Generalized Doubly-Reparameterized Gradient Estimators

Matthias Bauer 1 Andriy Mnih 1

Abstract

Efficient low-variance gradient estimation enabled by the reparameterization trick (RT) has been essential to the success of variational autoencoders. Doubly-reparameterized gradients (DREGs) improve on the RT for multi-sample variational bounds by applying reparameterization a second time for an additional reduction in variance. Here, we develop two generalizations of the DREGs estimator and show that they can be used to train conditional and hierarchical VAEs on image modelling tasks more effectively. First, we extend the estimator to hierarchical models with several stochastic layers by showing how to treat additional score function terms due to the variational posterior. We then generalize DREGs to score functions of arbitrary distributions instead of just those of the sampling distribution, which makes the estimator applicable to the parameters of the prior in addition to those of the posterior.

1. Introduction

In probabilistic machine learning we often optimize expectations of the form \( \mathcal{L}_{\phi, \theta} = \mathbb{E}_{q_\phi(z)} [f_{\phi, \theta}(z)] \) w.r.t. to their parameters, where \( f_{\phi, \theta}(z) \) is some objective function, and \( \phi \) and \( \theta \) denote the parameters of the sampling distribution \( q_\phi(z) \) and other (e.g. model) parameters, respectively. In the case of the influential variational autoencoder (VAE, Kingma & Welling (2014), Rezende et al. (2014)), \( q_\phi(z) \) is the variational posterior, \( \theta \) denotes the model parameters, and \( \mathcal{L}_{\phi, \theta} \) is typically either the ELBO (Jordan et al., 1999; Blei et al., 2017) or IWAE (Burda et al., 2016) objective.

In most cases of interest, this expectation is intractable, and we estimate it and its gradients, \( \nabla_\phi \mathcal{L} \) and \( \nabla_\theta \mathcal{L} \), using Monte Carlo samples \( z \sim q_\phi(z) \). The resulting gradient estimators are characterized by their bias and variance. We usually prefer unbiased estimators as they tend to be better-behaved and are better understood. Lower variance is also preferable because it enables faster training by allowing using higher learning rates.

In this paper, we address gradient estimation for continuous variables in variational objectives. A naive implementation of \( \nabla_\phi \mathcal{L} \) results in a score function, or REINFORCE, estimator (Williams, 1992), which tends to have high variance; however, if \( f_{\phi, \theta}(z) \) depends on \( \phi \) only through \( z \), we can use reparameterization (Kingma & Welling, 2014; Rezende et al., 2014) to obtain an estimator with lower variance by replacing the score function estimator of the gradient with a pathwise estimator.

In variational inference, \( f_{\phi, \theta}(z) \) typically depends on \( \phi \) not only through \( z \) but also through the value of the log density \( \log q_\phi(z) \). Then, the gradient estimators still involve the score function \( \nabla_\phi \log q_\phi(z) \) despite using reparameterization. Roeder et al. (2017) propose the sticking the landing (STL) estimator, which simply drops these score function terms to reduce variance. Tucker et al. (2019) show that STL is biased in general, and introduce the doubly-reparameterized gradient (DREGs) estimator for IWAE objectives, which again yields unbiased lower-variance gradient estimates. This is achieved by applying reparameterization a second time, targeting the remaining score function terms.

However, the DREGs estimator has two major limitations: 1) it only applies to latent variable models with a single latent layer; 2) it only applies in cases where the score function depends on the same parameters as the sampling distribution. In this work we address both limitations. Moreover, we show that for hierarchical models with several stochastic layers, gradients that look like pathwise gradients can actually contain additional score function gradients that are not doubly reparameterizable. Despite this, we show that we can still obtain a simple estimator with a sizable reduction in gradient variance for hierarchical IWAE objectives.

Our main contributions are:

- We extend DREGs to hierarchical models;
- We introduce GDREGs, a generalization of DREGs to score functions that depend on a different distribution than the sampling distribution;
2. Background

In this work we are interested in computing gradients of variational objectives of the form

$$\mathcal{L}_{\theta, \phi} = \mathbb{E}_{z \sim q_\phi(z)} [f_{\theta, \phi}(z)]$$ (1)

w.r.t. the variational parameters $\phi$ of the sampling distribution $q_\phi(z)$, and parameters $\theta$ of a second distribution $p_\theta(z)$, such as a learnable prior. Here $f_{\theta, \phi}(z)$ is a general function of $z$ that can also explicitly depend on both $q_\phi(z)$ and $p_\theta(z)$. More precisely, we wish to compute

$$\nabla_{\phi}^{TD} \mathcal{L}_{\theta, \phi} \quad \text{and} \quad \nabla_{\theta}^{TD} \mathcal{L}_{\theta, \phi},$$ (2)

where $\nabla_x^{TD}$ denotes the total derivative, which we explicitly distinguish from the partial derivative $\nabla_x$.

Arguably the simplest objectives of this form are the negative entropy $\mathcal{L}^\text{ent}_{\theta, \phi} = \mathbb{E}_{z \sim q_\phi(z)} [\log q_\phi(z)]$ and negative cross-entropy $\mathcal{L}^\text{ce}_{\theta, \phi} = \mathbb{E}_{z \sim q_\phi(z)} [\log p_\theta(z)]$.

Importance weighted autoencoders. Another such objective is the importance weighted autoencoder (IWAE) bound (Burda et al., 2016). For a VAE with likelihood $p_\lambda(x|z)$, (learnable) prior $p_\theta(z)$, and variational posterior (or proposal) $q_\phi(z|x)$ the IWAE bound with $K$ importance weights $w_k = \frac{p_\theta(z)p_\lambda(z|x)}{q_\phi(z|x)}$ is given by

$$\mathcal{L}^\text{IWAE}_{\theta, \phi} = \mathbb{E}_{z_1, \ldots, z_K \sim q_\phi(z|x)} \left[ \log \left( \frac{1}{K} \sum_{k=1}^K w_k \right) \right].$$ (3)

Eq. (3) reduces to the regular ELBO objective for $K = 1$ (Rezende et al., 2014; Kingma & Welling, 2014),

$$\mathcal{L}^\text{ELBO}_{\theta, \phi} = \mathbb{E}_{z \sim q_\phi(z|x)} \left[ \log p_\theta(z)p_\lambda(z|x)q_\phi(z|x) \right].$$ (4)

Burda et al. (2016) showed that using multiple importance samples ($K > 1$) provides the model with more flexibility to learn rich representations (fewer inactive units), and results in better log-likelihood estimates compared to VAEs trained with the single sample ELBO. The estimators discussed in this paper build on these results and lead to further improvements. While we focus on the IWAE objective, our proposed GDREGs estimator applies generally.

Gradient estimation. In practice, the expectation in Eq. (1) and its gradients are intractable, so we approximate them using Monte Carlo sampling, which makes the estimates of the objective and its gradients random variables. The resulting gradient estimators will be unbiased but have non-zero variance. We prefer estimators with lower variance, as they enable fast training by allowing higher learning rates.

