# Automatic Differentiation Variational Inference

Philip Schulz and Wilker Aziz

https://github.com/philschulz/VITutorial

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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

Multivariate calculus recap

Reparameterised gradients revisited

ADVI

Example

# 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

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

# Differential (or inifinitesimal)

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- Scalar case

$$\mathrm{d}y = \mathcal{T}'(x)\mathrm{d}x = \frac{\mathrm{d}y}{\mathrm{d}x}\mathrm{d}x = \frac{\mathrm{d}}{\mathrm{d}x}T(x)\mathrm{d}x$$

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- Multivariate case

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

the absolute value absorbs the orientation

# Integration by substitution

We can integrate a function $g(x)$ by substituting $x = \mathcal{T}^{-1}(y)$

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and then it follows that

$$p_X(x) = p_Y(\mathcal{T}(x))|\det J_{\mathcal{T}}(x)|$$

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

# Reparameterised expectations

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$$= \int \pi(\epsilon)g(\mathcal{S}_\lambda^{-1}(\epsilon))\mathrm{d}\epsilon = \mathbb{E}_{\pi(\epsilon)}\left[g(\mathcal{S}_\lambda^{-1}(\epsilon))\right]$$

# Reparameterised gradients

For optimisation, we need tractable gradients

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since now the density does not depend on $\lambda$, we can obtain a gradient estimate

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

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

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and

$$\frac{\partial}{\partial\lambda}\mathbb{E}_{\mathcal{N}(z|\mu,\sigma^2)}\left[g(z)\right]$$

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# Beyond

Many interesting densities cannot easily be reparameterised

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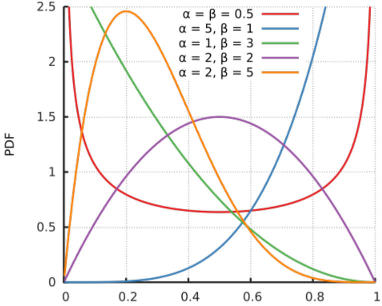
Beta



# Beyond

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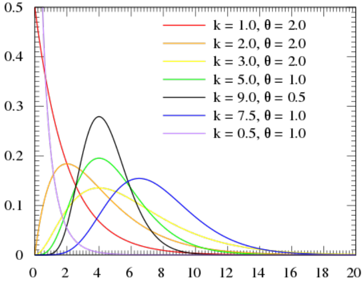
Gamma



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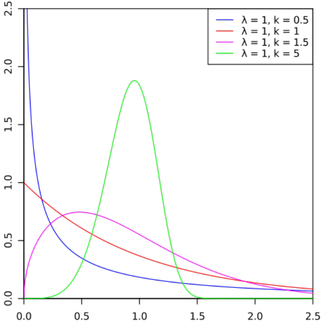
Weibull



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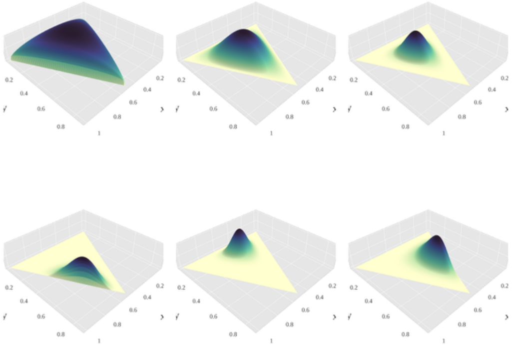
Dirichlet



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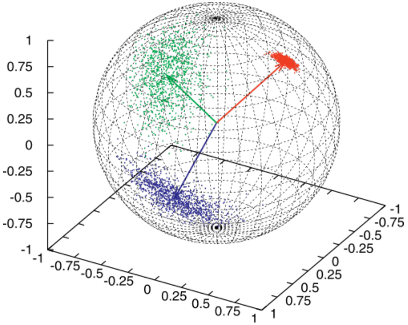
von Mises-Fisher



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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: Weibull-Poisson model

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

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\begin{aligned}
z|r, k &\sim \text{Weibull}(r, k) \quad & r \in \mathbb{R}_{>0}, k \in \mathbb{R}_{>0} \\
X|z &\sim \text{Poisson}(z) \quad & z \in \mathbb{R}_{>0}
\end{aligned}
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# VI for Weibull-Poisson model

Generative model

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No! $\mathrm{supp}(\mathcal{N}(z|\mu, \sigma^2)) = \mathbb{R}$

# Strategy

Build a change of variable into the model

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Can we use a Gaussian approximate posterior? Yes!

