Advanced Approximate Inference for Discrete LVMs

Deep Learning 2 – 2022

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Outline

Gradients of the evidence lowerbound

ELBO

$$\mathcal{E}(\lambda, \theta) = \mathbb{E}_{q_{Z|X}(z|x,\lambda)}\left[\log \frac{p_{ZX}(z, x|\theta)}{q_{Z|X}(z|x, \lambda)}\right]$$

Updating generative model

$$\nabla_\theta \mathcal{E}(\lambda, \theta) = \mathbb{E}_{q_{Z|X}(z|x,\lambda)}\left[\nabla_\theta \log \frac{p_{ZX}(z, x|\theta)}{q_{Z|X}(z|x, \lambda)}\right]$$

Updating inference model

$$\nabla_\lambda \mathcal{E}(\lambda, \theta) = \nabla_\lambda \mathbb{E}_{f_Z(z|\lambda)}[\psi(z)]$$

$f_Z(z|\lambda) = q_{Z|X}(z|x, \lambda)$ and $\psi(z) = \log \frac{p_{ZX}(z,x|\theta)}{q_{Z|X}(z|x,\lambda)}$

Score function estimator

$$\frac{\partial}{\partial\lambda}\mathbb{E}_{f_{Z|\lambda}(z)}\left[\psi(z)\right] = \mathbb{E}_{f_{Z|\lambda}(z)}\left[\psi(z)\frac{\partial}{\partial\lambda}\log f_{Z|\lambda}(z)\right]$$

Easy to MC estimate, but noisy.

Reparameterised gradient

$$\begin{aligned}\frac{\partial}{\partial \lambda}\mathbb{E}_{f_{Z|\lambda}(z)}\left[\psi(z)\right] &= \mathbb{E}_{s(\epsilon)}\left[\frac{\partial}{\partial \lambda}\psi(t(\epsilon,\lambda))\right] \\ &= \mathbb{E}_{s(\epsilon)}\left[\frac{\partial}{\partial z}\psi(z)\frac{\partial}{\partial \lambda}t(\epsilon,\lambda)\right]\end{aligned}$$

Easy to MC estimate.

Reparameterisation

- $t(\epsilon, \lambda)$ is invertible and differentiable
- $z = t(\epsilon, \lambda)$ has density $f_Z(z|\lambda)$
- $\epsilon = t^{-1}(z, \lambda)$ has density $s(\epsilon)$

Change of density

$$f_{Z|\lambda}(z) = s(\underbrace{t^{-1}(z,\lambda)}_{\epsilon})|\det J_{t^{-1}}(z,\lambda)|$$

As a result

$$\begin{aligned}\mathbb{E}_{f_Z(z|\lambda)}[\psi(z)] &= \int f_Z(z|\lambda)\psi(z)\mathrm{d}z \\ &= \int s(t^{-1}(z,\lambda))|\det J_{t^{-1}}(z,\lambda)|\psi(z)\mathrm{d}z \\ &= \int s(\epsilon)|\det J_t(\epsilon,\lambda)|^{-1}\psi(t(\epsilon,\lambda))|\det J_t(\epsilon,\lambda)|\mathrm{d}\epsilon \\ &= \int s(\epsilon)\psi(t(\epsilon,\lambda))\mathrm{d}\epsilon\end{aligned}$$

Gradient Estimators

Basic problem: we want to differentiate an expected value wrt λ

$$\frac{\partial}{\partial\lambda}\mathbb{E}_{f_{Z|\lambda}}[\psi(z)] \qquad \text{e.g., } \psi(z) := \log p(x|z,\theta)$$

$$f_{Z|\lambda}(z) := q(z|x,\lambda)$$

but the distribution of Z depends on λ.

We have met the SFE and the reparameterised gradient estimator:

$$\mathbb{E}_{f_\lambda(z)}\left[\underbrace{\color{red}{\psi(z)}\frac{\partial}{\partial\lambda}\log f_{Z|\lambda}(z)}_{\hat{g}_{\text{sfe}}}\right] = \mathbb{E}_{s(\epsilon)}\left[\underbrace{\color{blue}{\frac{\partial}{\partial z}\psi(z)}\frac{\partial}{\partial\lambda}t(\epsilon,\lambda)}_{\hat{g}_{\text{rep}}}\right]$$