We can distinguish between two general types of gradient estimators in this setting: (i) score function estimators and (ii) pathwise estimators. Score functions are gradients of a log probability density w.r.t. its parameters, such as $\nabla_{\phi} \log q_\phi(z)$; they treat the function $f_{\theta, \phi}(z)$ as a black box and often yield high variance gradients. In contrast, pathwise estimators move the parameter-dependence from the probability density into the argument $z$ of the function $f_{\theta, \phi}(z)$ and derive the computation path to often achieve lower variance gradients by using the knowledge of $\nabla_z f_{\theta, \phi}(z)$; see Mohamed et al. (2020) for a recent review.

When computing gradients of the objective $\mathcal{L}_{\theta, \phi}$ we have to differentiate both the sampling distribution of the expectation, $q_\phi(z)$, as well as the function $f_{\theta, \phi}(z)$,

$$\nabla_{\phi}^{TD} \mathbb{E}_{q_\phi(z)} [f_{\theta, \phi}(z)] = \mathbb{E}_{q_\phi(z)} \left[ \nabla_{\phi} f_{\theta, \phi}(z) + f_{\theta, \phi}(z) \nabla_{\phi} \log q_\phi(z) \right] \quad \text{(5)}$$

$$\nabla_{\theta}^{TD} \mathbb{E}_{q_\phi(z)} [f_{\theta, \phi}(z)] = \mathbb{E}_{q_\phi(z)} \left[ \nabla_{\theta} f_{\theta, \phi}(z) \right], \quad \text{and}$$ (6)

and both can give rise to score functions. To see that all of the underlined terms indeed contain score functions, note that we can rewrite $\nabla_{\phi} f_{\theta, \phi}(z)$ as $\nabla_{\phi} f_{\theta, \phi}(z) = \nabla_{\log q_\phi(z)} f_{\theta, \phi}(z) \nabla_{\phi} \log q_\phi(z)$ and similarly for $\nabla_{\theta} f_{\theta, \phi}(z)$.

In the following we recapitulate how to address the score functions w.r.t. $\phi$ in Eq. (5) using the reparameterization trick and doubly-reparameterized gradient estimators (DREGs, Tucker et al. (2019)), respectively. In Sec. 4 we introduce GDREGs, a generalization of DREGs, that eliminates the score function w.r.t. $\theta$ in Eq. (6).

Reparameterization. We can use the reparameterization trick (Kingma & Welling, 2014; Rezende et al., 2014) to turn the score function $\nabla_{\phi} \log q_\phi(z)$ inside the expectation in Eq. (5) into a pathwise derivative of the function $f_{\theta, \phi}(z)$ as follows: we express the latent variables $z \sim q_\phi(z)$ through a bijection of new random variables $\epsilon \sim q(\epsilon)$, which are independent of $\phi$,

$$z = \mathcal{T}_{q}(\epsilon; \phi) \iff \epsilon = \mathcal{T}_{q}^{-1}(z; \phi).$$ (7)

This allows us to rewrite expectations w.r.t. $q_\phi(z)$ as $\mathbb{E}_{q_\phi(z)} [f_{\theta, \phi}(z)] = \mathbb{E}_{q(\epsilon)} [f_{\theta, \phi}(\mathcal{T}_{q}(\epsilon; \phi))]$, which moves the parameter dependence into the argument of $f_{\theta, \phi}(z)$ and gives rise to a pathwise gradient:

$$\nabla_{\phi}^{TD} \mathbb{E}_{q_\phi(z)} [f_{\theta, \phi}(z)] = \mathbb{E}_{q(\epsilon)} \left[ \nabla_{\phi} f_{\theta, \phi}(\mathcal{T}_{q}(\epsilon; \phi)) + \nabla_{\epsilon} f_{\theta, \phi}(\mathcal{T}_{q}(\epsilon; \phi)) \nabla_{\phi} \mathcal{T}_{q}(\epsilon; \phi) \right]_{z=\mathcal{T}_{q}(\epsilon; \phi)}.$$ (8)
In Sec. 3 we discuss that this seemingly pathwise gradient in Eq. (8) can actually contain score functions for more structured or hierarchical models and explain how to extend DREGs to this case. For the remainder of this section we restrict ourselves to simple (single stochastic layer) models.

**Double reparameterization.** Tucker et al. (2019) further reduce gradient variance by replacing the remaining score function in the reparameterized gradient Eq. (8), \( \nabla_{\phi} \log q(z) = \nabla_{\log q(z)} f_{\theta}(z) \nabla_{\phi} \log q_{\phi}(z) \), with its reparameterized counterpart. Double reparameterization is based on the identity Eq. (9) (Eq. 5 in Tucker et al. (2019)),

\[
E_{\varepsilon \sim q_\varepsilon(z)} [ g_{\phi, \theta}(z) \nabla_{\phi} \log q_{\phi}(z) ] = \nabla_{\phi} \log q_\varepsilon(z) \nabla_{\phi} \log q_{\phi}(z) \frac{1}{m} \sum_{i=1}^{m} y_i \nabla_{\phi} T_q(\varepsilon_i, \theta, \phi) \tag{9}
\]

which follows from the fact that both the score function and the reparameterization estimators are unbiased and thus equal in expectation. This identity holds for arbitrary \( g_{\phi, \theta}(z) \); to match the score function in Eq. (8) with the LHS of Eq. (9), we have to choose \( g_{\phi, \theta}(z) = \nabla_{\log q_\varepsilon(z)} f_{\theta}(z) \). In Eq. (10) we have rewritten the expectation over \( \varepsilon \sim q_\varepsilon(z) \) in terms of \( z \sim q_{\varepsilon}(z) \), as this will become useful for our later generalization. Note how, to compute the pathwise gradient, the sample \( z \) is mapped back to the noise variable \( \varepsilon = T_q^{-1}(z; \phi) \), \( \nabla_{\phi} T_q(\varepsilon_i, \theta, \phi) \) is also sometimes written as \( \nabla_{\phi} z(\varepsilon_i; \theta, \phi) \) (Tucker et al., 2019).

**Gradient estimation for the IWAE objective.** For the IWAE objective Eq. (3), Tucker et al. (2019) derived the following doubly-reparameterized gradients (DREGs) estimator, which supersedes the previously proposed STL estimator (Roeder et al., 2017):

\[
\nabla_{\phi}^{\text{DREGs}} L_{\text{IWAE}} = \frac{1}{K} \sum_{k=1}^{K} \nabla_{\phi} T_q(\varepsilon_k, \theta, \phi) \frac{1}{M} \sum_{i=1}^{M} w_i \nabla_{\phi} T_q(\varepsilon_i; \theta, \phi) \tag{11}
\]

\[
\nabla_{\phi}^{\text{STL}} L_{\text{IWAE}} = \frac{1}{K} \sum_{k=1}^{K} \nabla_{\phi} T_q(\varepsilon_k, \theta, \phi) \frac{1}{M} \sum_{i=1}^{M} w_i \nabla_{\phi} T_q(\varepsilon_i; \theta, \phi) \tag{12}
\]

with normalized importance weights \( w_k = \frac{\hat{w}_k}{\sum_{k'}^{K} \hat{w}_{k'}} \) and \( \varepsilon_1:K \sim q_\varepsilon(z) \). While the DREGs estimator double-reparameterizes the score function in Eq. (8), the STL estimator simply drops it and is biased as a result. Crucially, because DREGs relies on reparameterization, it is limited to score functions of the sampling distribution \( q_\varepsilon(z) \), making it inapplicable in the more general setting of arbitrary score functions, such as \( E_{\varepsilon \sim q_\varepsilon(z)} [ \nabla_{\phi} f_{\theta}(z) ] \) in Eq. (6).

