Latent Transformations for Discrete-Data Normalising Flows

Rob Hesselink 1  Wilker Aziz 1

Abstract
Normalising flows (NFs) for discrete data are challenging because parameterising bijective transformations of discrete variables requires predicting discrete/integer parameters. Having a neural network architecture predict discrete parameters takes a non-differentiable activation function (e.g., the step function) which precludes gradient-based learning. To circumvent this non-differentiability, previous work has employed biased proxy gradients, such as the straight-through estimator. We present an unbiased alternative where rather than deterministically parameterising one transformation, we predict a distribution over latent transformations. With stochastic transformations, the marginal likelihood of the data is differentiable and gradient-based learning is possible via score function estimation. To test the viability of discrete-data NFs we investigate performance on binary MNIST. We observe great challenges with both deterministic proxy gradients and unbiased score function estimation. Whereas the former often fails to learn even a shallow transformation, the variance of the latter could not be sufficiently controlled to admit deeper NFs.

1. Introduction
Normalising flows (Tabak et al., 2010; Rezende & Mohamed, 2015) have been shown to be powerful density estimators for high-dimensional continuous data (Papamakarios et al., 2019). For discrete data, NFs have received little attention thus far. The foremost reason is the problem of gradient estimation of discrete functions. Tran et al. (2019) and Hoogeboom et al. (2019) have resorted to a deterministic proxy gradient known as straight-through estimator (STE; Bengio et al., 2013). STE is a biased estimator and its effects as a function of the number of discrete variables (related to the dimensionality of the data) and/or the depth of the flow (a hyperparameter that controls expressiveness) are little understood.

To gain insight into the viability of discrete-data NFs, we propose to give transformations a latent treatment by means of turning their parameters into stochastic latent variables. While this sacrifices tractable likelihood assessments, gradient-based learning is still possible via optimisation of the evidence lowerbound (ELBO), as in variational inference (VI; Jordan et al., 1999), and score function estimation (SFE; Rubinstein, 1976; Paisley et al., 2012). We use a generalised XOR transformation (Tran et al., 2017) to parameterise autoregressive flows (Kingma et al., 2016; Papamakarios et al., 2017) and compare the performance of STE and SFE to model binary data (MNIST). Our experiments show that STE struggles in general and that SFE struggles with depth.1

2. Normalising Flows
A normalising flow (NF; Tabak et al., 2010) is built upon an invertible and differentiable transformation of a continuous random variable with known density, i.e.,

\[ p_X(x) = p_Y(t^{-1}(x)) | \det J_{t^{-1}}(x) | \] (1)

where \( J_{t^{-1}}(x) \) is the matrix of partial derivatives of \( t^{-1} \) assessed at \( x \). NFs have been used extensively in deep latent variable models (Rezende & Mohamed, 2015; Kingma et al., 2016), where they play the role of a variational approximation to the model’s true posterior, but also in density estimation (Dinh et al., 2015; 2017; Kingma & Dhariwal, 2018; Papamakarios et al., 2017), where they enable exact likelihood-based learning with expressive distributions.

If \( X \) takes on values in some discrete space, a bijective mapping corresponds to an unambiguous relabelling of the sample space and thus incurs no distortion in volume (there is no notion of volume). The mass function of the transformed discrete variable is simply

\[ p_X(x) = p_Y(t^{-1}(x)) , \] (2)

We can parameterise the transformation (either directly or

1Institute for Logic, Language, and Computation, University of Amsterdam, Netherlands. Correspondence to: Rob Hesselink <rob.hesselink@pm.me>, Wilker Aziz <w.aziz@uva.nl>.

1Code available on github.com/robdhess/Latent-DNFs
we address in this work.

An invertible transformation for binary data can be designed with sigmoid outputs. An elementwise threshold function can constrain the outputs \( o = f(x; \theta) \) to \( \{0, 1\}^D \), i.e.

\[
h_d(o_d) = \begin{cases} 
1 & \text{if } o_d > 0.5 \\
0 & \text{otherwise} 
\end{cases}
\]

and we could design \( u = h(f(x; \theta)) \). However \( \frac{\partial}{\partial o_d} h(o) \) is undefined for \( o_d = 0.5 \) and 0 everywhere else. A model specified this way leads to a non-differentiable likelihood, that is, for a given \( x \), \( p_{X|\theta,\beta}(x) \) is not a differentiable function of the parameters \( \theta \). In the next section we will give \( u \) stochastic treatment. Effectively, we specify a distribution \( p_{XU|\theta,\beta}(x,u) \), differentiable with respect to its parameters, and above all, whose marginal \( p_{X|\theta,\beta}(x) \) too is differentiable with respect to its parameters. Note that STE ignores the non-differentiability of \( h \) by defining \( J_h(o) = \mathbb{I}_D \) where \( \mathbb{I}_D \) is the \( D \times D \) identity matrix.

