Automatic Differentiation Variational Inference

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https://vitutorial.github.io/tour/ua2020

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gourmet

1. Multivariate calculus recap

2. Reparameterised gradients revisited

3. ADVI

4. Example

What we know so far

- DGMs:

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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

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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 $J_{\mathcal{T}}(x)$ of $\mathcal{T}$
assessed at x is the matrix of partial derivatives

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Inverse function theorem

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

Differential (or inifinitesimal)

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- Scalar case

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

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

Reparameterised expectations

If we are interested in

$$\mathbb{E}_{q(z|\lambda)}\left[g(z)\right]$$

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$$= \int \pi(\epsilon)$$

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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

$$\frac{\partial}{\partial \lambda}\mathbb{E}_{q(z|\lambda)}\left[g(z)\right] = \frac{\partial}{\partial \lambda}\mathbb{E}_{\pi(\epsilon)}\left[g(\mathcal{S}_{\lambda}^{-1}(\epsilon))\right]$$

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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

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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\end{aligned}$$

Reparameterised gradients: Inverse cdf

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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Example: Kumaraswamy distribution

- $f_Z(z; a, b) = abz^{a-1}(1 - z^a)^{b-1}$
- $F_Z(z; a, b) = 1 - (1 - z^a)^b$
- $F_Z^{-1}(p; a, b) = (1 - (1 - p)^{1/b})^{1/a}$

Beyond

Many interesting densities cannot be easily reparameterised

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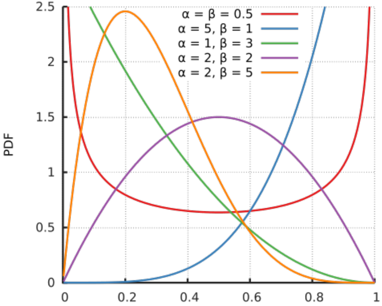
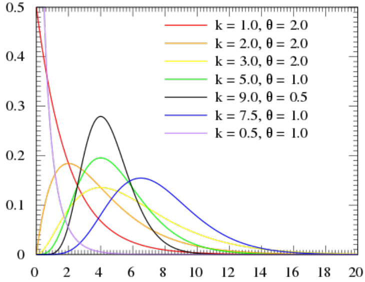
Beta



Beyond

Many interesting densities cannot be easily reparameterised

Gamma



Beyond

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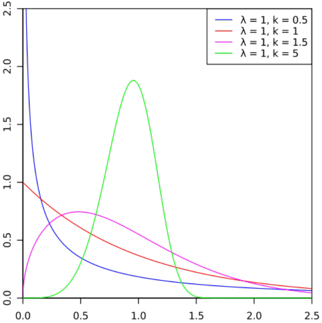
Weibull



Beyond

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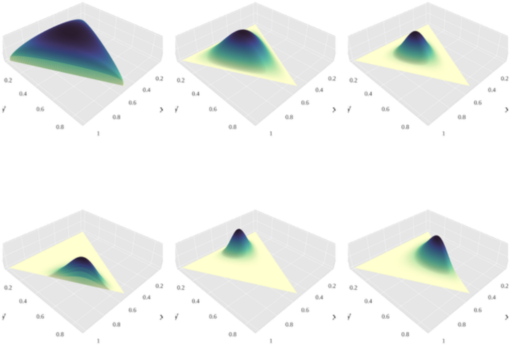
Dirichlet



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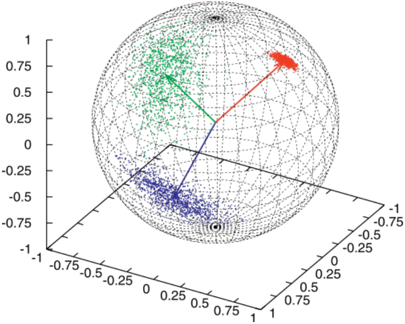
von Mises-Fisher



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- but many models are differentiable
  that's the main constraint for using NNs

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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$$\begin{aligned} z|r,k &\sim \text{Weibull}(r,k) & r \in \mathbb{R}_{>0}, k \in \mathbb{R}_{>0} \\ X|z &\sim \text{Poisson}(z) & z \in \mathbb{R}_{>0} \end{aligned}$$

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VI for Weibull-Poisson model

Generative model

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

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Can we make $q(z|\lambda)$ Gaussian?

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

Strategy

Build a change of variable into the model

$$p(x, z|r, k) = p(z|r, k)p(x|z)$$
$$= \text{Weibull}(z|r, k)\,\text{Poisson}(x|z)$$

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ELBO

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\mathbb{E}_{q(\zeta|\lambda)}\left[f(x, \zeta)\right] + \mathbb{H}\left(q(\zeta)\right)
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ELBO

$$\mathbb{E}_{q(\zeta|\lambda)}[f(x, \zeta)] + \mathbb{H}(q(\zeta))$$

Can we use a Gaussian approximate posterior?

