Variational Inference

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February 27, 2023

Introduction and Background

Approximate Inference Methods

- Laplace approximation
  - Procedure to give Gaussian
  - Fixed and limited approximation quality
  - No way to use better approximating distributions
  - No measure of quality of approximation
- Markov Chain Monte Carlo (to sample from the posterior)
  - Would always converge to the right answer
  - No idea about how long it takes to converge
- **Variational inference** (Jordan et al., 1999)
  - Somewhere in between
  - Can (in principle) use complicated approximating distributions
  - Has measure of approximation quality

Further Reading

- Pattern Recognition and Machine Learning, Chapter 10 (Bishop, 2006)
- Machine Learning: A Probabilistic Perspective, Chapter 21 (Murphy, 2012)
- Variational Inference: A Review for Statisticians (Blei et al., 2017)
- NIPS-2016 Tutorial by Blei, Ranganath, Mohamed
  `https://nips.cc/Conferences/2016/Schedule?showEvent=6199`
- Tutorials by S. Mohamed
  `http://shakirm.com/papers/VITutorial.pdf`
  `http://shakirm.com/slides/MLSS2018-Madrid-ProbThinking.pdf`

Variational Inference

- Variational inference is the most scalable approximate inference method available (at the moment)
- Can handle (arbitrarily) large datasets
- Applications include:
  - Topic modeling (Hoffman et al., 2013)
  - Community detection (Gopalan & Blei, 2013)
  - Genetic analysis (Gopalan et al., 2016)
  - Reinforcement learning (e.g., Eslami et al., 2016)
  - Neuroscience analysis (Manning et al., 2014)
  - Compression and content generation (Gregor et al., 2016)
  - Traffic analysis (Kucukelbir et al., 2016; Salimbeni & Deisenroth, 2017)

Key Idea: Approximation by Optimization

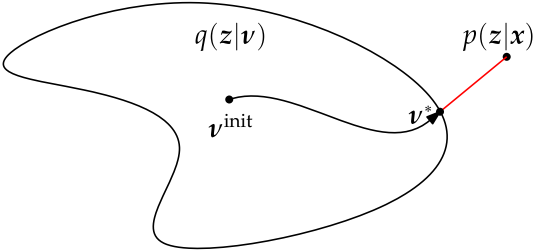


Figure adopted from Blei et al.'s NIPS-2016 tutorial

- Find approximation of a probability distribution (e.g., posterior) by optimization:
    1. Define a (parametrized) family of approximating distributions $q_{\boldsymbol{\nu}}$
    2. Define a measure of similarity of distributions to the true posterior
    3. Optimize objective function w.r.t. variational parameters $\boldsymbol{\nu}$
- Inference ⏩ Optimization

From importance sampling to variational inference

Problem setting

- We have the joint $p(\mathbf{x}, \mathbf{z})$.
- We are interested in posterior $p(\mathbf{z}|\mathbf{x})$.
- Marginal likelihood is $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z})\mathrm{d}\mathbf{z}$.

This is a very general formulation, as $\mathbf{z}$ can be a vector containing many random variables. We will consider variational bounds for more structured graphical models later.

Importance sampling

In Q34 we saw a connection between the **variance of importance sampling** and the **proposal being the posterior**.

$$I = \int p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z} \tag{1}$$

$$\hat{I} = \frac{1}{S} \sum_{s=1}^{S} \frac{p(\mathbf{x} \,|\, \mathbf{z}^{[s]}) p(\mathbf{z}^{[s]})}{q(\mathbf{z}^{[s]})}\,, \qquad \mathbf{z}^{[s]} \sim q(\mathbf{z})\,. \tag{2}$$

$$\mathbb{V}_{q(\mathbf{z})}[\hat{I}] = 0 \quad \text{iff} \quad q(\mathbf{z}) = p(\mathbf{z} \,|\, \mathbf{x}) = \frac{p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z})}{p(\mathbf{x})} \tag{3}$$

Importance sampling

Importance sampling gave an **unbiased** approximation of the marginal likelihood.

