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Approximate Bayesian inference

2021

Slides are partially based on lectures of Dmitry Vetrov, Dmitry Kropotov and Kirill Struminsky, deepbayes.ru/2018

Bayesian ML models

Training stage:

$$p\left(\theta \mid X_{tr}, Y_{tr}\right) = \frac{p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta)}{\boxed{\int p\left(Y_{tr} \mid X_{tr}, \theta\right) p(\theta) d\theta}}$$

May be intractable

Testing stage:

$$p\left(y \mid x, X_{tr}, Y_{tr}\right) = \boxed{\int p(y \mid x, \theta) p\left(\theta \mid X_{tr}, Y_{tr}\right) d\theta}$$

What can we do if they are intractable?

Approximate inference

Probabilistic model: $p(x, \theta) = p(x \mid \theta)p(\theta)$

Variational Inference

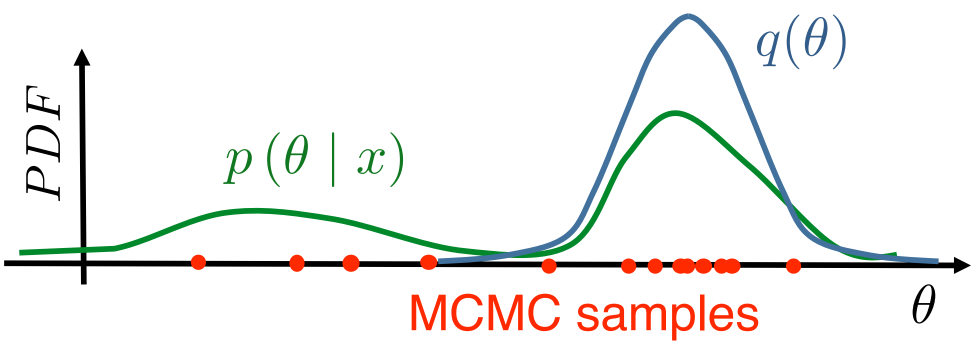
Approximate $p(\theta \mid x) \approx q(\theta) \in \mathcal{Q}$

- Biased
- Faster and more scalable

MCMC

Samples from unnormalized $p(\theta \mid x)$

- Unbiased
- Need a lot of samples



Variational inference

Probabilistic model: $p(x, \theta) = p(x \mid \theta)p(\theta)$

Main idea: find posterior approximation $p(\theta \mid x) \approx q(\theta) \in \mathcal{Q}$, using the following criterion function:

$$F(q) := KL(q(\theta) \| p(\theta \mid x)) \to \min_{q(\theta) \in \mathcal{Q}}$$

Kullback-Leibler divergence
a good mismatch measure between two distributions over the **same domain**

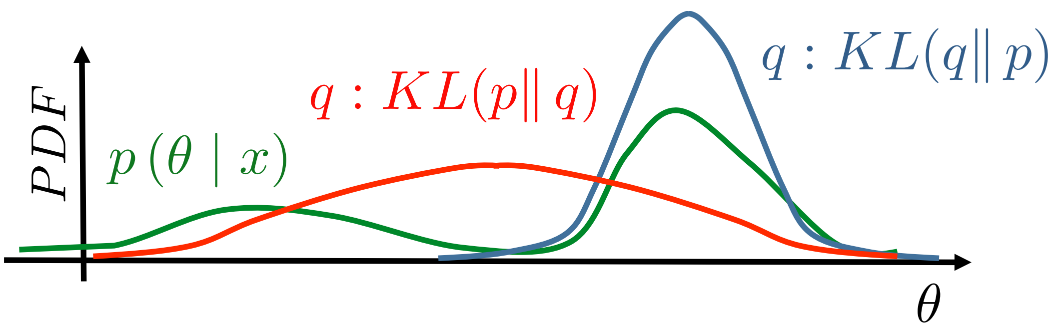
Kullback-Leibler divergence

A good mismatch measure between two distributions over the **same domain**

$$KL(q(\theta) \| p(\theta \mid x)) = \int q(\theta) \log \frac{q(\theta)}{p(\theta \mid x)} d\theta$$

Properties:

- $KL(q \| p) \geq 0$
- $KL(q \| p) = 0 \;\Leftrightarrow\; q = p$
- $KL(q \| p) \neq KL(p \| q)$



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We could not compute the posterior in the first place

How to perform an optimization w.r.t. a distribution?