- $\hat{g}_{\text{sfe}}$ is typically cursed with variance

From VAEs, you know the *reparameterised gradient estimator*

$$\begin{aligned}\frac{\partial}{\partial\lambda}\mathbb{E}_{f_{Z|\lambda}(z)}[\psi(z)] &= \mathbb{E}_{s(\epsilon)}\left[\frac{\partial}{\partial\lambda}\psi(t(\epsilon,\lambda))\right] \\ &= \mathbb{E}_{s(\epsilon)}\left[\frac{\partial}{\partial z}\psi(z)\frac{\partial}{\partial\lambda}t(\epsilon,\lambda)\right]\end{aligned}$$

it takes an invertible and differentiable transformation t such that

$$t(\epsilon,\lambda) \sim f_{Z|\lambda}$$
$$t^{-1}(z,\lambda) \sim s(\epsilon)$$

Goals Understand why there can't be a $\hat{g}_{\text{rep}}$ for discrete rvs. Meet alternatives to SFE.

A general reparameterisation

For univariate Z, what transformation will always absorb the parameters of the density $f_{Z|\lambda}(z)$?

The argument extends to a vector of independent univariate rvs.

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$$\underbrace{F_{Z|\lambda}(z)}_{\text{cdf}} \sim \mathcal{U}(\underbrace{0, 1}_{\text{fixed}})$$

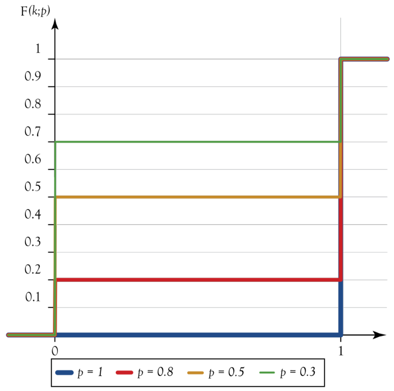
So, if I know the inverse cdf,

$$\epsilon \sim \mathcal{U}(0, 1)$$
$$F^{-1}_{Z|\lambda}(\epsilon) \sim Z|\lambda$$

I have access to $\hat{g}_{\text{rep}}$.

The argument extends to a vector of independent univariate rvs.

Let's reparameterise a Bernoulli



$$Z \sim \text{Bernoulli}(p)$$

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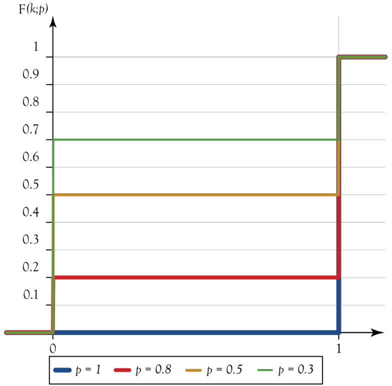

$$Z \sim \text{Bernoulli}(p)$$

$$F^{-1}_{Z|p}(\epsilon) = \begin{cases} 1 & \text{if } \epsilon < p \\ 0 & \text{otherwise} \end{cases}$$

$$= \mathbb{1}_{(0,p)}(\epsilon)$$

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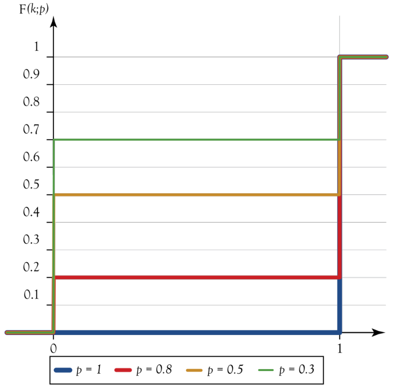

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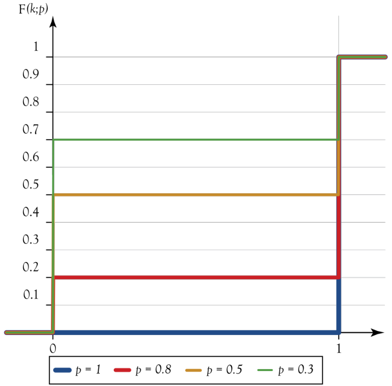

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How about $\frac{\partial}{\partial p} F^{-1}_{Z|p}(\epsilon)$? Mostly 0, sometimes undefined!

Discrete case

Discrete variables do not admit a differentiable reparameterisation. The derivatives of the inverse cdf are either 0 or undefined :/

STE's original paper (Bengio et al., 2013).

There are other pseudo-gradients in the literature, for example for relaxed combinatorial random variables (Peng et al., 2018; Mihaylova et al., 2021).