- View $q(\mathbf{z})$ as an approximation to $p(\mathbf{z} \mid \mathbf{x})$
- Estimator variance is a measure of quality of $q(\mathbf{z}) \approx p(\mathbf{z} \mid \mathbf{x})$

By comparing the variance of approximations we could compare different $q(\mathbf{z})$ as approximations to $p(\mathbf{z} \mid \mathbf{x})$.

How to compare approximations?

- Draw many samples
- Estimate variance using samples

Problem: High variance makes it hard to compare

Lower bounds

Instead of **unbiased** estimates where we try to **minimise the variance**, we can have a **biased** estimate, where we try to **minimise the bias**.

Lower bound

$$\log p(\mathbf{x}) \geqslant \mathcal{L}(q(\mathbf{z})) \tag{4}$$

Wishlist of properties:

- The posterior recovers the marginal likelihood $\mathcal{L}(p(\mathbf{z} \mid \mathbf{x})) = \log p(\mathbf{x})$
- Continuous in $q(\mathbf{z})$
- Easily computable estimate

Procedure: **Adjust $q(\mathbf{z})$ to maximise $\mathcal{L}$**.

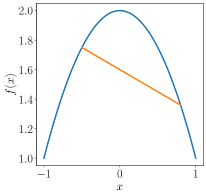
Jensen's Inequality

An important result from convex analysis:

Jensen's Inequality

For concave functions f:

$$f(\mathbb{E}[z]) \geqslant \mathbb{E}[f(z)]$$



Logarithms are concave. Therefore:

$$\log \mathbb{E}[g(z)] = \log \int g(z)p(z)dz \geqslant \int p(z) \log g(z)dz = \mathbb{E}[\log g(z)]$$

Idea: For estimating the log marginal likelihood, use Jensen's inequality instead of Monte Carlo.

Deriving the Variational Lower Bound

Look at log-marginal likelihood (log-evidence):

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})d\boldsymbol{z} \\
&= \log \int p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})\frac{q(\boldsymbol{z})}{q(\boldsymbol{z})}d\boldsymbol{z} \\
&= \log \int p(\boldsymbol{x}|\boldsymbol{z})\frac{p(\boldsymbol{z})}{q(\boldsymbol{z})}q(\boldsymbol{z})d\boldsymbol{z} \\
&= \log \mathbb{E}_q\left[p(\boldsymbol{x}|\boldsymbol{z})\frac{p(\boldsymbol{z})}{q(\boldsymbol{z})}\right] \\
&\geqslant \mathbb{E}_q \log\left(p(\boldsymbol{x}|\boldsymbol{z})\frac{p(\boldsymbol{z})}{q(\boldsymbol{z})}\right) \\
&= \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \mathbb{E}_q\left[\log\left(\frac{q(\boldsymbol{z})}{p(\boldsymbol{z})}\right)\right] \\
&= \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}[q(\boldsymbol{z})||p(\boldsymbol{z})]
\end{aligned}
$$

What have we gained?

Marginal likelihood bound[1]:

$$\mathcal{L}(q) = \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}[q(\boldsymbol{z})||p(\boldsymbol{z})] \tag{5}$$

- Objective function that can be optimised to find $q(\mathbf{z})$
  - Terms only include prior and likelihood (can evaluate)
  - Often, integrals **can** be found in closed form!
- Bound allows us to compare approximations! Higher is better.
  - Compare to importance sampling: Two estimates with unknown variances. Don't know which one to believe!

With parameterised $q_{\mathbf{v}}(\mathbf{z})$, use gradient-based optimisation to find $\mathbf{v}$.

[1] Also called **negative variational free energy**, or **Evidence Lower BOund** (ELBO).

A different derivation:

Minimising the KL

What is the measure of similarity?