### 3. DREGs for hierarchical models

We now show that for models with hierarchically structured latent variables even terms that look like pathwise gradients, such as \( \nabla_{\phi} f_{\theta}(z) \) in Eq. (8) or \( \nabla_{\phi}^{\text{DREGs}} \) in the DREGs or STL estimator for the IWAE objective Eqs. (11) and (12), can give rise to additional score functions. These additional score functions appear because the distribution parameters of one stochastic layer depend on the latent variables of another layer. Their appearance is contrary to the intuition that doubly-reparameterized gradient estimators only contain pathwise gradients.

#### 3.1. An illustrative example

To illustrate this, consider a hierarchical model with two layers where we first sample \( z_2 \sim q_{\phi_2}(z_2) \) and then \( z_1 \sim q_{\phi_1}(z_1 | z_2) \). Note that the conditioning on \( z_2 \) is through the distribution parameters of \( q_{\phi_1}(z_1 | z_2) \); to highlight this dependence of \( z_1 \) on \( z_2 \), we rewrite \( q_{\phi_1}(z_1 | z_2) = q_{\alpha_1 | z_2}(z_1; \alpha_1) \), where we explicitly distinguish between the distribution parameters \( \alpha_1 \), such as the mean and covariance of a Gaussian, and the network parameters \( \phi_1 \) that parameterize them together with the previously sampled latent \( z_2 \). A derivative w.r.t. \( z_2 \) that looks like a pathwise gradient actually gives rise to a score function term at a subsequent level:

\[
\nabla_{z_2}^{\text{DREGs}} \log q_{\phi_1}(z_1 | z_2) = \nabla_{z_2}^{\text{DREGs}} \log q_{\alpha_1 | z_2}(z_1; \alpha_1) \tag{13}
\]

\[
= \nabla_{z_2}^{\text{DREGs}} \log q_{\alpha_1 | z_2}(z_1) \nabla_{z_2} \alpha_1(z_2, \phi_1) + \ldots \tag{14}
\]

We omitted (true) pathwise gradients \( \ldots \), as the samples \( z_1 \) also depend on \( z_2 \) through reparameterization. Similar additional score functions arise for seemingly pathwise gradients of hierarchical or autoregressive priors and variational posteriors.

#### 3.2. Extending DREGs to hierarchical VAEs

Here we show how to extend DREGs to hierarchical VAEs to effectively reduce gradient variance for the variational posterior despite the results in the previous section. We still consider the IWAE objective (Eq. (3)), but now the latent space \( z \) is structured, and both \( \theta \) and \( \phi \) are hierarchically factorized distributions.

Let us consider a 2-layer VAE \( \overrightarrow{z_2} \overrightarrow{z_1} \overrightarrow{z} \) and examine the term \( \nabla_{z_2}^{\text{DREGs}} \log q_{\phi_1}(z_1; z_2) \), which appears in the total derivative of the IWAE objective, as a concrete example. We have sampled \( z_1 \) and \( z_2 \) hierarchically using reparameterization: \( z_2(\phi_2) \equiv T_{\phi_2}(\varepsilon_2, \alpha_2(\phi_2)) \) and \( z_1(\phi_1, \phi_2) \equiv T_{\phi_1}(\varepsilon_1; \alpha_1(\phi_2), \phi_1) \):}

\[
\nabla_{z_2}^{\text{DREGs}} \log q_{\alpha_2}(\phi_2) = \nabla_{z_2}^{\text{DREGs}} \log q_{\alpha_2}(\phi_2) q_{\alpha_1 | z_2}(z_1(\phi_1, \phi_2), \phi_1) \tag{15}
\]

When computing total derivatives w.r.t. parameters \( \phi_2 \) of the upper layer, we distinguish between three types of gradients: the (true) pathwise gradients w.r.t. \( z_1 \) and \( z_2 \), a direct score function because the distribution parameters \( \alpha_2(\phi_2) \)...
directly depend on $\phi_2$, and an indirect score function because the distribution parameter $\alpha_{i|2}(z_2(\phi_2), \phi_1)$ indirectly depends on $\phi_2$ through $z_2(\phi_2)$. Indirect score functions do not arise in single stochastic layer models considered by Tucker et al. (2019), and we have three options to estimate them: (1) leave them—this naive estimator is unbiased but potentially has high variance; (2) drop them, similar to STL—this estimator is generally biased; (3) doubly-reparameterize them using DREGs again—this estimator is unbiased, but can generate further indirect score functions.

Total derivatives of other terms in the objective similarly decompose into pathwise gradients as well as direct and indirect score functions. Notably, this includes indirect score functions of the prior $\log p_\theta(z_1, z_2)$, to which DREGs do not apply. In Sec. 4 we introduce the generalized DREGs (GDREGs) estimator that applies in this case.

3.3. DREGs for hierarchical IWAE objectives

For IWAE objectives we find that the indirect score functions come up twice: once when computing pathwise gradients of the initial reparameterization, and a second time (with a different prefactor) when computing pathwise gradients for the double-reparameterization of the direct score functions. The same happens for the (true) pathwise gradients, and it is this double-appearance and the resulting cancellation of prefactors that helps reduce gradient variance for DREGs. Moreover, for general model structures it is impossible to replace all successively arising indirect score functions with pathwise gradients, even by applying GDREGs. For example, when the prior and posterior do not factorize in the same way, double-reparameterization of one continuously creates indirect score functions of the other and vice versa, see Apps. C and C.4 for more details.

Thus, to extend DREGs to hierarchical models, we leave the indirect score functions unchanged and only doubly-reparameterize the direct score functions. The extended DREGs estimator for IWAE models with arbitrary hierarchical structures is given by Eq. (20).

\[
\mathbb{E}_{z \sim q_\phi(z)}[g_{\phi, \theta}(z) \nabla_\theta \log p_\theta(z)] = \mathbb{E}_{z \sim q_\phi(z)} \left[ \left( g_{\phi, \theta}(z) \nabla_z \log q_\phi(z) + \nabla_z g_{\phi, \theta}(z) \right) \nabla_\theta T_p(\epsilon; \theta) \right]_{\epsilon = T_{\theta}^{-1}(z, \theta)}
\]

(16)

\[
\nabla^2_{\theta} \mathbb{E}_{q_\phi(z)}[g_{\phi, \theta}(z)] = \nabla^2_{\theta} \mathbb{E}_{p_\phi(z)} \left[ \frac{q_\phi(z)}{p_\phi(z)} g_{\phi, \theta}(z) \right] = \nabla^2_{\theta} \mathbb{E}_{q(\epsilon)} \left[ \frac{q_\phi(T_p(\epsilon; \theta))}{p(\epsilon; \theta)} g_{\phi, \theta}(T_p(\epsilon; \theta)) \right]; \quad q(\epsilon) = \mathcal{N}(0, 1)
\]