4. Latent Transformations

A straight-forward way to define a differentiable likelihood model that employs a discrete parameter \( u \) is to sample the parameter from a distribution with discrete support and compute gradients in expectation. This is equivalent to thinking of the transformation as latent.

We design a latent variable model

\[
p_{U|X,\theta}(u|x) = \prod_{d=1}^{D} \text{Bern}(u_d|f_d(x; \theta)) \tag{6a}
\]

\[
p_{X|\theta,\beta}(x) = \sum_{u \in \{0, 1\}^D} p_{Y|\beta}(y_t(x; u)) p_{U|X,\theta}(u|x) \tag{6b}
\]

where \( f_d(x; \theta) \) depends on \( x \) only through \( x_{<d} \). Equation (6a) specifies a distribution over transformations, rather over the parameters of transformations. The marginalisation is clearly intractable—the sum ranges over \( \mathcal{O}(2^D) \) outcomes—thus we approach this via variational inference (VI; Jordan et al., 1999) with an approximate posterior

\[
q_{U|X,\lambda}(u|x) = \prod_{d=1}^{D} \text{Bern}(u_d|g_d(x; \lambda)) \tag{7}
\]

where, unlike \( f(x; \theta) \), \( g(x; \lambda) \) need not be auto-regressive. We then optimise parameters using gradient estimates of the evidence lowerbound (ELBO) with respect to \( \theta \) and \( \lambda \) (and possibly \( \beta \) too, though we typically leave the base fixed):

\[
\log p_{X|\theta,\beta}(x) \geq \mathbb{E} \left[ \log \frac{p_{Y|\beta}(y_t(x; u)) p_{U|X,\theta}(u|x)}{q_{U|X,\lambda}(u|x)} \right] . \tag{8}
\]

where the expectation is taken w.r.t. \( q_{U|X,\lambda}(u|x) \). This model learns a distribution over latent transformations, from

Note on STE
Suppose \( f(x; \theta) \) is a differentiable function from \( \{0, 1\}^D \) to \( \{0, 1\}^D \) (for example, a feed-forward NN

\cite{tran2019latent}, for example, design expressive non-auto-regressive likelihoods for language problems, where autoregressiveness is the norm, and highlight efficiency as a motivation.

\text{Note on STE} \hspace{1cm} \text{Suppose } f(x; \theta) \text{ is a differentiable function from } \{0, 1\}^D \text{ to } \{0, 1\}^D \text{ (for example, a feed-forward NN}

\cite{tran2019latent}, for example, design expressive non-auto-regressive likelihoods for language problems, where autoregressiveness is the norm, and highlight efficiency as a motivation.
which a sample parameterises a discrete-data normalising flow. Clearly, unlike a standard normalising flow, we do not have exact marginal likelihood assessments, but we can estimate a lowerbound via importance sampling (this is the common practice with VAEs). NFs have been used in VAEs, but usually to model the latent space (Rezende & Mohamed, 2015), in this proposal we use VI to train a model whose sampling distribution is itself an NF. We do maintain tractability of sampling though.

### Multiple layers

In general, we have a sequence of $L$ transformations $u = \langle u^{(1)}, \ldots, u^{(L)} \rangle$, each $u^{(l)} \in \{0, 1\}^D$. We then obtain a base sample $y = t(x; u)$ by iteratively transforming the data sample: $x^{(l)} = x^{(l-1)} \oplus u^{(l)}$ for $l = 1, \ldots, L$, where $x = x^{(0)}$ and $y = x^{(L)}$ and with $\oplus$ applying elementwise. To model with multiple flows we make a conditional independence assumption, namely, that $u^{(l)}$ depends only on $u^{(l-1)}$, both in the generative model $p_{U|X, \theta}(u|x) = \prod_{l=1}^L p(u^{(l)}|u^{(l-1)}, \theta_l)$, and in the approximate posterior $q_{U|X, \lambda}(u|x) = \prod_{l=1}^L q(u^{(l)}|u^{(l-1)}, \lambda_l)$, where $u^{(0)} := x$ and we omit subscripts to avoid clutter. Appendix A contains more information about the factorisation.

### Other latent transformation NFs

Marginalisation of latent transformations has been proposed as a means to increase flexibility of continuous-data NFs, which struggle to accommodate topological differences between the target and the base distribution. Dinh et al. (2019) introduce a finite mixture of transformations, where marginalisation is possible if the number of components is small. For increased expressiveness, Cornish et al. (2019) propose continuously indexed NFs (i.e., a compound distribution whose sampling distribution is an NF) and approach approximate marginalisation via variational inference. Rather than (exactly or approximately) marginalising out members of a parametric family of transformations, one can realise the mapping between target and base distributions as a stochastic process (Sohl-Dickstein et al., 2015; Wu et al., 2020).

