Automatic Differentiation Variational Inference

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https://github.com/philschulz/VITutorial

What we know so far

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- But the MC estimator is not differentiable
  - Score function estimator: applicable to any model
  - Reparameterised gradients
    so far seems applicable only to Gaussian variables

Reparameterised gradients: Gaussian

We have seen one case, namely,
if $\epsilon \sim \mathcal{N}(0, I)$ and $Z \sim \mathcal{N}(\mu, \sigma^2)$

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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

The Jacobian matrix $\mathbf{J} = J_{\mathcal{T}}(x)$ of $\mathcal{T}$ assessed at x is the matrix of partial derivatives

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Inverse function theorem

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

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where $\mathrm{d}y/\mathrm{d}x$ is the *derivative* of y wrt x

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- Multivariate case

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

the absolute value absorbs the orientation

Integration by substitution

We can integrate a function $g(x)$
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and then it follows that

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

Standardisation functions

Location-scale family

- a family of distributions where for
  $F_X(x) = \Pr\{X \leq x\}$
  if $Y = a + bX$, then $F_Y(y|a,b) = F_X(\frac{z-a}{b})$

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Examples: Gaussian, Laplace, Cauchy, Uniform

Standardisation functions (cont.)

Inverse cdf

- for univariate Z with pdf $f_Z(z)$ and cdf $F_Z(z)$

$$P \sim \mathcal{U}(0,1) \qquad Z \sim F_Z^{-1}(P)$$

where $F_Z^{-1}(p)$ is the *quantile function*

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Gumbel distribution

- $f_Z(z|\mu,\beta) = \beta^{-1} \exp(-z - \exp(-z))$
- $F_Z(z|\mu,\beta) = \exp\left(-\exp\left(-\frac{z-\mu}{\beta}\right)\right)$
- $F_Z^{-1}(p) = \mu - \beta \log(-\log p)$

Beyond

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The inverse cdf of a multivariate rv is seldom known in closed-form

- Dirichlet, von Mises-Fisher

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- many models have intractable posteriors
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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 standardisation function 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

Differentiable models

We focus on *differentiable probability models*

$$p(x, z) = p(x|z)p(z)$$

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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 $\mathrm{supp}(p(z)) = \{z \in \mathbb{R}^K : p(z) > 0\} \subseteq \mathbb{R}^K$

VI optimisation problem

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

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To automatise the search for a variational approximation $q(z)$ we must ensure that

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- otherwise KL is not defined
  $\mathrm{KL}\left(q \,||\, p\right) = \mathbb{E}_q\left[\log q\right] - \mathbb{E}_q\left[\log p\right] = \infty$

Support matching constraint

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

$$\operatorname*{arg\,min}_{q(z)\in\mathcal{Q}} \mathrm{KL}\left(q(z)\;||\;p(z|x)\right)$$

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- typically the same as the support of $p(z)$ as long as $p(x, z) > 0$ if $p(z) > 0$

Parametric family

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

Constrained optimisation for the ELBO

We maximise the ELBO

$$\arg\max_{\phi \in \Phi} \mathbb{E}_{q(z;\phi)}\left[\log p(x, z)\right] + \mathbb{H}\left(q(z|\phi)\right)$$

subject to

$$\mathcal{Q} = \{q(z;\phi) : \phi \in \Phi, \operatorname{supp}(q(z;\phi)) \subseteq \operatorname{supp}(p(z))\}$$

Constrained optimisation for the ELBO

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$$\arg\max_{\phi \in \Phi} \mathbb{E}_{q(z;\phi)} [\log p(x, z)] + \mathbb{H}\left(q(z|\phi)\right)$$

subject to

$$\mathcal{Q} = \{q(z;\phi) : \phi \in \Phi, \mathrm{supp}(q(z;\phi)) \subseteq \mathrm{supp}(p(z))\}$$

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- Φ can be an intricate subset of $\mathbb{R}^D$
  e.g. univariate Gaussian location lives in $\mathbb{R}$ but scale lives in $\mathbb{R}_{>0}$

ADVI

From the point of view of a black-box procedure, this objective poses two problems

1. intractable expectations

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1. intractable expectations Reparameterised Gradients!
2. custom $\text{supp}(q(z;\phi))$

Idea

1. let's find a way to transform $\text{supp}(p(z))$ to the complete real coordinate space
2. then we pick a variational family over the complete real coordinate space for which a standardisation exists!