(17)

\[
\mathbb{E}_{q(\epsilon)} \left[ \nabla^2_{\theta} \left( \frac{q_\phi(z)}{p_\phi(z)} g(z) \right) \nabla_\theta T_p(\epsilon; \theta) + \frac{q_\phi(z)}{p_\phi(z)} \nabla_\theta g_{\phi, \theta}(z) - g(z) \nabla_\theta \log p_\theta(z) \right]_{\epsilon = T_{\theta}^{-1}(z; \theta)}
\]

(18)

\[
\mathbb{E}_{q_\phi(z)} \left[ \left( g(z) \nabla^2_{\theta} \log q_\phi(z) + \nabla^2_{\theta} g(z) \right) \nabla_\theta T_p(\epsilon; \theta) \right]_{\epsilon = T_{\theta}^{-1}(z; \theta)} + \nabla_\theta g_{\phi, \theta}(z) - g(z) \nabla_\theta \log p_\theta(z)
\]

(19)

**Figure 1:** The GDREGs identity and a brief derivation in three steps: (1) temporarily change the path so that it depends on $\theta$; (2) perform the reparameterized gradient computation; (3) change the path back so we can use samples $z \sim q_\phi(z)$ to estimate the expectation. See App. A for details and an alternative derivation using the change of density formula.

where $l$ denotes the stochastic layer, $p_{\alpha_i}(l)$ is the set of latent variables that $z_{kl}$ depends on, and $z_{kl} = \tilde{T}_q(\epsilon_{kl}; \alpha_i(p_{\alpha_i}(l), \phi_l))$ through reparameterization. We provide a detailed derivation in App. C and a worked example for a VAE with two stochastic layers in App. D. In Apps. E and E.1 we show how to implement this estimator using automatic differentiation by using a surrogate loss function, whose forward computation we discard, but whose backward computation exactly corresponds to the estimator in Eq. (20). Alternatively, one could implement a custom gradient for the objective that directly implements Eq. (20); however, we found our approach using a surrogate loss function to be simpler both conceptually and implementation-wise.

Roeder et al. (2017) apply the STL estimator to hierarchical ELBO objectives but do not discuss indirect score functions. Their experimental results are consistent with maintaining the indirect score functions, similar to how we extend DREGs to hierarchical models; the STL estimator is biased for IWAE objectives (Tucker et al., 2019).

4. Generalized DREGs

Here, we generalize DREGs to score functions that involve distributions $p_\phi(z)$ different from the sampling distribution $q_\phi(z)$, as in Eq. (6). In other words, we would like to replace score function terms of the form $\mathbb{E}_{q_\phi(z)}[g_{\phi, \theta}(z) \nabla_\theta \log p_\theta(z)]$ with doubly-reparameterized pathwise gradients. Such terms appear, for example, when training a VAE with a trainable prior $p_\theta(z)$ with the ELBO or IWAE objectives. DREGs cannot be used directly in this case as it relies on reparameterization of the sampling distribution $q_\phi(z)$, so that the path depends on the parameters $\phi$, 

\[
\mathbb{E}_{z \sim q_\phi(z)}[g_{\phi, \theta}(z) \nabla_\theta \log p_\theta(z)] = \mathbb{E}_{z \sim q_\phi(z)} \left[ \left( g_{\phi, \theta}(z) \nabla_z \log q_\phi(z) + \nabla_z g_{\phi, \theta}(z) \right) \nabla_\theta T_p(\epsilon; \theta) \right]_{\epsilon = T_{\theta}^{-1}(z, \theta)}
\]

(20)
whereas the score function is with w.r.t. parameters $\theta$ of a different distribution $p_\theta(z)$.

To make progress we need to make the path depend on $\theta$ while still sampling $z \sim q_\phi(z)$ during training. Our solution consists of three steps (also see Fig. 1):

1. temporarily change the path so that it depends on $\theta$;
2. perform the reparameterized gradient computation;
3. change the path back so we can use samples $z \sim q_\phi(z)$ to estimate the expectation.

We change the path by first using an importance sampling reweighting to temporarily re-write the expectation, $E_{q_\phi(z)}[*] = E_{p_\theta(z)}[q_\phi(z) p_\theta(z)]$, and then employing reparameterization on the new sampling distribution $p_\theta(z)$: $z = T_p(\epsilon; \theta)$ with $\epsilon \sim q(\epsilon)$. Following this recipe, we derive the gradient identity in Eq. (16) for general $q_\phi, p_\theta(z)$ that we refer to as generalized DREGS (or GDREGS for short) identity.

Like DREGS (Eq. 10), GDREGS allows us to transform score functions into pathwise gradients. Yet, unlike DREGS, GDREGS applies to general score functions and contains a correction term that vanishes when $p_\theta(z)$ and $q_\phi(z)$ are identical ($\log q_\phi(z)/p_\theta(z)$ term in Eq. 16).

Note that the pathwise derivative $\nabla_\theta T_p(\epsilon; \theta)$ in Eq. (16) looks like we reparameterized an independent noise variable $\epsilon$ using $p_\theta(z)$, where the numerical value of the noise variable is given by $\epsilon = T_p^{-1}(z; \theta)$ and $z \sim q_\phi(z)$. We can interpret this sequence of transformations as a normalizing flow (Rezende & Mohamed, 2015) $z \rightarrow \epsilon \rightarrow z$, such that $T_p(\epsilon; \theta) = T_p^{-1}(z; \theta); \theta = z$. We can think of this procedure as re-expressing the sample $z \sim q_\phi(z)$ as if it came from $p_\theta(z)$: Its numerical value $z$ remains unchanged and it is still distributed according to $q_\phi(z)$, yet its pathwise gradient $\nabla_\theta T_p(\epsilon; \theta)$ depends on $\theta$. We illustrate the corresponding computational flow in Fig. 2 and provide an example implementation with code in App. F.

Note that to derive the GDREGS identity, we only require $p_\theta(z)$ to be reparameterizable (\(\square\) in Fig. 2). While $q_\phi(z)$ may be reparameterizable as well (\(\square\) in Fig. 2), this is not necessary; we only need to be able to evaluate its density in Eq. 16.

In the simplest case of the cross-entropy objective $L^{ce}$ because $\epsilon \sim q(\epsilon)$, we only require

$$L^{ce} = \mathbb{E}_{q_\phi(z)}[\log p_\theta(z)]$$

(as in the ELBO with a sample-based KL estimate), $q_{\phi, 0}(z) = 1$, and the GDREGS identity Eq. (16) gives rise to the following GDREGS estimator:

$$\hat{\nabla}_\theta L^{ce} = \nabla_\epsilon \mathbb{E}_{p_\theta(z)}[q_\phi(z) p_\theta(z)]\nabla_\theta T_p(\epsilon; \theta)|_{\epsilon = T_p^{-1}(z, \theta)}$$

(21)

with $z \sim q_\phi(z)$. For Gaussian distributions $q_\phi(z)$ and $p_\theta(z)$, the cross-entropy and its gradients can be computed in closed form, which we can think of as a perfect estimator with zero bias and zero variance. Moreover, the expectation and variance of both the naive score function as well as the GDREGS estimator in Eq. (21) can be computed in closed form. We provide full derivations and a discussion of this special case in App. H as well as an example implementation in terms of (pseudo-)code in App. F. The main results are: (i) GDREGS has lower variance gradients than the score function when $q_\phi(z)$ and $p_\theta(z)$ overlap substantially, which is typically the case at the beginning of training; (ii) we can derive a closed-form control variate that depends on a ratio of the means and variances of the two distributions and that is strictly superior to the naive score function estimator and the GDREGS estimator in terms of gradient variance. However, the analytic expression for the cross-entropy has even lower (zero) gradient variance in this case.