## 5. Gradient Estimation

The intractability of the marginal likelihood extends to the ELBO and for that reason we must resort to Monte Carlo (MC) gradient estimation. The gradient of the ELBO w.r.t. the parameters $\beta$ of the base distribution is straightforward to estimate using a sample $u \sim q_{U|X=x, \lambda}$, $\nabla_{\beta} \text{ELBO} \approx \nabla_{\beta} \log p_{Y|\beta}(t(x; u))$. That is because $\beta$ is not involved in the sampling of $u$. Similarly, estimating the gradient w.r.t. the parameters $\theta$ of the generative model poses no challenge, $\nabla_{\theta} \text{ELBO} \approx \nabla_{\theta} \log p_{U|X, \theta}(u|x)$. The gradient w.r.t. the parameters $\lambda$ of the approximate posterior, $\nabla_{\lambda} \text{ELBO} = \nabla_{\lambda} \mathbb{E} \left[ \log p_{Y|\beta}(t(x; u)) \right] - \nabla_{\lambda} \text{KL}(q_{U|X, \lambda} || p_{U|X, \theta})$ (9)

is less trivial to estimate since $\lambda$ is involved in sampling $u$, but it can be rewritten as follows,

$$
\mathbb{E} \left[ \log p_{Y|\beta}(t(x; u)) \nabla_{\lambda} \log q_{U|X, \lambda}(u|x) \right] - \mathbb{E} \left[ \frac{p_{U|X, \theta}(u|x)}{q_{U|X, \lambda}(u|x)} \nabla_{\lambda} \log q_{U|X, \lambda}(u|x) \right],
$$

for which MC estimation is possible. The result is the SFE, which is generally very noisy. For variance reduction we follow the steps of Mnih & Gregor (2014) closely. That is, to reduce variance of the first term (10a), we subtract from the learning signal a self-critic (Rennie et al., 2017) and standardise the result using moving estimates of mean and standard deviation. These baselines can be defined for each observed variable since $\log p_{Y|\beta}(t(x; u)) = \sum_{d=1}^D \log p_{Y|\beta}(x_d \oplus u_d^{(0)} \oplus \cdots \oplus u_d^{(L)})$. For the second term (10b), in addition to using baselines, we rewrite the SFE factoring out of the computation as many terms as possible in order to reduce variance.

### Local KL

The gradient of the KL term is expressed in terms of nested expectations, and due to conditional independence assumptions in the model and in the posterior approximation, we can improve upon a vanilla SFE in manner reminiscent of how Mnih & Gregor (2014) improved the SFE for hidden layers with binary hidden units. The first-order Markov assumption we make over latent parameters implies weighing the score of $u^{(l)}$ by the sum of log-ratios due to two KL terms: the one w.r.t. the distribution of $U^{(l)}$ and the one w.r.t. the distribution of $U^{(l+1)}$. Thus, we can rewrite the SFE for the KL term (complete derivation in Appendix B). For each layer $l$, $\nabla_{\lambda_l} \text{KL} \approx \log \frac{p(u^{(l)}|u^{(l-1)}, \theta_l)}{q(u^{(l)}|u^{(l-1)}, \lambda_l)} \nabla_{\lambda_l} \log q(u^{(l)}|u^{(l-1)}, \lambda_l)$ (11a)

$$
+ \log \frac{p(u^{(l+1)}|u^{(l)}, \theta_l)}{q(u^{(l+1)}|u^{(l)}, \lambda_l)} \nabla_{\lambda_l} \log q(u^{(l)}|u^{(l-1)}, \lambda_l),
$$

where $\lambda_l$ corresponds to the parameters of the neural network $g$ that maps from $u^{(l-1)}$ to a distribution over possible assignments to the $l$th transformation. Finally, (11a) can

---

4 A self-critic here corresponds to $\log p_{Y|\beta}(t(x; u'))$ for an independently sampled transformation $u'$.  
5 We could potentially estimate the two terms independently, which then allows scaling the second SFE by $\gamma > 0$.  

We compare SFE and STE on binarised MNIST. We binarise the gradient w.r.t. \( \frac{\partial U}{\partial u} \) by factoring out the closed-form entropy of and realising that \( u_d^{(t)} \) cannot affect \( \log p(u_{d'}^{(t-1)}, u_{d'}^{(t)}) \). For further variance reduction of the SFE in (12b), we can again employ a self-critic and standardisation of the learning signal, though this time, these techniques are applied independently for each layer.