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p(x, z|r, k) &= p(z|r, k)p(x|z) \\
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&= \text{Weibull}(\underbrace{\exp(\zeta)}_{z}|r, k)\,\text{Poisson}(x|\underbrace{\exp(\zeta)}_{z})|\det J_{\exp}(\zeta)| \\
&= f(x, \zeta)
\end{aligned}
$$

ELBO

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

Can we use a Gaussian approximate posterior? Yes!

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

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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$$\frac{\partial}{\partial \lambda} \mathbb{E}_{q(z;\lambda)} [\log p(x, z)] = \mathbb{E}_{\pi(\epsilon)} \left[\frac{\partial}{\partial \lambda} \log p(x, z = \mathcal{S}_{\lambda}^{-1}(\epsilon)) \right]$$

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VI optimisation problem

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

$$\arg\min_{q(z)} \mathrm{KL}\left(q(z) \,||\, p(z|x)\right)$$

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

Support matching constraint

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

$$\arg\min_{q(z)\in\mathcal{Q}} \mathrm{KL}\left(q(z) \mid\mid p(z|x)\right)$$

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$$\mathcal{Q} = \{q(z) : \mathrm{supp}(q(z)) \subseteq \mathrm{supp}(p(z|x))\}$$

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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

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where

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

Constrained optimisation for the ELBO

We maximise the ELBO

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

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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

Consider the Gaussian case: $Z \sim \mathcal{N}(\mu, \sigma)$

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how can we get v from $\lambda_v \in \mathbb{R}^d$?

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

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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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    - Express $z \in \mathrm{supp}(p(z)) \subseteq \mathbb{R}^K$ as a transformation of some unconstrained $\zeta \in \mathbb{R}^K$

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   - basically, pick a Gaussian!
3. Intractable expectations
   - Reparameterised Gradients!

Joint model in real coordinate space

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We can design a posterior approximation whose support is $\mathbb{R}^K$

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

where

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

ELBO in real coordinate space

$\log p(x)$

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$$\log p(x) = \log \int p(x, z) \mathrm{d}z$$

ELBO in real coordinate space

$$\log p(x) = \log \int p(x, z)\mathrm{d}z$$

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

ELBO in real coordinate space

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

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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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&\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\left|\det J_{\mathcal{T}^{-1}}(\zeta)\right|\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 $\epsilon_i \sim \mathcal{N}(0, I)$

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

Gradient estimate

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

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

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$$+ \frac{\partial}{\partial \lambda} \log \underbrace{p(\mathcal{T}^{-1}(\mathcal{S}_\lambda^{-1}(\epsilon_i)))}_{\text{prior}}$$
$$+ \frac{\partial}{\partial \lambda} \log \underbrace{\left| \det J_{\mathcal{T}^{-1}}(\mathcal{S}_\lambda^{-1}(\epsilon_i)) \right|}_{\text{change of volume}}$$

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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`

Weibull-Poisson model

Build a change of variable into the model

$$
\begin{aligned}
p(x, z \mid r, k) &= p(z \mid r, k) p(x \mid \rho) \\
&= \text{Weibull}(z \mid r, k) \, \text{Poisson}(x \mid z)
\end{aligned}
$$

Weibull-Poisson model

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\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})
\end{aligned}
$$

Weibull-Poisson model

Build a change of variable into the model

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

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p(x, z \mid r, k) &= p(z \mid r, k)\, p(x \mid \rho) \\
&= \text{Weibull}(z \mid r, k)\, \text{Poisson}(x \mid z) \\
&= \text{Weibull}(\underbrace{\log^{-1}(\zeta)}_{z} \mid r, k)\, \text{Poisson}(x \mid \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

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

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$$

ELBO

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

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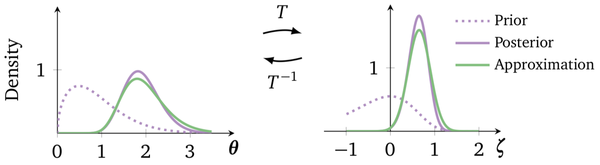
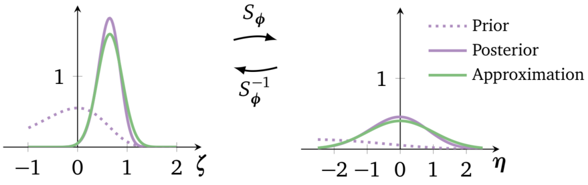
$$

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

Visualisation



(a) Latent variable space **(b)** Real coordinate space



(a) Real coordinate space **(b)** Standardized space

Images from ?

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!

Summary

ADVI is a big step towards blackbox VI

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What's left?

Summary

ADVI is a big step towards blackbox VI

- we knew how to map parameters to the unconstrained real coordinate space
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Think of ADVI as reparameterised gradients and autodiff expanded to many more models!

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.