4.1. GDREGS for VAE objectives

We can now use the GDREGS identity Eq. (16) to derive generalized doubly-reparameterized estimators for expectations of general score functions of the form $\mathbb{E}_{q_\phi(z)}[g_{\phi, \theta}(z) \nabla_\theta \log p_\theta(z)]$, also see Eq. (6). In App. B we derive the following GDREGS estimator of the IWAE objective w.r.t. the prior parameters $\theta$:

$$\hat{\nabla}_{\theta} L^{IWAE}_{\phi, \theta} = \sum_{k=1}^{K}(\bar{w}_k \nabla_{z_k}^{TD} \log p_\lambda(x|z_k) - \nabla_{z_k}^{TD} \log \bar{w}_k) \nabla_\theta T_p(\epsilon_k; \theta)|_{\epsilon_k = T_p^{-1}(z_k, \theta)}$$

(22)

with $z_{1:K} \sim q_\phi(z|x)$. The second term in Eq. (22) looks like the DREGS estimator for $\phi$ in Eq. (11) except that the samples $z_k$ are now re-expressed as if they came from $p_\theta(z)$. In addition we obtain a term that involves the likelihood $p_\lambda(x|z)$ and is linear in $\bar{w}_k$. Note that we do not apply GDREGS to the likelihood parameters $\lambda$ because $p_\lambda(x|z)$...
4.2. Extending GDREGs to hierarchical VAEs

When extending GDREGs to hierarchical models, we again encounter direct and indirect score functions (see Sec. 3). Like for the posterior parameter $\phi$ we apply GDREGs to the direct score functions but leave the indirect score functions unchanged. The full GDREGs estimator for IWAE objectives with arbitrary hierarchical structure is given in App. C Eq. (C.16), see App. C for a derivation. In App. D we provide a worked example and in App. E we again show how to use surrogate losses to implement the estimator in practice.

To apply GDREGs we need to re-express samples from $q_\phi(z)$ as if they came from $p_\theta(z)$. We do this for the entire hierarchy jointly. In Fig. 3 we illustrate the necessary computational flow for the example of a 2-layer VAE with the variational posterior factorized in the opposite direction from the generative process; see App. C for the general case. We draw samples $z_1, z_2 \sim q_\phi(z_1, z_2) = q_{\phi_1}(z_1)q_{\phi_2}(z_2|z_1)$ (by transforming independent variables $\epsilon_i$) and then re-express them as if they were sampled from the prior $p_\theta(z_2)p_\theta(z_1|z_2)$, which factorizes in the opposite direction. While the numerical values of $z_1$ and $z_2$ remain unchanged, $z_1$ is now dependent on $z_2$ and both depend on the respective $\theta$ parameters when computing gradients; we can view $(z_1, z_2)$ as samples that were obtained by transforming independent variables $(\epsilon_1, \epsilon_2)$ that follow a more complicated distribution than $(\epsilon_1, \epsilon_2)$. As in the single-layer case, only $p_\theta(z)$ needs to be reparameterizable.

5. Experiments

In this section we empirically evaluate the hierarchical extension of DREGs and its generalization to GDREGs, and compare them to the naive IWAE gradient estimator (labelled as IWAE) as well as STL (Roeder et al., 2017). First, we illustrate that DREGs and GDREGs increase the gradient signal-to-noise ratio (SNR) and reduce gradient variance compared to the naive estimator on a simple hierarchical example (Sec. 5.1); second, we show that they also reduce gradient variance in practice and improve test performance on several generative modelling tasks with VAEs with one or more stochastic layers (Sec. 5.2). We highlight that both the extension of DREGs to more than one stochastic layer as well as training the prior with GDREGs are novel contributions of this work.

5.1. Illustrative example: linear VAE

We first consider an extended version of the illustrative example by Rainforth et al. (2018) and Tucker et al. (2019) to show that hierarchical DREGs and GDREGs increase the gradient signal-to-noise ratio (SNR) and reduce gradient variance compared to the naive IWAE gradient estimator.

We consider a 2-layer linear VAE with hierarchical prior $z_2 \sim \mathcal{N}(0, I)$, $z_1|z_2 \sim \mathcal{N}(\mu_\theta(z_2), \sigma_\theta^2(z_2))$, Gaussian noise likelihood $x|z_1 \sim \mathcal{N}(z_1, \|)$, and bottom up variational posterior $q_{\phi_1}(z_1|x) = \mathcal{N}(\mu_{\phi_1}(x), \sigma_{\phi_1}^2(x))$ and $q_{\phi_2}(z_2|z_1) = \mathcal{N}(\mu_{\phi_2}(z_1), \sigma_{\phi_2}^2(z_1))$. All $\mu_i$ and $\sigma_i$ are linear functions, and $z_1, z_2, x \in \mathbb{R}^D$. We sample 512 datapoints in $D = 5$ dimensions from a model with $\mu_\theta(z_2) = z_2$ and $\sigma_\theta(z_2) = 1$. We then train the parameters $\phi$ and $\theta$ using SGD and the IWAE objective til convergence and evaluate the gradient variance and signal-to-noise ratio for each estimator. For the proposal parameters $\phi$ we compare DREGs to the naive score function (labelled as IWAE) and to STL; for the prior parameters $\theta$ we compare GDREGs to IWAE.
We consider both single layer and hierarchical (multi-layer) VAEs and evaluate them on unconditional and conditional modelling tasks using the IWAE objective, Eq. (3). In the hierarchical case, the generative path (prior and likelihood) is top-down whereas the variational posterior is bottom-up, see Fig. 5 and Eq. (23) for a full description of the model and a 2-layer unconditional example. For conditional modelling we predict the bottom half of an image given its top half, as in Tucker et al. (2019); in this case, both the prior and variational posterior also depend on a context variable \( c \), \( q_\phi(z|x,c) \) and \( p_\theta(z|c) \), respectively. We use a factorized Bernoulli likelihood along with factorized Gaussians for the variational posterior and prior. Every conditional distribution in Eq. (23) is parameterized by an MLP with two hidden layers of 300 \( \tanh \) units each, and all latent spaces have 50 dimensions. Unless stated otherwise, we train all models for 1000 epochs using the Adam optimizer (Kingma & Ba, 2015) with default learning rate of \( 3 \cdot 10^{-4} \), a batch size of 64, and \( K = 64 \) importance samples; see App. G for details.