**Special case** Since including both a variational posterior and an autoregressive generative model can be computationally costly, we also consider the situation where we choose \( q_U|X,\lambda(u|x) := p_U|X,\theta(u|x) \). This corresponds to a simpler form of VI where rather than introducing an independent posterior approximation we estimate a lowerbound on log-likelihood by sampling from the generative model directly. This leads to KL evaluating to zero, and makes gradient estimation w.r.t. \( \theta \) a matter of score function estimation. In this case, we use the bound \( \log p_X|\beta,\theta(x) \geq \mathcal{L} = \mathbb{E}_{p_{U|X,\theta}(u|x)} \left( \log p_{Y|\beta}(t^{-1}(x); u) \right) \), (13)

While the gradient w.r.t. \( \beta \) is unchanged, the gradient w.r.t. \( \theta \) can be split in two terms. For this, we group the \( L \) parameters \( \{u_d^{(1)}, \ldots, u_d^{(L)}\} \) that transform the \( d \)th observation, and denote them simply by \( u_d \). Then \( \nabla_\theta \mathcal{L} = \sum_{d=1}^{D} \mathbb{E} \left[ r(u_d) \nabla_\theta \log p(u_d|u_{<d}) + r(u_d) \nabla_\theta \log p(u_{<d}) \right] \)

(14a)

with expectations taken w.r.t. \( p_{U|X,\theta}(u|x), \) and \( r(u_d) := \log p_{Y|\beta}(x_d \oplus u_d^{(1)} \ldots \oplus u_d^{(L)}) \). For the full derivation, see appendix C. Note how the reward for the \( d \)th observation scales the score of its transformation (first term) as well as the score of the transformations of preceding observations (second term). We want to note similarities to the Bellman equation, where rewards are discounted for past actions. If we estimate the two terms independently, that is, using two independent samples \( u \) and \( u' \), stochastic gradient optimisation allows us to choose different scaling constants for each term. We opt for an impatient approach and set the constant for the second term negligibly small.

6. Experiments

We compare SFE and STE on binarised MNIST. We binarise stochastically by interpreting the pixel intensities as Bernoulli probabilities. Every layer uses a 784-dimensional MADE (Germain et al., 2015) and models are trained using Adam with learning rate 1e-3. The base distribution is fixed with Bernoulli parameters [0.9, 0.1]. Stochastic models are evaluated using 1,000 samples, and we also report the performance of a single flow, namely the one specified by a greedy approximation to \( \arg \max_u q_U|X,\lambda(u|x) \).

| Model                  | Depth | NLL ↓ | Greedy |
|------------------------|-------|-------|--------|
| STE                    | 1     | 222.1 |        |
|                        | 2     | 211.2 |        |
|                        | 4     | 205.6 |        |
|                        | 8     | 209.1 |        |
| SFE (full posterior)   |       |       |        |
| greedy self-critic     | 1     | 293.7 | 205.3 |
| running average        | 1     | 242.4 | 207.3 |
| SFE (special case)     |       |       |        |
| greedy self-critic     | 1     | 267.9 | 267.7 |
| running average        | 1     | 190.1 | 189.6 |

Table 1 shows that by applying proper variance reduction techniques, SFE can outperform STE, even for architectures with fewer parameters. In the special case where \( q_U|X,\lambda(u|x) := p_U|X,\theta(u|x) \) performance is highest, possibly due to lower gradient variance. We did find, however, that performance did not increase with depth. Multiple stochastic layers increases variance in performance and the model encourages deeper layers to become fixed. Samples of SFE and STE can be found in appendix D.

We want to emphasize the possibility of treating the flow stochastically during training to compute the gradients, but reverting to a deterministic forward pass after that. By doing this, we train using unbiased estimates of the gradient, without losing exact likelihood assessment.

7. Conclusion

We have presented a new technique for training discrete normalising flows by treating the transformation parameters as latent variables. Our unbiased gradients lead to better performance on binarised MNIST compared to straight-through, while we sacrifice exact likelihood assessment. Further work could experiment with more powerful architectures and recent developments in discrete gradient estimation, such as (Grathwohl et al., 2018).

Acknowledgements

This project is supported by the European Union’s Horizon 2020 research and innovation programme under grant agree-
ment No 825299 (Gourmet). We thank Emiel Hoogeboom for insightful discussions.

References

Bengio, Y., Léonard, N., and Courville, A. Estimating or propagating gradients through stochastic neurons for conditional computation. *arXiv preprint arXiv:1308.3432*, 2013.

Cornish, R., Caterini, A. L., Deligiannidis, G., and Doucet, A. Relaxing bijectivity constraints with continuously indexed normalising flows. *arXiv preprint arXiv:1909.13833*, 2019.

Dinh, L., Krueger, D., and Bengio, Y. Nice: Non-linear independent components estimation. In *ICLR*, 2015.

Dinh, L., Sohl-Dickstein, J., and Bengio, S. Density estimation using real NVP. In *ICLR*, 2017.

