Automatic Differentiation Variational Inference

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https://github.com/philschulz/VITutorial

What we know so far

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- Objective: lowerbound on likelihood (ELBO)
    - cannot be computed exactly
      we resort to Monte Carlo estimation
- 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

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if $\epsilon \sim \mathcal{N}(0, I)$ and $Z \sim \mathcal{N}(\mu, \sigma^2)$

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Multivariate calculus recap

Let $x \in \mathbb{R}^D$ and let $\mathcal{T} : \mathbb{R}^D \to \mathbb{R}^D$ 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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- $\mathcal{S}_\lambda(z)$ absorbs dependency on λ

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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

Many interesting densities are not location-scale families

- e.g. Beta, Gamma

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

- 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 standardisation function is known

Example

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

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

and suppose we want to impose

Differentiable models

We focus on *differentiable probability models*

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

VI optimisation problem

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

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- otherwise KL is not defined
- but what is the support of $p(z|x)$?
- typically the same as the support of $p(z)$ as long as $p(x,z) > 0$ if $p(z) > 0$

Parametric family

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

$$\mathcal{Q} = \{q(z;\phi) : \phi \in \Phi\}$$

- a parameter vector ϕ picks out a member $q(z;\phi)$ of the family

Our objective now is

$$\underset{\phi \in \Phi}{\arg\min} \, \mathrm{KL}\left(q(z;\phi) \,||\, p(z|x)\right)$$

ADVI

Minimising the original VI problem is equivalent to maximising the ELBO

$$\mathcal{L}(\phi) = \mathbb{E}_{q(z;\phi)}\left[\log p(x, z)\right] + \mathbb{H}\left(q(z|\phi)\right) \qquad (1)$$

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 $\mathrm{supp}(q(z;\phi))$

Idea

1. let's find a way to transform $\mathrm{supp}(p(z))$ to the complete real coordinate space