As mentioned in Sec. 4.1, we use separate surrogate objectives to compute the gradient estimators for the likelihood, posterior, and prior parameters. While we always train the likelihood parameters \( \lambda \) on the naive IWAE objective, we consider the naive IWAE estimator (labelled as IWAE), STL, and DREGs for the variational posterior parameters \( \phi \), and IWAE and DREGs for the prior parameters \( \theta \). See App. E for details on the implementation of the estimators. We present the results for conditional modelling in Tab. 1 and Fig. 6, and for unconditional modelling in Tab. 2 and Fig. 7; see App. G for more experimental results.

**Estimators for the variational parameters \( \phi \).** First, we evaluate the choice of estimator for the parameters of \( q_\phi(z) \). Like Tucker et al. (2019) for the single layer case, we find that our extension of DREGs to hierarchical models leads to a dramatic reduction in gradient variance for the variational posterior parameters \( \phi \) on all tasks (third column in Figs. 6 and 7), which translates to an improved test objective in all cases considered. DREGs is unbiased and typically outperforms the (biased) STL estimator. We also observed similar improvements on the training objective.

**Estimators for the prior parameters \( \theta \).** Second, we consider the estimators for the \( \theta \) parameters of the prior \( p_\theta(z) \). Using the DREGs estimator instead of the naive IWAE estimator consistently improves the train and test objective when combined with any estimator for the variational posterior, especially for conditional image modelling with deeper models. For unconditional image modelling the improvements are only marginal, though using DREGs never hurts. In terms of gradient variance for the prior parameters \( \theta \), DREGs consistently performs better in the beginning of

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**Figures:**

- **Figure 4**: Average gradient variance (left) and signal-to-noise ratio (SNR) (right) for the proposal parameters \( \phi \) (top) and the prior parameters \( \theta \) (bottom).

- **Figure 5**: Model specification and 2-layer example for conditional and unconditional image modelling.
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| estimator $\nabla^T_{TD} \theta$ | IWAЕ | GDREGs | IWAЕ | IWAЕ | IWAЕ | GDREGs |
|--------------------------------|------|--------|------|------|------|--------|
| MNIST 1 layer                   | −38.77 ± 0.01 | −38.71 ± 0.02 | −38.76 ± 0.03 | −38.68 ± 0.03 | −38.50 ± 0.01 | −38.44 ± 0.01 |
| 2 layer                         | −38.55 ± 0.02 | −38.42 ± 0.03 | −38.24 ± 0.02 | −38.14 ± 0.02 | −38.20 ± 0.01 | −38.02 ± 0.02 |
| 3 layer                         | −38.63 ± 0.01 | −38.44 ± 0.02 | −38.20 ± 0.01 | −38.10 ± 0.02 | −38.20 ± 0.01 | −38.04 ± 0.01 |
| Omniglot 1 layer                | −55.84 ± 0.02 | −55.66 ± 0.03 | −55.80 ± 0.05 | −55.62 ± 0.05 | −55.34 ± 0.02 | −55.24 ± 0.02 |
| 2 layer                         | −55.27 ± 0.03 | −54.98 ± 0.03 | −54.66 ± 0.03 | −54.28 ± 0.02 | −54.73 ± 0.02 | −54.36 ± 0.03 |
| 3 layer                         | −55.35 ± 0.02 | −54.93 ± 0.03 | −54.64 ± 0.04 | −54.21 ± 0.03 | −54.72 ± 0.02 | −54.28 ± 0.02 |
| FMNIST 1 layer                  | −102.82 ± 0.02 | −102.80 ± 0.02 | −102.99 ± 0.02 | −102.88 ± 0.02 | −102.61 ± 0.01 | −102.58 ± 0.01 |
| 2 layer                         | −102.74 ± 0.02 | −102.68 ± 0.01 | −102.65 ± 0.02 | −102.48 ± 0.03 | −102.40 ± 0.01 | −102.30 ± 0.02 |
| 3 layer                         | −102.86 ± 0.01 | −102.71 ± 0.01 | −102.68 ± 0.02 | −102.42 ± 0.02 | −102.46 ± 0.01 | −102.26 ± 0.01 |

Table 1: Test objective values (higher is better) on conditional image modelling with a VAE model trained with IWAЕ. Higher is better; errorbars denote ±1.96 standard errors ($\sigma/\sqrt{5}$) over 5 reruns.

Figure 6: Conditional image modelling of MNIST with a VAE with 1 layer (top) and 2 layers (bottom). Shaded areas denote ±1.96 standard deviations $\sigma$ over 5 reruns.

training, when it always has lower variance. However, later in training this is only consistently true when also using the DREGs estimator for the variational posterior parameters $\phi$. We hypothesize that the GDREGs estimator yields larger improvements for conditional modelling because the prior and posterior distribution are closer to each other due to the conditioning, and we saw that GDREGs works particularly well in this case for Gaussian distributions, also see App. H. To quantify this “closeness” we compared the KL of the variational posterior to the prior on the same dataset and found it to be about twice as large for unconditional modelling than for conditional modelling, see App. G.

We also note that the gradient variance for the prior parameters $\theta$ is higher when using the DREGs estimator for the variational posterior parameters $\phi$, compared to the naive IWAЕ estimator (compare orange and blue lines in the middle column of Figs. 6 and 7). This is an indirect effect of altered learning dynamics. We suspect that better posterior gradient estimates with DREGs lead to generative models that fit the data better, which in turn results in larger gradient variance for the prior. This effect is absent in the illustrative example in Fig. 4 because we evaluate the gradient variance on the same fixed model for all estimators. In App. G.3 we compare the estimators offline for different combinations of estimators during training. The results are in line with our online results in this section: for the gradients of the variational posterior the DREGs estimator always has lower variance than the naive (IWAЕ) estimator; for the gradients of the prior the GDREGs estimator typically has lower variance, though in some cases only in the beginning of training.

6. Related work

Roeder et al. (2017) observed that the reparameterization gradient estimator for the ELBO contains a score function term and proposed the STL estimator that simply drops this term to reduce the estimator variance. They considered
hierarchical ELBO models but do not discuss how to treat indirect score functions. While the STL estimator is unbiased for the ELBO objective, Tucker et al. (2019) showed that it is biased for more general objectives such as the IWAE. They proposed the DREGs estimator that yields unbiased and low variance gradients for IWAE and resolves the diminishing signal-to-noise issue of the naive IWAE gradients first discussed by Rainforth et al. (2018). We extend DREGs to hierarchical models, discuss how to treat the indirect score functions, and generalize it to general score functions by introducing GDRGs.

Several classic techniques from the variance reduction literature have been applied to variational inference and reparameterization. For example, Miller et al. (2017) and Geffner & Domke (2020) proposed control variates for reparameterization gradients; Ruiz et al. (2016) used importance sampling with a proposal optimized to reduce variance. Such approaches are orthogonal to methods such as (G)DREGs and STL, and can be combined with them for greater variance reduction (Agrawal et al., 2020).