- So far, the justification for VI came from that if $q(\mathbf{z}) = p(\mathbf{z} \,|\, \mathbf{x})$, then $\mathcal{L} = \log p(\mathbf{x})$.
- Measure of similarity to $p(\mathbf{z} \,|\, \mathbf{x})$ was defined simply as "how good a bound" does the $q(\mathbf{z})$ give.

Can we understand more about the measure of similarity?

What is the measure of similarity?

We can find an equation for the measure of similarity by investigating the difference between $\mathcal{L}$ and $\log p(\mathbf{x})$:

$$\begin{aligned}
\log p(\mathbf{x}) - \mathcal{L} &= \log p(\mathbf{x}) - \int q(\mathbf{z}) \log \frac{p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z})}{q(\mathbf{z})} \mathrm{d}\mathbf{z} \\
&= \int q(\mathbf{z}) \log p(\mathbf{x}) \mathrm{d}\mathbf{z} - \int q(\mathbf{z}) \log \frac{p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z})}{q(\mathbf{z})} \mathrm{d}\mathbf{z} \\
&= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}) q(\mathbf{z})}{p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z})} \mathrm{d}\mathbf{z} \\
&= \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z} \,|\, \mathbf{x})} \mathrm{d}\mathbf{z} \\
&= \mathrm{KL}[q(\mathbf{z}) || p(\mathbf{z} \,|\, \mathbf{x})]
\end{aligned}$$

VI minimises the KL from the true posterior!

Properties of Variational Inference

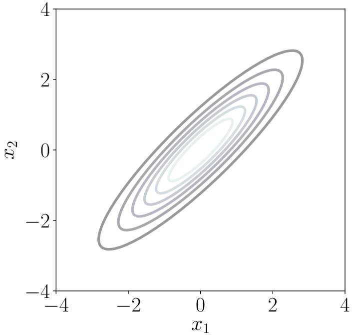
Properties of the KL divergence

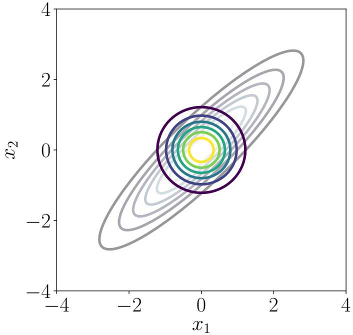
The KL divergence is a **measure of difference** between probability distributions.

$$\mathrm{KL} = \mathrm{KL}[q(\mathbf{z})||p(\mathbf{z})] = \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z})} \mathrm{d}\mathbf{z} \tag{6}$$

- $\mathrm{KL} \geqslant 0$
- $\mathrm{KL} = 0$ iff $q(\mathbf{z}) = p(\mathbf{z})$
- Related to information theory and code lengths
- Related to decision theory and betting returns
- Intuitively:
  - Strong penalty for $q(\mathbf{z})$ for placing mass where $p(\mathbf{z})$ doesn't
  - Weak penalty for $q(\mathbf{z})$ for placing too much mass compared to $p(\mathbf{z})$

Example: Gaussian KL divergence





$$\mathrm{KL}\left[\mathcal{N}\left(\mathbf{x};\boldsymbol{\mu}_0,\Sigma_0\right)||\mathcal{N}\left(\mathbf{x};\boldsymbol{\mu}_1,\Sigma_1\right)\right] =$$
$$\frac{1}{2}\left[\mathrm{Tr}\left(\Sigma_1^{-1}\Sigma_0\right) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^\intercal\Sigma_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)) - D + \log\frac{\det\Sigma_1}{\det\Sigma_0}\right]$$