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How about we fake a Jacobian and call it a pseudo-gradient?

$$J_t(\epsilon, \lambda) = \text{diag}(\mathbf{1})$$

This is the ingredient behind the straight-through estimator (STE).

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Optimising the ELBO via reparameterised samples requires

$$\hat{g}_{\text{rep}} = \frac{\partial}{\partial \lambda} \log p(x|z = t(\epsilon, \lambda)) = \frac{\partial}{\partial z} \log p(x|z) \frac{\partial}{\partial \lambda} t(\epsilon, \lambda)$$

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Let's use our *pseudo gradient*

$$\hat{g}_{\text{ste}} := \frac{\partial}{\partial\lambda} t(\epsilon,\lambda) = \frac{\partial}{\partial\lambda} g(x;\lambda) \cancel{\frac{\partial}{\partial p} \mathbb{1}_{(0,p)}(\epsilon)} := 1$$

Concrete Distribution

We can sample from a Categorical distribution via

$$\epsilon_k \sim \text{Gumbel}(0, 1)$$
$$\underbrace{\arg\max_k \; \{\lambda_k + \epsilon_k\}_{k=1}^K}_{z = t(\epsilon, \lambda)} \sim \text{Cat}(\text{softmax}(\lambda))$$

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$$\text{softmax}\left(\frac{\lambda + \epsilon}{\tau}\right) \to \text{onehot}(z) \qquad \text{as } \tau \to 0$$

and now the transformation is differentiable, but the outcome is dense.

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STE: use sparse encoding for z

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Mixed Binary Variables

Continuous random variables that take on sparse outcomes with non-zero probability mass.
Example I:

- sample $\zeta \sim \mathcal{N}(0, 1)$
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When $\zeta < 0$ or $\zeta > 1$ the derivative of hardsigmoid is 0, when $0 < \zeta < 1$ the derivative is 1. Hardsigmoid has undefined derivatives for $\zeta = 0$ and $\zeta = 1$, but we will never sample those.

If we had a parameterised Gaussian, we could sample with a reparameterisation and learn the Gaussian parameters.

This has been applied to generate mixed random variables in the support $[0, 1]$.

Spike-and-slab (Rolfe, 2017); HardConcrete (Louizos et al., 2018); Hard-Kumaraswamy (Bastings et al., 2019).

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Construction:

- start with a continuous univariate rv ζ with density $s(\zeta)$
- project it to $[0, 1]$ using a function that hits the boundaries of the set
- the projection function is differentiable everywhere except at $\zeta = 0$ and $\zeta = 1$ which have 0 measure under $s(\zeta)$

The path derivative is defined *almost everywhere*, a g-rep can be used.

Can we go beyond univariates?

Yes, if we look into *sparse projections to the probability simplex*.

It turns out the 'hard sigmoid' is the a special case of a more general projection known as *sparsemax*.

Sparsemax

$$\mathrm{sparsemax}(\zeta) = \arg \max_{\zeta \in \Delta_{K-1}} \min ||p - \zeta||^2$$

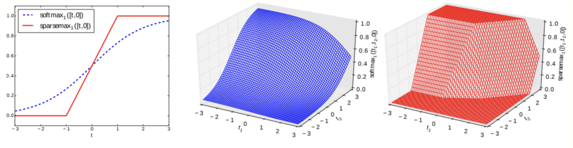


Figure 1. Comparison of softmax and sparsemax in 2D (left) and 3D (two righmost plots).

When $K = 2$, sparsemax is equivalent to hardsigmoid.

Mixed Random Variables

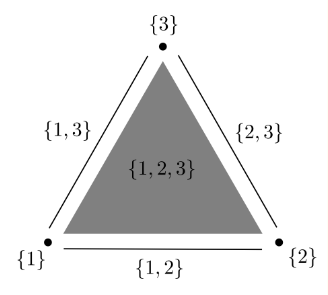
Generalisation of mixed binary random variables to the multivariate case.

Intrinsic view:

- draw ζ in $\mathbb{R}^K$ (e.g., from a multivariate Gaussian)
- project it to Δ_{K-1} (e.g., using sparsemax)

What is the probability that we have a point in one of the faces of the simplex?

The faces of the simplex (e.g., with 3 vertices):



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What is the probability that we have a point in one of the faces of the simplex? In this example, we would have to integrate the multivariate Gaussian pdf over the set of points in the inverse of sparsemap.

