{A}^{-1}\mathbf{K}(\mathbf{Z},\mathbf{Z})),$$

where $\mathbf{A} = \mathbf{K}(\mathbf{Z},\mathbf{Z}) + \sigma_n^{-2}\mathbf{K}(\mathbf{Z},\mathbf{X})\mathbf{K}(\mathbf{X},\mathbf{Z})$.

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