# Differentiable models

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

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

# 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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Reparameterisation requires $\frac{\partial}{\partial z}$

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# VI optimisation problem

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

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- a parameter vector $\lambda$ picks out a member of the family

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We maximise the ELBO

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  e.g. univariate Gaussian location lives in $\mathbb{R}$ but scale lives in $\mathbb{R}_{>0}$

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It is typically possible to work with unconstrained parameters, it only takes an appropriate activation

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A gradient-based black-box VI procedure

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

where

- $\mu_k = \lambda_{\mu_k}$ for $\lambda_{\mu_k} \in \mathbb{R}^K$
- $\sigma_k = \text{softplus}(\lambda_{\sigma_k})$ for $\lambda_{\sigma_k} \in \mathbb{R}^K$

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$$= \log \int q(\zeta) \frac{p(x, \mathcal{T}^{-1}(\zeta)) |\det J_{\mathcal{T}^{-1}}(\zeta)|}{q(\zeta)} \mathrm{d}\zeta$$

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

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

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

# Gradient estimate

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

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

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$$\frac{\partial}{\partial \lambda} \mathsf{ELBO}(\lambda) \overset{\mathsf{MC}}{\approx} \frac{1}{M} \sum_{i=1}^{M} \frac{\partial}{\partial \lambda} \log \underbrace{p(x|\mathcal{T}^{-1}(\mathcal{S}_\lambda^{-1}(\epsilon_i)))}_{\text{likelihood}}$$

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+ \frac{\partial}{\partial \lambda} \log \underbrace{\left| \det J_{\mathcal{T}^{-1}}(\mathcal{S}_\lambda^{-1}(\epsilon_i)) \right|}_{\text{change of volume}} \\
+ \frac{\partial}{\partial \lambda} \underbrace{\mathbb{H}\left(q(\zeta; \lambda)\right)}_{\text{analaytic}}
\end{aligned}
$$

# Practical tips

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

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

# Weibull-Poisson model

Build a change of variable into the model

$$
\begin{aligned}
p(x, z \mid r, k) &= p(z \mid r, k)\, p(x \mid \rho) \\
&= \mathrm{Weibull}(z \mid r, k)\, \mathrm{Poisson}(x \mid z)
\end{aligned}
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p(x, z|r, k) &= p(z|r, k)p(x|\rho) \\
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&= \text{Weibull}(\underbrace{\log^{-1}(\zeta)}_{z}|r, k)\,\text{Poisson}(x|\underbrace{\log^{-1}(\zeta)}_{z})\left|\det J_{\log^{-1}}(\zeta)\right|
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&= p(x, z = \log^{-1}(\zeta)) \left|\det J_{\log^{-1}}(\zeta)\right|
\end{aligned}
$$

# Weibull-Poisson model

Build a change of variable into the model

$$
\begin{aligned}
p(x, z|r, k) &= p(z|r, k)p(x|\rho) \\
&= \text{Weibull}(z|r, k)\,\text{Poisson}(x|z) \\
&= \text{Weibull}(\underbrace{\log^{-1}(\zeta)}_{z}|r, k)\,\text{Poisson}(x|\underbrace{\log^{-1}(\zeta)}_{z})\left|\det J_{\log^{-1}}(\zeta)\right| \\
&= p(x, z = \log^{-1}(\zeta))\left|\det J_{\log^{-1}}(\zeta)\right|
\end{aligned}
$$

ELBO

$$\mathbb{E}_{q(\zeta|\lambda)}\left[\ldots\right] + \mathbb{H}\left(q(\zeta)\right)$$

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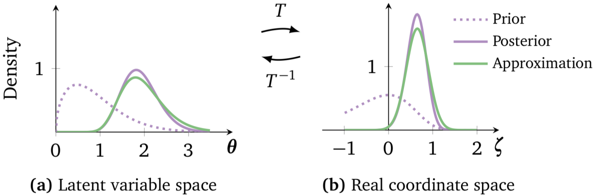
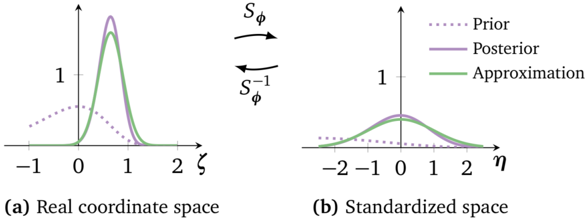
$$

$$
\mathbb{E}_{\phi(\epsilon)} \left[ \log p(x, z = \log^{-1}(\mathcal{S}^{-1}(\epsilon))) \left| \det J_{\log^{-1}}(\mathcal{S}^{-1}(\epsilon)) \right| \right] + \mathbb{H}\left(q(\zeta)\right)
$$

# Visualisation




Images from Kucukelbir et al. (2017)

# Wait... no deep learning?

Sure! Parameters may well be predicted by NNs

- approximate posterior location and scale
- Weibull rate and shape

Everything is now differentiable, reparameterisable, and the optimisation is unconstrained!

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What's left? Our posteriors are still rather simple, aren't they?

Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, and David M. Blei. Automatic differentiation variational inference. *Journal of Machine Learning Research*, 18(14):1–45, 2017. URL http://jmlr.org/papers/v18/16-107.html.