Dinh, L., Sohl-Dickstein, J., Pascanu, R., and Larochelle, H. A rad approach to deep mixture models. In *ICLR: Workshop track*, 2019.

Germain, M., Gregor, K., Murray, I., and Larochelle, H. Made: Masked autoencoder for distribution estimation. In *ICML*, pp. 881–889, 2015.

Grathwohl, W., Choi, D., Wu, Y., Roeder, G., and Duvenaud, D. Backpropagation through the void: Optimizing control variates for black-box gradient estimation. In *ICLR*, 2018.

Hoogeboom, E., Peters, J., van den Berg, R., and Welling, M. Integer discrete flows and lossless compression. In Wallach, H., Larochelle, H., Beygelzimer, A., d’Alché Buc, F., Fox, E., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems* 32, pp. 12134–12144. Curran Associates, Inc., 2019.

Jordan, M., Ghahramani, Z., Jaakkola, T., and Saul, L. An introduction to variational methods for graphical models. *Machine Learning*, 37(2):183–233, 1999.

Kingma, D. P. and Dhariwal, P. Glow: Generative flow with invertible 1x1 convolutions. In *Advances in Neural Information Processing Systems*, pp. 10236–10245, 2018.

Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., and Welling, M. Improved variational inference with inverse autoregressive flow. In *Advances in Neural Information Processing Systems*, pp. 4743–4751, 2016.

Mnih, A. and Gregor, K. Neural variational inference and learning in belief networks. In *Proceedings of the 31st International Conference on International Conference on Machine Learning - Volume 32, ICML’14*, pp. II–1791–II–1799. JMLR.org, 2014.

Paisley, J., Blei, D., and Jordan, M. Variational bayesian inference with stochastic search. In *ICML*, 2012.

Papamakarios, G., Pavlakou, T., and Murray, I. Masked autoregressive flow for density estimation. In *Advances in Neural Information Processing Systems*, pp. 2338–2347, 2017.

Papamakarios, G., Nalisnick, E., Rezende, D. J., Mohamed, S., and Lakshminarayanan, B. Normalizing flows for probabilistic modeling and inference. *arXiv preprint arXiv:1912.02762*, 2019.

Rennie, S. J., Marcheret, E., Mroueh, Y., Ross, J., and Goel, V. Self-critical sequence training for image captioning. In *CVPR*, 2017.

Rezende, D. and Mohamed, S. Variational inference with normalizing flows. In Bach, F. and Blei, D. (eds.), *ICML*, volume 37 of *Proceedings of Machine Learning Research*, pp. 1530–1538, Lille, France, 07–09 Jul 2015. PMLR.

Rubinstein, R. A monte carlo method for estimating the gradient in a stochastic network. *Unpublished manuscript, Technion, Haifa, Israel*, 1976.

Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., and Ganguli, S. Deep unsupervised learning using nonequilibrium thermodynamics. In Bach, F. and Blei, D. (eds.), *ICML*, volume 37 of *Proceedings of Machine Learning Research*, pp. 2256–2265, Lille, France, 07–09 Jul 2015. PMLR.

Tabak, E. G., Vanden-Eijnden, E., et al. Density estimation by dual ascent of the log-likelihood. *Communications in Mathematical Sciences*, 8(1):217–233, 2010.

Tran, D., Ranganath, R., and Blei, D. Hierarchical implicit models and likelihood-free variational inference. In *Advances in Neural Information Processing Systems*, pp. 5523–5533, 2017.

Tran, D., Vafa, K., Agrawal, K., Dinh, L., and Poole, B. Discrete flows: Invertible generative models of discrete data. In *ICLR Workshop DeepGenStruct*, 2019.

Wu, H., Köhler, J., and Noé, F. Stochastic normalizing flows. *arXiv preprint arXiv:2002.06707*, 2020.
A. Model

A.1. Specification

Generative model We make a first-order Markov assumption across layers and model the units within a layer autoregressively:

\[ p_{u|x,\theta}(u|x) = \prod_{\ell=1}^{L} p(u^{(\ell)}|u^{(\ell-1)}, \theta_\ell) \]  
\[ p(u^{(\ell)}|u^{(\ell-1)}, \theta_\ell) = \prod_{d=1}^{D} p(u_d^{(\ell)}|u_{<d}^{(\ell-1)}, \theta_\ell) \]  
\[ U_d^{(\ell)}|\theta_\ell, u^{(\ell-1)}, u_{<d}^{(\ell)} \sim \text{Bern}(f_d(u^{(\ell-1)}, u^{(\ell)}; \theta_\ell)), \]  
where \( u^{(0)} := x \) and \( f_d(\cdot; \theta_\ell) \) depends on \( u^{(\ell)} \) only through \( u_{<d}^{(\ell)} \).

