Automatic Differentiation Variational Inference

Deep Learning 2 – 2023

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

Outline

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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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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- Multivariate case

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

  the absolute value absorbs the orientation

Integration by substitution

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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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Revisiting reparameterised gradients

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  we call it a *base density*
- $\mathcal{S}_\lambda(z)$ absorbs dependency on λ

Reparameterised expectations

If we are interested in

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

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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

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since now the density does not depend on λ, we can obtain a gradient estimate

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

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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and

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

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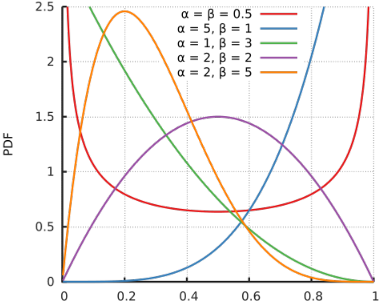
Beta



Beyond

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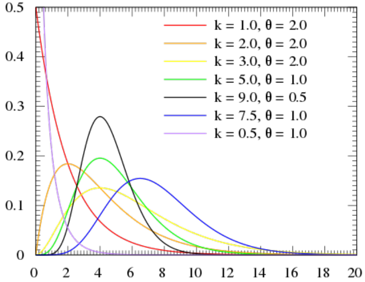
Gamma



Beyond

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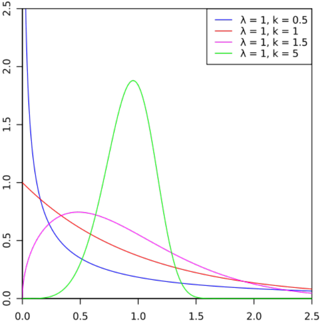
Weibull



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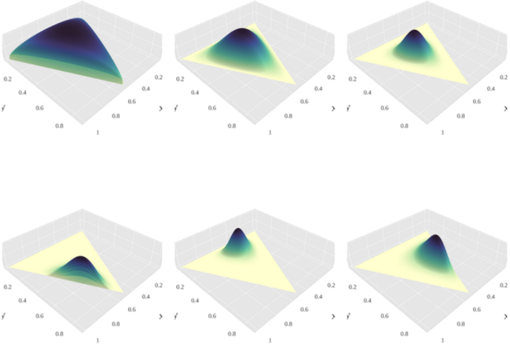
Dirichlet



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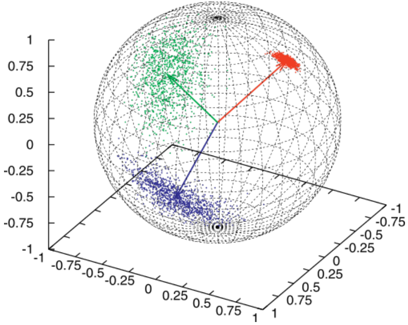
von Mises-Fisher



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Automatic Differentiation VI

Motivation

- many models have intractable posteriors
  their normalising constants (evidence) lack analytic solutions

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Reparameterised gradients are a step towards automating VI for differentiable models

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

Example: Weibull-Poisson model

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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

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

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Can we make $q(z|\lambda)$ Gaussian?
No! $\text{supp}(\mathcal{N}(z|\mu, \sigma^2)) = \mathbb{R}$

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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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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Can we use a Gaussian approximate posterior? Yes!

Differentiable models

We focus on *differentiable probability 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 $\text{supp}(p(z)) = \{z \in \mathbb{R}^K : p(z) > 0\} \subseteq \mathbb{R}^K$

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

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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

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

where

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

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

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We maximise the ELBO

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

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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 $\mathbb{R}^K$

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A gradient-based black-box VI procedure

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3. Intractable expectations
   - Reparameterised Gradients!

Joint model in real coordinate space

Let's introduce an invertible and differentiable transformation

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

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

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

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

ELBO in real coordinate space

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

Reparameterised ELBO

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

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

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

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

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$$+ \frac{\partial}{\partial \lambda} \log \underbrace{p(\mathcal{T}^{-1}(\mathcal{S}_\lambda^{-1}(\epsilon_i)))}_{\text{prior density of } z}$$

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

$$+ \frac{\partial}{\partial \lambda} \underbrace{\mathbb{H}\left(q(\zeta; \lambda)\right)}_{\text{analaytic}}$$

Practical tips

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

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

Outline

Weibull-Poisson model

Build a change of variable into the model

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

Weibull-Poisson model

Build a change of variable into the model

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\begin{aligned}
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|
\end{aligned}
$$

Weibull-Poisson model

Build a change of variable into the model

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ELBO

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

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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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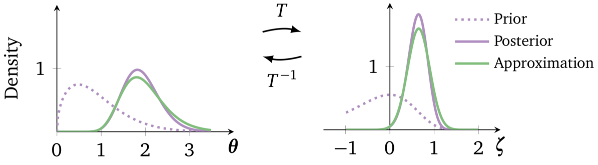
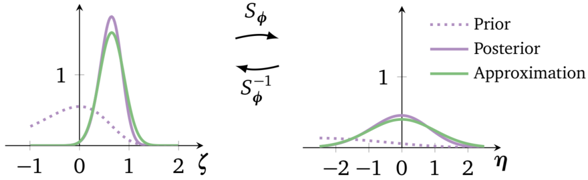
ELBO

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

Visualisation



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



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

Images from 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!

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?

References I

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. ISSN 1533-7928. URL http://jmlr.org/papers/v18/16-107.html.