### 7. Conclusion

In this paper we generalized the recently proposed doubly-reparameterized gradients (DREGs, Tucker et al. (2019)) estimator for variational objectives in two ways. First, we showed that for hierarchical models such as VAEs seemingly pathwise gradients can actually contain score functions, and how to consistently and effectively extend DREGs in this case. Second, we introduced GDRGs, a doubly-reparameterized gradient estimator that applies to general score functions, while DREGs is limited to score functions of the variational distribution. Finally, we demonstrated that both generalizations can improve performance on conditional and unconditional image modelling tasks.

While we present and discuss the GDRGs estimator in the context of deep probabilistic models, it applies generally to score function gradients of the form $\mathbb{E}_{q_\phi(z)}[\nabla_\theta \log p_\theta(z)]$. Applying it to other problem settings of this type such as normalizing flows is an exciting area of future research.

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Appendix to Generalized Doubly-Reparameterized Gradient Estimators

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A. Derivation of the GDREgs identity

Here, we detail the derivation of our main result, the GDREgs identity (Eq. (16)), which we restate here.

\[
\mathbb{E}_{z \sim q_{\phi}(z)}[g_{\phi, \theta}(z) \nabla_\theta \log p_{\theta}(z)] = \mathbb{E}_{z \sim q_{\phi}(z)} \left[ \left( g_{\phi, \theta}(z) \nabla^T_{\theta} \log \frac{q_{\phi}(z)}{p_{\theta}(z)} + \nabla_{\theta} \log p_{\theta}(z) \right) \nabla_{\theta} T_p(\tilde{e}; \theta) |_{\tilde{e} = T_p^{-1}(z, \theta)} \right]
\] (16)

We can derive this identity in two ways: (1) through a reweighting correction as presented in the main paper, see App. A.1; (2) through a flow-like transformation of \( z \sim q_{\phi}(z|x) \), see App. A.2.

A.1. Derivation via reweighting

In the main paper (Sec. 4), we explained that we need to make the sampling path of \( z \) depend on the parameters \( \theta \) to replace the score function \( \nabla_\theta \log p_{\theta}(z) \) with a pathwise derivative. At the same time, we evaluate the objective on samples \( z \) from the variational posterior \( q_{\phi}(z|x) \) during training. The derivation consists of the following three steps:

1. Temporarily change the path such that it depends on \( \theta \). We change the path by first using importance sampling reweighting to temporarily re-write the expectation, \( \mathbb{E}_{q_{\phi}(z)}[\cdot] = \mathbb{E}_{p_{\theta}(z)} \left[ \frac{q_{\phi}(z)}{p_{\theta}(z)} \cdot \right] \) (step (\( \Theta \))), and then by employing reparameterization on \( p_{\theta}(z) \): \( z = T_p(\tilde{e}; \theta) \) with \( \tilde{e} \sim p(\tilde{e}) = \mathcal{N}(0, I) \) (step (\( \Theta \))).
2. Perform the gradient computation and collect all the terms.
3. Change the path back by un-doing the reparameterization and the reweighting so we can use samples \( z \sim q_{\phi}(z|x) \) to estimate the expectation.

\[
\nabla^T_{\theta} \mathbb{E}_{q_{\phi}(z)}[g_{\phi, \theta}(z)] \stackrel{(1)}{=} \nabla^T_{\theta} \mathbb{E}_{p_{\theta}(z)} \left[ \frac{q_{\phi}(z)}{p_{\theta}(z)} g_{\phi, \theta}(z) \right] \stackrel{(2)}{=} \nabla^T_{\theta} \mathbb{E}_{p(\tilde{e})} \left[ \frac{q_{\phi}(T_p(\tilde{e}; \theta))}{p_{\theta}(T_p(\tilde{e}; \theta))} g_{\phi, \theta}(T_p(\tilde{e}; \theta)) \right] \\
\mathbb{E}_{p(\tilde{e})} \left[ \nabla_{\theta} T_p(\tilde{e}; \theta) \right] \frac{q_{\phi}(z)}{p_{\theta}(z)} g_{\phi, \theta}(z) \nabla_{\theta} \log p_{\theta}(z) \right|_{z = T_p(\tilde{e}; \theta)} \right]
\] (A.1)

\[
\mathbb{E}_{q_{\phi}(z)} \left[ \left( g_{\phi, \theta}(z) \nabla^T_{\theta} \log \frac{q_{\phi}(z)}{p_{\theta}(z)} + \nabla_{\theta} \log p_{\theta}(z) \right) \nabla_{\theta} T_p(\tilde{e}; \theta) |_{\tilde{e} = T_p^{-1}(z, \theta)} + \nabla_{\theta} g_{\phi, \theta}(z) - g_{\phi, \theta}(z) \nabla_{\theta} \log p_{\theta}(z) \right]
\] (A.3)
In the derivation we have used the identity \( x \nabla_x \log x = \nabla_x x \) repeatedly. By noting that \( \nabla^\text{TD}_\theta \mathbb{E}_{q_\theta(z)} \left[ g_{\theta,\theta}(z) \right] = \mathbb{E}_{q_\theta(z)} \left[ \nabla_\theta g_{\theta,\theta}(z) \right] \), we can cancel these terms on the left hand side of Eq. (A.1) and right hand side of Eq. (A.3). By moving \(- \mathbb{E}_{q_\theta(z)} \left[ g_{\theta,\theta}(z) \nabla_\theta \log p_\theta(z) \right]\) to the other side we obtain the desired result.

A.2. Derivation via flow-like transformation

Here we provide a second derivation of the GDREGs identity (Eq. (16)) that does not explicitly use a re-weighting of the expectation as in App. A.1, but uses flow-like transformations instead (Rezende & Mohamed, 2015). We already noted in the main text that we can interpret the change of paths as a flow \( z \to \tilde{\epsilon} \to z \), where \( \tilde{\epsilon} \) follows a more complicated distribution than the original \( \epsilon \) that might have been used to reparameterize samples \( z \) from \( q_{\phi}(z|x) \). Here, we make this connection to normalizing flows more explicit.

We make use of the usual change of probability density formula for flows (see, e.g., Rezende & Mohamed (2015)):

\[
y = f(x); x \sim p_x(x) \implies p_y(y) = p_x(x) |\nabla_x f(x)|^{-1}.
\]

(A.4)

Our main insight is that we can reparameterize \( z \sim q_{\phi}(z|x) \) in many different ways. Usually we sample an independent noise variable from a simple base distribution, for example, \( \epsilon \sim q(\epsilon) = \mathcal{N}(0, I) \), and use it to reparameterize \( z \) as \( z = T_\theta(q(\epsilon)) \). However, we can equally use a different base distribution \( \tilde{q}(\tilde{\epsilon}) \) and reparameterize \( z \) as \( z = T_\theta(\tilde{\epsilon}, \theta), \tilde{\epsilon} \sim \tilde{q}(\tilde{\epsilon}) \). Note that we reparameterize using \( p_\theta(z) \) in this case. In order for \( z \) still to be distributed according to \( q_{\phi}(z|x) \), we have to choose \( \tilde{q}(\tilde{\epsilon}) \) to be itself given by the normalizing flow \( \tilde{\epsilon} = T_\theta^{-1}(z; \theta) \), \( z \sim q_{\phi}(z) \), such that \( \tilde{q}(\tilde{\epsilon}) = \tilde{q}(\tilde{\epsilon}; \theta) \). It may appear counter-intuitive to transform \( z \) as \( z \to \tilde{\epsilon} \to z \) because we are doing and then undoing a transformation; however, it allows us to make the computation path depend on \( \theta \) when computing the gradients. We then separate the forward flow \( z = T_\theta(\tilde{\epsilon}; \theta) \) and the backward flow \( \tilde{\epsilon} = T_\theta^{-1}(z; \theta) \) by moving the forward flow into the path through reparameterization and the backward flow into the integration measure, see Eq. (A.7) below. To move the backward flow into the integration measure, we express \( \tilde{q}(\tilde{\epsilon}) \) as a change of density:

\[
\tilde{\epsilon} = T_\theta^{-1}(z; \theta), z \sim q_{\phi}(z|x) \implies \tilde{q}(\tilde{\epsilon}) = q_{\phi}(z) |\nabla_z T_\theta^{-1}(z; \theta)|^{-1}
\]