Mathematical magic

$$\log p(x) = \int q(\theta) \log p(x) d\theta = \int q(\theta) \log \frac{p(x,\theta)}{p(\theta \mid x)} d\theta =$$

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$$= \boxed{\mathcal{L}(q(\theta))} + \boxed{KL(q(\theta) \| p(\theta \mid x))}$$

Evidence lower bound (ELBO) KL-divergence we need for VI

ELBO = Evidence Lower Bound

$$\log p(x) = \mathcal{L}(q(\theta)) + KL(q(\theta) \| p(\theta \mid x))$$

Evidence:

$$p(\theta \mid x) = \frac{p(x \mid \theta)p(\theta)}{p(x)} = \frac{p(x \mid \theta)p(\theta)}{\int p(x \mid \theta)p(\theta)d\theta} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

Evidence of the probabilistic model shows the total probability of observing the data.

Lower Bound: KL is non-negative $\longrightarrow$ $\log p(x) \geq \mathcal{L}(q(\theta))$

Variational inference

Optimization problem with intractable posterior distribution:

$$F(q) := KL(q(\theta) \| p(\theta \mid x)) \to \min_{q(\theta) \in \mathcal{Q}}$$

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$$KL(q(\theta) \| p(\theta \mid x)) \to \min_{q(\theta) \in \mathcal{Q}} \quad \Leftrightarrow \quad \mathcal{L}(q(\theta)) \to \max_{q(\theta) \in \mathcal{Q}}$$

Variational inference

Final optimisation problem:

$$\mathcal{L}(q(\theta)) = \int q(\theta) \log \frac{p(x, \theta)}{q(\theta)} d\theta \to \max_{q(\theta) \in \mathcal{Q}}$$

Variational inference: ELBO interpretation

Final optimisation problem:

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this is not the same KL-divergence!

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How to perform an optimization w.r.t. a distribution?

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How to perform an optimization w.r.t. a distribution?

Parametric approximation

Parametric family

$$q(\theta) = q(\theta \mid \lambda)$$

Parametric approximation

Parametric family of variational distributions:

$$q(\theta) = q(\theta \mid \lambda), \qquad \lambda \text{ — some parameters}$$

Why is it a restriction? We choose a family of some fixed form:

- It may be too simple and insufficient to model the data
- If it is complex enough then there is no guaranty we can train it well to fit the data

Parametric approximation

Parametric family of variational distributions:

$$q(\theta) = q(\theta \mid \lambda), \qquad \lambda \text{ — some parameters}$$

Variational inference transforms to parametric optimization problem:

$$\mathcal{L}(q(\theta \mid \lambda)) = \int q(\theta \mid \lambda) \log \frac{p(x, \theta)}{q(\theta \mid \lambda)} d\theta \to \max_{\lambda}$$

If we're able to calculate derivatives of ELBO w.r.t. λ then we can solve this problem using some numerical optimization solver.

Inference methods: summary

Probabilistic model: $p(x, \theta)$ We want to compute: $p(\theta \mid x)$

Approximation		Inference
Exact	$p(\theta \mid x)$	Full Bayesian inference
Parametric	$p(\theta \mid x) \approx q(\theta) = q(\theta \mid \lambda)$	Parametric VI
Delta function	$p(\theta \mid x) \approx \delta(\theta - \theta_{MP})$	MP inference
No prior	θ_{ML}	MLE