Automatic Differentiation Variational Inference

Philip Schulz and Wilker Aziz

https://github.com/philschulz/VITutorial

What we know so far

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  - Score function estimator: applicable to any model
  - Reparameterised gradients
    so far seems applicable only to Gaussian variables

Multivariate calculus recap

Let $x \in \mathbb{R}^K$ and let $\mathcal{T} : \mathbb{R}^K \to \mathbb{R}^K$ be differentiable and invertible

- $y = \mathcal{T}(x)$
- $x = \mathcal{T}^{-1}(y)$

Jacobian

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Inverse function theorem

$$J_{\mathcal{T}^{-1}}(y) = \left(J_{\mathcal{T}}(x)\right)^{-1}$$

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- Multivariate case

$$\mathrm{d}y = |\det J_{\mathcal{T}}(x)|\mathrm{d}x$$

  the absolute value absorbs the orientation

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and then it follows that

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- $\mathcal{S}_\lambda(z)$ absorbs dependency on λ

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Reparameterised gradients

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$$\overset{\text{MC}}{\approx} \frac{1}{M} \sum_{\substack{i=1 \\ \epsilon_i \sim \pi(\epsilon)}}^{M} \frac{\partial}{\partial \lambda} g(\mathcal{S}_\lambda^{-1}(\epsilon_i))$$

Reparameterised gradients: Gaussian

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&= \mathbb{E}_{\mathcal{N}(0,I)}\left[\frac{\partial}{\partial z}g(z = \mu + \sigma\epsilon)\frac{\partial z}{\partial\lambda}\right]
\end{aligned}$$

Beyond

Many interesting densities cannot easily be reparameterised

- e.g. Beta, Gamma, Dirichlet, von Mises-Fisher

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Reparameterised gradients are a step towards automatising VI for differentiable models

- but not every model of interest employs rvs for which a reparameterisation is known

Example

Suppose we have some ordinal data which we assume to be Poisson-distributed

$$X|\lambda \sim \text{Poisson}(\lambda)$$

and suppose we want to impose
FINISH EXAMPLE, GIVE THE OVERVIEW OF ADVI "PSEUDO-CODE" FIRST

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- members of this class have continuous latent variables z
- and the gradient $\nabla_z \log p(x, z)$ is valid within the *support* of the prior
  $\text{supp}(p(z)) = \{z \in \mathbb{R}^K : p(z) > 0\} \subseteq \mathbb{R}^K$

Why do we need differentiable models?

Recall the gradient of the ELBO

$$\frac{\partial}{\partial \lambda} \mathbb{E}_{q(z;\lambda)} \left[\log p(x, z) \right] + \frac{\partial}{\partial \lambda} \mathbb{H} \left(q(z; \lambda) \right)$$

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Let's focus on the design and optimisation of the variational approximation

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- otherwise KL is not a real number
  $\mathrm{KL}\left(q \,||\, p\right) = \mathbb{E}_q\left[\log q\right] - \mathbb{E}_q\left[\log p\right] \stackrel{\text{def}}{=} \infty$

Support matching constraint

So let's constrain $q(z)$ to a family $\mathcal{Q}$ whose support is included in the support of the posterior

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- a parameter vector λ picks out a member of the family

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We maximise the ELBO

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- Λ may be constrained to a subset of $\mathbb{R}^D$
  e.g. univariate Gaussian location lives in $\mathbb{R}$ but scale lives in $\mathbb{R}_{>0}$

Parameters in real coordinate space

It is easy to make sure parameters are unconstrained

- we just need to use an appropriate activation

Example

- $Z \sim \mathcal{N}(\mu, \sigma)$
  where $\mu \in \mathbb{R}^d$ and $\sigma \in \mathbb{R}^d_{>0}$

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We maximise the ELBO

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- support of $q(z;\lambda)$ depends on the choice of prior and thus may be a subset of $\mathbb{R}^K$

ADVI

A gradient-based black-box VI procedure

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Joint model in real coordinate space

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$$p(x, \zeta) = p(x, \mathcal{T}^{-1}(\zeta))|\det J_{\mathcal{T}^{-1}}(\zeta)|$$

ASK FILL-IN THE GAP QUESTION

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$$q(\zeta;\lambda) = \underbrace{\prod_{k=1}^{K} q(\zeta_k;\lambda)}_{\text{mean field}} = \prod_{k=1}^{K} \mathcal{N}(\zeta_k|\mu_k,\sigma_k^2)$$

where

- $\mu_k = \lambda_{\mu_k}$ for $\lambda_{\mu_k} \in \mathbb{R}^K$
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$$= \log \int q(\zeta) \frac{p(x, \mathcal{T}^{-1}(\zeta)) |\det J_{\mathcal{T}^{-1}}(\zeta)|}{q(\zeta)} \mathrm{d}\zeta$$

ELBO in real coordinate space

$$
\begin{aligned}
\log p(x) &= \log \int p(x, z) \mathrm{d}z \\
&= \log \int p(x, \mathcal{T}^{-1}(\zeta)) |\det J_{\mathcal{T}^{-1}}(\zeta)| \mathrm{d}\zeta \\
&= \log \int q(\zeta) \frac{p(x, \mathcal{T}^{-1}(\zeta)) |\det J_{\mathcal{T}^{-1}}(\zeta)|}{q(\zeta)} \mathrm{d}\zeta \\
&\overset{\text{JI}}{\geq} \int q(\zeta) \log \frac{p(x, \mathcal{T}^{-1}(\zeta)) |\det J_{\mathcal{T}^{-1}}(\zeta)|}{q(\zeta)} \mathrm{d}\zeta
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&= \mathbb{E}_{q(\zeta)} \left[\log p(x, \mathcal{T}^{-1}(\zeta)) + \log |\det J_{\mathcal{T}^{-1}}(\zeta)| \right] + \mathbb{H}\left(q(\zeta)\right)
\end{aligned}
$$

Reparameterised ELBO

Recall that for Gaussians we have a standardisation procedure $\mathcal{S}_\lambda(\zeta) \sim \mathcal{N}(\epsilon|0, I)$

$$\mathbb{E}_{q(\zeta;\lambda)}\left[\log p(x, \mathcal{T}^{-1}(\zeta)) + \log\left|\det J_{\mathcal{T}^{-1}}(\zeta)\right|\right] + \mathbb{H}\left(q(\zeta;\lambda)\right)$$

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$$= \mathbb{E}_{\mathcal{N}(\epsilon|0,I)}\left[\log p(x, \underbrace{\mathcal{T}^{-1}(\overbrace{\mathcal{S}_\lambda^{-1}(\epsilon)}^{\zeta})}_{z}) + \log\left|\det J_{\mathcal{T}^{-1}}(\mathcal{S}_\lambda^{-1}(\epsilon))\right|\right]$$

$$+ \mathbb{H}\left(q(\zeta;\lambda)\right)$$

Gradient estimate

For $\epsilon_i \sim \mathcal{N}(0, I)$

$$\frac{\partial}{\partial \lambda} \mathrm{ELBO}(\lambda)$$

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Practical tips

Many software packages know how to transform the support of various distributions

- Stan
- Tensorflow `tf.probability`
- Pytorch `torch.distributions`

LDA

Wait... no deep learning?