Approximate posterior We make a first-order Markov assumption across layers and mean field assumption within layers:

\[ q_{u|x,\lambda}(u|x) = \prod_{\ell=1}^{L} q(u^{(\ell)}|u^{(\ell-1)}, \lambda_\ell) \]  
\[ q(u^{(\ell)}|u^{(\ell-1)}, \lambda_\ell) = \prod_{d=1}^{D} q(u_d^{(\ell)}|u_{<d}^{(\ell-1)}, \lambda_\ell) \]  
\[ U_d^{(\ell)}|\lambda_\ell, u^{(\ell-1)} \sim \text{Bern}(g_d(u^{(\ell-1)}; \lambda_\ell)), \]  
where \( u^{(0)} = x \). Here \( g_d(\cdot; \lambda_\ell) \) conditions freely on all of its inputs.

ELBO

\[ \mathbb{E}_{q_{u|x,\lambda}(u|x)} \left[ \log p_Y|\beta(t^{-1}(x; u)) + \log \frac{p_{u|x,\theta}(u|x)}{q_{u|x,\lambda}(u|x)} \right] = \mathbb{E}_{q_{u|x,\lambda}(u|x)} \left[ \log p_Y|\beta(t^{-1}(x; u)) \right] - \text{KL}(q_{u|x,\lambda}||p_{u|x,\theta}) \]  

A.2. Gradient estimation

Unless otherwise noted, we derive MC estimates on a single sample \( u \sim q_{u|x=x,\lambda} \).

Base distribution

\[ \nabla_\beta \text{ELBO} \approx \nabla_\beta \log p_Y|\beta(t^{-1}(x; u)) . \]  

Generative model

\[ \nabla_\theta \text{ELBO} \approx \nabla_\theta \log p_{u|x,\theta}(u|x) . \]  

Approximate posterior

\[ \nabla_\lambda \text{ELBO} \approx \nabla_\lambda \mathbb{E}_{q_{u|x,\lambda}(u|x)} \left[ \log p_Y|\beta(t^{-1}(x; u)) \right] - \nabla_\lambda \text{KL}(q_{u|x,\lambda}||p_{u|x,\theta}) \]  

For the first term we employ the score function estimator (SFE):

\[ \mathbb{E}_{q_{u|x,\lambda}(u|x)} \left[ \log p_Y|\beta(t^{-1}(x; u)) \right] \nabla_\lambda \log q_{u|x,\lambda}(u|x) . \]  

For variance reduction we subtract a self-critic, namely, \( \log p_Y|\beta(t^{-1}(x; u')) \) for an independent sample \( u' \), and standardise the result using moving estimates of mean and standard deviation. These baselines are applied per pixel since the reward factorises: \( \log p_Y|\beta(t^{-1}(x; u)) = \sum_{d=1}^{D} \log p_Y|\beta(x_d \oplus u_d^{(1)} \oplus \ldots \oplus u_d^{(L)}) \). The second term is made of nested KL terms, and due to conditional independence assumptions in the model and in the approximation, we can improve upon a vanilla SFE (see next).
B. Gradient of KL

We make a conditional independence assumption, namely, \(u^{(\ell)}\) is independent of all but the previous assignment \(u^{(\ell-1)}\), which can be exploited to rewrite the SFE for the KL term. We are looking to simplify

\[
\nabla_{\lambda} \text{KL}(q_{U|x,\lambda}||p_{U|x,\theta}) = \mathbb{E}_{q_{U|x,\lambda}(u|x)} \left[ \log \frac{p_{U|x,\theta}(u|x)}{q_{U|x,\lambda}(u|x)} \nabla_{\lambda} \log q_{U|x,\lambda}(u|x) \right].
\]

(26)

Define a “local reward” as

\[
r(u^{(\ell)}, u^{(\ell-1)}) := \sum_{d=1}^{D} \log \frac{p(u^{(\ell)}_d|u^{(\ell-1)}_d, u_{<d}^{(\ell-1)})}{q(u^{(\ell)}_d|u^{(\ell-1)}_d, \lambda^{(\ell)})}.
\]

(27)

Let expectations be expressed w.r.t. \(q_{U|x,\lambda}\), then the gradient of the KL with respect to the parameters of the \(\ell\)-th layer is:

\[
\nabla_{\lambda_{\ell}} \text{KL} = \mathbb{E} \left[ \left( \sum_{k=1}^{L} r(u^{(k)}, u^{(k-1)}) \right) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right].
\]

(28a)

Note that we only need the \(\ell\)-th score.

\[
= \mathbb{E} \left[ \left( \sum_{k=1}^{L} r(u^{(k)}, u^{(k-1)}) \right) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\]

(28b)

And that we can expand the reward explicitly to identify constant terms.