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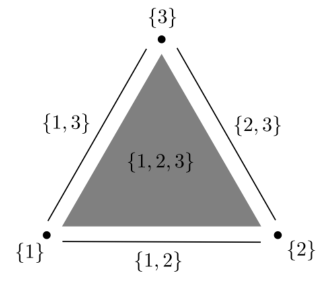

Mixed Random Variables

Generalisation of mixed binary random variables to the multivariate case.

Extrinsic view:

- choose a face f of the simplex with probability $P_F(f)$
- draw z from the relative interior of f (e.g., using a LogisticNormal distribution)

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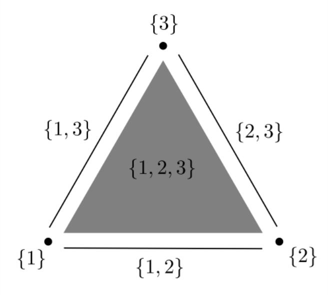

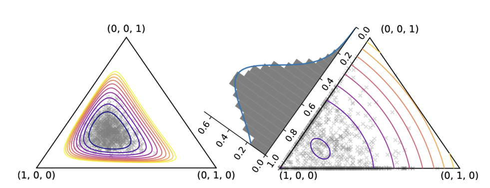

Farinhas et al. (2022)

Outline

Latent Computation Graphs

Estimators built on reparameterisation require

- z to be of some fixed finite dimensionality
- the decoder's computation graph must be independent of z.

Some composition functions are parameterised by their inputs (e.g., a tree-LSTM), they are dynamic computation graphs controlled by the discrete latent.

STE is not an option, so we are back to SFE. Or are we?

$\hat{g}_{\text{rep}}$ differentiates the decoder wrt z

$$\hat{g}_{\text{rep}} = \frac{\partial}{\partial z}\psi(z) \times \frac{\partial}{\partial \lambda} t(\epsilon, \lambda)$$

This cannot work when the computation graph of ψ depends on z (i.e., whenever z cannot be treated as a point in the relative interior of a fixed and finite-dimensional polytope). For example, a tree-LSTM updates its states following a depth-first traversal of an input tree.

Parameterise for Tractability

We can use sparse projections to the probability simplex to parameterise discrete distributions that assign 0 probability mass to most of the outcomes in their supports.

$$
\begin{aligned}
&\nabla_\lambda \mathbb{E}_{q(z|x,\lambda)}[\log p(x,z|\theta) - \log q(z|x,\lambda)] \\
=&\nabla_\lambda q(c_1|x,\lambda)(\log p(x,c_1|\theta) - \log q(c_1|x,\lambda)) \\
&+ \dots \\
&+ \nabla_\lambda q(c_k|x,\lambda)(\log p(x,c_k|\theta) - \log q(c_k|x,\lambda)) \\
&+ \nabla_\lambda \sum_{z=c_{k+1}}^{c_K} \underbrace{q(z|x,\lambda)}_{=0}(\log p(x,z|\theta) - \log q(z|x,\lambda))
\end{aligned}
$$

Effectively, we have an inference network that parameterises a model whose support is small enough for *enumeration*.

Sparse projections: (Martins and Astudillo, 2016; Niculae et al., 2018a)

Latent dynamic computation graphs: (Niculae et al., 2018b)

Sparse marginals: (Correia et al., 2020)

Outline

1. Reparameterised Gradients
2. Sparse Gradients
3. Variance reduction

Control variates

Intuition

To estimate $\mathbb{E}[\psi(z)]$ via Monte Carlo we compute the empirical average of $\hat{\psi}(z)$ where $\hat{\psi}(z)$ is chosen so that $\mathbb{E}[\hat{\psi}(z)] = \mathbb{E}[\psi(z)]$ and $\text{Var}(\psi) > \text{Var}(\hat{\psi})$.

Equivalent expectations

Let $\bar{\psi} = \mathbb{E}[\psi(z)]$ be an expectation of interest

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  it holds that $\mathbb{E}[\hat{\psi}(z)] = \mathbb{E}[\psi(z)]$
- and $\mathrm{Var}(\hat{\psi}) = \mathrm{Var}(\psi) - 2b\,\mathrm{Cov}(\psi, c) + b^2\,\mathrm{Var}(c)$

Choosing the control variate

1. $\hat{\psi}(z) \triangleq \psi(z) - b(c(z) - \mathbb{E}[c(z)])$
2. $\mathsf{Var}(\hat{\psi}) = \mathsf{Var}(\psi) - 2b\,\mathsf{Cov}(\psi, c) + b^2\,\mathsf{Var}(c)$

How do we choose b and $c(z)$?