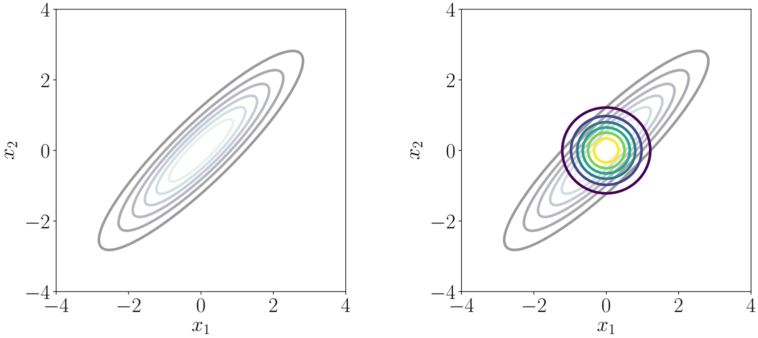
- $\Sigma_0 \to \mathbf{0} \qquad \implies \qquad \mathrm{KL} \to \infty$

Approximating Distributions

Trade-off

- More expressive gets closer to the true posterior
- Less expressive is easier to handle
- Expressive distributions may not allow integrals in ELBO to be computed

Mean-Field Approximation: Limitation



- Mean-field VI to approximate a correlated Gaussian with a factorized Gaussian
- Generally, mean-field VI tends to yield an approximation that is too compact ⏩ Need better classes of posterior approximations

Interpretation of terms

$$\log p(\boldsymbol{x}) \geqslant \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}[q(\boldsymbol{z})||p(\boldsymbol{z})] =: \mathrm{ELBO}$$

- Data-fit term (expected log-likelihood): Measures how well samples from $q(\boldsymbol{z})$ explain the data ("reconstruction cost").
  ▶▶ Place q's mass on the MAP estimate.
- Regularizer: Variational posterior $q(\boldsymbol{z})$ should not differ much from the prior $p(\boldsymbol{z})$

Alternative form of ELBO

$$
\begin{aligned}
\mathcal{L}(q_{\mathbf{v}}) &= \int q_{\mathbf{v}}(\mathbf{z}) \log p(\mathbf{x} \,|\, \mathbf{z}) \mathrm{d}\mathbf{z} && - \underbrace{\int q_{\mathbf{v}}(\mathbf{z}) \log \frac{q_{\mathbf{v}}(\mathbf{z})}{p(\mathbf{z})} \mathrm{d}\mathbf{z}}_{\text{KL}} \\
&= \int q_{\mathbf{v}}(\mathbf{z}) \log p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z} && - \int q_{\mathbf{v}}(\mathbf{z}) \log q_{\mathbf{v}}(\mathbf{z}) \mathrm{d}\mathbf{z} \\
&= \int q_{\mathbf{v}}(\mathbf{z}) \log p(\mathbf{x} \,|\, \mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z} && + \mathcal{H}(q_{\mathbf{v}}(\mathbf{z}))
\end{aligned}
$$

Comparison to MAP

$$\mathcal{L}(q_{\mathbf{v}}) = \int q_{\mathbf{v}}(\mathbf{z}) \log p(\mathbf{x} \mid \mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z} \qquad + \mathcal{H}(q_{\mathbf{v}}(\mathbf{z})) \tag{7}$$

$$L_{\mathrm{MAP}}(\mathbf{z}) = \log p(\mathbf{x}|\mathbf{z}) + \log p(\mathbf{z}) \tag{8}$$

- Fit the data like MAP
- but also be as **uncertain** as possible (entropy)

Properties of the differential entropy

$$\mathcal{H}[q(\mathbf{z})] = -\int q(\mathbf{z}) \log q(\mathbf{z}) \mathrm{d}\mathbf{z} \tag{9}$$

- Generalises entropy to continuous variables
- Limit of: Entropy of quantised $q(\mathbf{z})$ minus uniform distribution
- Can be negative! (i.e. more certain than a uniform)

Summary

- Variational turns inference into optimisation
- Two ways to derive:
  - We minimise the KL divergence to the posterior
  - Lower bound marginal likelihood with Jensen's inequality
- Constrained approximation families (e.g. mean-field) tend to underestimate uncertainty

Next time:

- How to compute ELBOs
- How to optimise ELBOs

References I

[1] C. M. Bishop. *Pattern Recognition and Machine Learning*. Information Science and Statistics. Springer-Verlag, 2006.