\[
= \mathbb{E} \left[ \left( \sum_{k=1}^{\ell-1} r(u^{(k)}, u^{(k-1)}) \right) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right] \quad \text{constant w.r.t. } u^{(\ell)}
\]

(28c)

\[
+ \mathbb{E} \left[ \left( \sum_{k=\ell+2}^{L} r(u^{(k)}, u^{(k-1)}) \right) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right] \quad \text{constant w.r.t. } u^{(\ell)}
\]

(28d)

\[
+ \mathbb{E} \left[ \left( r(u^{(\ell)}, u^{(\ell-1)}) + r(u^{(\ell+1)}, u^{(\ell)}) \right) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right] \quad \text{local rewards}
\]

(28e)

Recall that the expected value of the score is 0, i.e., \(\mathbb{E}_{q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell})} \left[ \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right] = 0\), thus the expectations involving rewards which are constant w.r.t. \(u^{(\ell)}\) disappear. This allows us to simplify the expression keeping only the part that includes the local rewards:

\[
= \mathbb{E} \left[ \left( r(u^{(\ell)}, u^{(\ell-1)}) + r(u^{(\ell+1)}, u^{(\ell)}) \right) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right].
\]

(28f)

This estimator can be further refined. In the part that accounts for \(r(u^{(\ell)}, u^{(\ell-1)})\) we can solve the entropy term exactly:

\[
\mathbb{E}_{q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell})} \left[ \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\]

(29a)

\[
= \mathbb{E}_{q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell})} \left[ \log \frac{p(u^{(\ell)}|u^{(\ell-1)}, \theta_{\ell})}{q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell})} \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\]

(29b)

\[
= \mathbb{E}_{q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell})} \left[ \log \frac{p(u^{(\ell)}|u^{(\ell-1)}, \theta_{\ell})}{q(u^{(\ell)}|u^{(\ell-1), \lambda_{\ell}})} \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1), \lambda_{\ell}}) \right]
\]

(29c)

\[
- \mathbb{E}_{q(u^{(\ell)}|u^{(\ell-1), \lambda_{\ell}})} \log q(u^{(\ell)}|u^{(\ell-1), \lambda_{\ell}}) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1), \lambda_{\ell}}).
\]

(29d)
Recall that with a mean field assumption the entropy can be computed exactly
\[
\mathbb{H}(U^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) = \sum_{d=1}^{D} \mathbb{H}(g(u_{d}^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell})).
\] (30)

The negative cross entropy term can not be computed exactly because the generative model is autoregressive, that is, \(u_{d}^{(\ell)}\) depends on \(u_{<d}^{(\ell)}\). Still, its SFE can be further simplified. The argument is once again based on iterated expectations:
\[
\mathbb{E} \left[ \log p(u^{(\ell)}|u^{(\ell-1)}, \theta_{\ell}) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\] (31a)
\[
= \sum_{d=1}^{D} \mathbb{E} \left[ \sum_{k=1}^{d-1} \log p(u_{k}^{(\ell)}|u^{(\ell-1)}, u_{<k}, \theta_{\ell}) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\] (31b)
\[
+ \sum_{d=1}^{D} \mathbb{E} \left[ \sum_{k=d}^{D} \log p(u_{k}^{(\ell)}|u^{(\ell-1)}, u_{<k}, \theta_{\ell}) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\] (31c)
\[
= \sum_{d=1}^{D} \mathbb{E} \left[ \sum_{k=d}^{D} \log p(u_{k}^{(\ell)}|u^{(\ell-1)}, u_{<k}, \theta_{\ell}) \nabla_{\lambda_{\ell}} \log q(u^{(\ell)}|u^{(\ell-1)}, \lambda_{\ell}) \right]
\] (31d)

C. Special case

Here we lowerbound the marginal log-likelihood of the data by direct application of Jensen’s inequality without an independent variational approximation. We are interested in the gradient
\[
\nabla_{\theta_{\ell}} \mathbb{E}_{p_{\omega(x|z(u|x))}} \left[ \log p_{Y|\beta}(t^{-1}(x; u)) \right]
\] (32)

We can first express the gradient for layer \(\ell\) as
\[
\nabla_{\theta_{\ell}} \sum_{\ell=1}^{L} \mathbb{E}_{p(u^{(\ell)}|\theta)} \mathbb{E}_{p(u^{(\ell-1)}, \theta_{\ell})} \left[ \log p_{Y|\beta}(t^{-1}(x; u)) \right]
\] (33a)
\[
= \nabla_{\theta_{\ell}} \sum_{\ell=1}^{L} \mathbb{E}_{p(u^{(\ell)}|\theta)} \sum_{d=1}^{D} \mathbb{E}_{p(u_{d}^{(\ell)}|u^{(\ell-1)}, \theta_{\ell})} \mathbb{E}_{p(u_{<d}^{(\ell)}|u^{(\ell-1)}, \theta_{\ell})} \left[ \log p_{Y|\beta}(t^{-1}(x; u)) \right]
\] (33b)