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- solving $\frac{\partial}{\partial b}\text{Var}(\hat{\psi}) = 0$ yields $b^\star = {}^{\text{Cov}(\psi, c)}/_{\text{Var}(c)}$
  when $\psi(z)$ and $c(z)$ are positively correlated, then we may reduce variance

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Of course, $\mathbb{E}[c(z)]$ must be known!

MC

We then use the estimate

$$\bar{\psi} \overset{\text{MC}}{\approx} \frac{1}{S}\left(\sum_{s=1}^{S} \psi(z^{(s)}) - bc(z^{(s)})\right) + b\bar{c}$$

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And recall that for us

$$\psi(z) = \log \frac{p_{ZX}(z, x|\theta)}{q_{Z|X}(z|x, \lambda)} \frac{\partial}{\partial \lambda} \log q_{Z|X}(z|x, \lambda)$$

and $z^{(s)} \sim q_{Z|X}(z|x, \lambda)$

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&= \int \frac{\partial}{\partial\lambda}q(z|x,\lambda)\mathrm{d}z \\
&= \frac{\partial}{\partial\lambda}\int q(z|x,\lambda)\mathrm{d}z \\
&= \frac{\partial}{\partial\lambda}1 = {\color{blue}0}
\end{aligned}
$$

Baselines

With

$$\psi(z) = \log \frac{p(z, x|\theta)}{q(z|x, \lambda)} \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

and

$$c(z) = \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

we have

$$\hat{\psi}(z) =$$

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b is known as *baseline* in RL literature.

Examples of baselines

- Moving average of $\log \frac{p(z,x|\theta)}{q(z|x,\lambda)}$ based on previous batches

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- Moving average of $\log \frac{p(z,x|\theta)}{q(z|x,\lambda)}$ based on previous batches
- A trainable constant b
- A neural network prediction based on x e.g. $b(x;\omega)$
- The reward assessed at a deterministic point, e.g. $b(x) = \log \frac{p(z^\star,x|\theta)}{q(z^\star|x,\lambda)}$ where $z^\star = \arg\max_z q(z|x,\lambda)$

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- The reward assessed at a stochastic point, e.g. $b(x) = \log \frac{p(z',x|\theta)}{q(z'|x,\lambda)}$ where $z' \sim q(z|x,\lambda)$

Trainable baselines

Baselines are predicted by a regression model (e.g. a neural net).

The model is trained using an L_2-loss.

$$\min_{\omega} \left(b(x;\omega) - \log \frac{p(z,x|\theta)}{q(z|x,\lambda)} \right)^2$$

Other techniques

- control variates beyond baselines: Tucker et al. (2017), Grathwohl et al. (2018)
- Rao-Blackwell: Liu et al. (2019)

Summary

Learning discrete LVMs poses challenges for gradient estimation, in particular, gradients of the inference network are challenging.

SFE is the most general, it requires tractable pmf and sampling, nothing else. It is too noisy to be useful without variance reduction techniques.

Summary

Alternatives to SFE are possible in some cases.

STE requires a relaxation of the decoder and introduces biases, violating the requirements for stochastic optimisation.

We can mix a pmf and a pdf to obtain reparameterised and unbiased gradients for a sparse rv. This addresses STE's bias.

Sparse parameterisation of the inference model leads to sparse gradients with many terms evaluating trivially to zero. Enumeration dispenses with relaxations and works for combinatorial variables.

Final Remarks

- Probabilistic models are extremely flexible tools.
- They are interesting precisely because we can make choices about unobserved aspects of the data.
- Discrete latent variables are oftentimes key to revealing interpretable structure, or to imposing some interpretable structure on a joint distribution.
- Learning discrete LVMs is challenging, but recent years have seen amazing progress.
- Join the party! Apply these models, extend them, discover problems with their estimation/evaluation, investigate solutions.
- Avoid approaching LVMs wondering whether they will beat some non-LVM NN. If such NN exists, then you are probably looking at an aspect of the problem that does not require latent variables.

What Next?

- For more material, check
  https://vitutorial.github.io/classes/
- We also have some coding exercises
  https://github.com/vitutorial/exercises
- Check this great tutorial by our friends from DeepSPIN
  https://deep-spin.github.io/tutorial/

See you around!

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