Where we first applied the Markov property and secondly iterated expectation within the layer. If we introduce a proposal distribution \(\rho(u_{<d}^{(\ell)}),\) independent of \(\theta_{\ell},\) and define
\[
\omega(u_{<d}^{(\ell)}, \theta) = \frac{p_{\theta}(u_{<d}^{(\ell)})}{\rho(u_{<d}^{(\ell)})}
\] (34)
\[
\mathcal{L}(u_{<d}^{(\ell)}, \theta) = \mathbb{E}_{p(u_{<d}^{(\ell)}|u_{<d}^{(\ell)}), \theta_{\ell}} \left[ \log p_{Y|\beta}(t^{-1}(x; u)) \right]
\] (35)

then
\[
\nabla_{\theta_{\ell}} \sum_{d=1}^{D} \mathbb{E}_{p(u_{d}^{(\ell)}|u^{(\ell-1)}, \theta_{\ell})} \left[ \mathcal{L}(u_{<d}^{(\ell)}, \theta_{\ell}) \right]
\]
\[
= \nabla_{\theta_{\ell}} \sum_{d=1}^{D} \mathbb{E}_{\rho(u_{d}^{(\ell)})} \left[ \omega(u_{<d}^{(\ell)}, \theta_{\ell}) \mathcal{L}(u_{<d}^{(\ell)}, \theta_{\ell}) \right]
\] (36a)
\[
= \sum_{d=1}^{D} \mathbb{E}_{\rho(u_{d})} \left[ \omega(u_{d}^{(\ell)}, \theta_{\ell}) \nabla_{\theta_{\ell}} \mathcal{L}(u_{<d}^{(\ell)}, \theta_{\ell}) + \mathcal{L}(u_{<d}^{(\ell)}, \theta_{\ell}) \nabla_{\theta_{\ell}} \omega(u_{<d}^{(\ell)}, \theta_{\ell}) \right].
\] (36b)
Note that the first term inside the expectation can be estimated via the score function estimator i.e.

\[ \omega(u_{<d}, \theta_t) \nabla_{\theta_t} \mathcal{L}(u_{<d}, \theta_t) = \omega(u_{<d}, \theta_t) \mathbb{E}_{p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t)} \left[ \log p_Y(t^{-1}(x; u)) \nabla_{\theta_t} p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t) \right] . \quad (37) \]

For the second term we can write

\[ \mathcal{L}(u_{<d}, \theta_t) \nabla_{\theta_t} \omega(u_{<d}, \theta_t) = \frac{\mathcal{L}(u_{<d}, \theta_t)}{\rho(u_{<d})} \nabla_{\theta_t} p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t) \]

\[ = \omega(u_{<d}, \theta_t) \mathcal{L}(u_{<d}, \theta_t) \mathbb{E}_{p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t)} \left[ \log p_Y(t^{-1}(x; u)) \nabla_{\theta_t} p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t) \right] . \quad (38a) \]

\[ \mathcal{L}(u_{<d}, \theta_t) \nabla_{\theta_t} \omega(u_{<d}, \theta_t) = \omega(u_{<d}, \theta_t) \mathcal{L}(u_{<d}, \theta_t) \mathbb{E}_{p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t)} \left[ \log p_Y(t^{-1}(x; u)) \nabla_{\theta_t} p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t) \right] . \quad (38b) \]

Where our proposal is \( \rho(u_{<d}) := p(u_{<d} | u^{(\ell-1)}, \theta_t) \), we have \( \omega(u_{<d}, \theta_t) = 1 \). This means that the first term becomes a local learning signal

\[ \sum_{\ell=1}^{L} \mathbb{E}_{p(u^{(\ell)} | \theta)} \mathbb{E}_{p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t)} \left[ \log p_Y(t^{-1}(x; u)) \nabla_{\theta_t} p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t) \right] , \quad (39) \]

where the learning signal derived from the \( d \)th observation interacts directly with the gradient of the log-probability of the \( d \)th latent variable. The second term becomes

\[ \sum_{\ell=1}^{L} \mathbb{E}_{p(u^{(\ell)} | \theta)} \mathbb{E}_{p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t)} \left[ \log p_Y(t^{-1}(x; u)) \nabla_{\theta_t} p(u_d^{(\ell)} | u_{<d}, u^{(\ell-1)}, \theta_t) \right] \quad (40) \]

where the learning signal derived from the \( d \)th observation interacts with the gradient of the log-probability of the \( d \)th latent prefix.

**D. Samples**