(A.5)

Note that \( \tilde{q}(\tilde{\epsilon}) \) is different from \( q(\epsilon) = \mathcal{N}(0, I) \) typically used to reparameterize samples of the approximate posterior \( z = T_\theta(\epsilon; \phi) : \epsilon \sim q(\epsilon) \). Using the change of density in Eq. (A.5) together with reparameterization as described above, we can re-write the following expectation over \( z \) as an integral over \( \tilde{\epsilon} \):

\[
\int q_{\phi}(z) g_{\theta,\theta}(z) d\epsilon = \int \tilde{q}(\tilde{\epsilon}) g_{\theta,\theta}(T_\theta(\tilde{\epsilon}; \theta)) d\tilde{\epsilon} = \int \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} \right]_{z = T_\theta(\tilde{\epsilon}; \theta)} g_{\theta,\theta}(T_\theta(\tilde{\epsilon}; \theta)) d\tilde{\epsilon}
\]

(A.6)

where reparameterization and change of density.

In the these integrals, \( \tilde{\epsilon} \) is an independent variable; its dependence on \( \theta \) has been moved into the path \( g_{\theta,\theta}(T_\theta(\tilde{\epsilon}; \theta)) \) as well as the change of density (Eq. (A.5)). This is one way to understand where the stop_gradient in Figs. 2 and 3 comes from.

To derive the GDREGs identity, we take the total derivative of Eq. (A.7) w.r.t. \( \theta \) and apply the chain- and product rule

\[
\nabla^\text{TD}_\theta \int q_{\phi}(z) g_{\theta,\theta}(z) \, dz = A^7 \nabla^\text{TD}_\theta \int \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} \right]_{z = T_\theta(\tilde{\epsilon}; \theta)} g_{\theta,\theta}(T_\theta(\tilde{\epsilon}; \theta)) \, d\tilde{\epsilon}
\]

(A.8)

\[
= \int \nabla^\text{TD}_\theta \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} g_{\theta,\theta}(z) \right]_{z = T_\theta(\tilde{\epsilon}; \theta)} \, d\tilde{\epsilon}
\]

(A.9)

\[
= \int \nabla^\text{TD}_z \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} g_{\theta,\theta}(z) \right]_{z = T_\theta(\tilde{\epsilon}; \theta)} \nabla_{\theta} T_\theta(\tilde{\epsilon}; \theta) + \nabla_{\theta} \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} g_{\theta,\theta}(z) \right]_{z = T_\theta(\tilde{\epsilon}; \theta)} \, d\tilde{\epsilon}
\]

(A.10)

\[
= \int \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} \right] \left( g_{\theta,\theta}(z) \nabla^\text{TD}_\theta \log \left( q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} \right) + \nabla^\text{TD}_z g_{\theta,\theta}(z) \right)_{z = T_\theta(\tilde{\epsilon}; \theta)} \nabla_{\theta} T_\theta(\tilde{\epsilon}; \theta) + \left[ q_{\phi}(z) \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} \right] \left( g_{\theta,\theta}(z) \nabla_{\theta} \log \left| \nabla_z T_\theta^{-1}(z; \theta) \right|^{-1} + \nabla_{\theta} g_{\theta,\theta}(z) \right)_{z = T_\theta(\tilde{\epsilon}; \theta)} \, d\tilde{\epsilon}
\]

(A.11)
where we have separated out the derivatives and used \( x \nabla_s \log x = \nabla_s x \). We can now further separate terms and undo the change of density to replace \( q_\phi(z) \left| \nabla_z T_p^{-1}(z; \theta) \right|^{-1} \) with \( \overline{q}(\epsilon) \) (Eq. (A.5)) after taking the derivatives. We obtain

\[
\nabla_T^\theta \int q_\phi(z) g_\phi, \theta(z) dz = \int \overline{q}(\epsilon) \left\{ \nabla_T^\theta \left[ \log q_\phi(z) + \log \left| \nabla_z T_p^{-1}(z; \theta) \right|^{-1} \right] g_\phi, \theta(z) \right|_{z = T_p(\epsilon; \theta)} \nabla_\theta T_p(\epsilon; \theta) + \nabla_T^2 g_\phi, \theta(z) \right|_{z = T_p(\epsilon; \theta)} \nabla_\theta T_p(\epsilon; \theta) + \nabla_\theta g_\phi, \theta(z) \right|_{z = T_p(\epsilon; \theta)} \nabla_\theta \log \left| \nabla_z T_p^{-1}(z; \theta) \right|_{z = T_p(\epsilon; \theta)} \right\} d\epsilon. \tag{A.12}
\]

To evaluate the gradients of the log Jacobians, \( \nabla_* \log \left| \nabla_z T_p^{-1}(z; \theta) \right| \), we can combine the log Jacobians with a simple base distribution \( q(\epsilon) \) to obtain \( p_\theta(z) \) because

\[
z = T_p(\epsilon; \theta); \epsilon \sim q(\epsilon) = \mathcal{N}(0, 1) \quad \Rightarrow \quad p_\theta(z) = q(\epsilon) \left| \nabla_z T_p^{-1}(z; \theta) \right| \tag{A.14}
\]

through reparameterization of \( p_\theta(z) \) and by noting that

\[
\nabla_* \log (f(x) \cdot c) = \nabla_* \log (f(x)) \quad \text{if } c \text{ is constant w.r.t. } \ast \tag{A.15}
\]

and that the simple base distribution \( q(\epsilon) \) is constant w.r.t. all gradients:

\[
\nabla_* \log \left| \nabla_z T_p^{-1}(z; \theta) \right|_{q(\epsilon)} = \nabla_* \log \left( \left| \nabla_z T_p^{-1}(z; \theta) \right| q(\epsilon) \right) = \nabla_* \log p_\theta(z). \tag{A.16}
\]

This allows us to simplify Eq. (A.13) as

\[
\nabla_T^\theta \int q_\phi(z) g_\phi, \theta(z) dz = \int q_\phi(z) \left\{ \left( g_\phi, \theta(z) \nabla_T^\theta \log \frac{q_\phi(z)}{p_\theta(z)} + \nabla_T^2 g_\phi, \theta(z) \right) \nabla_\theta T_p(\epsilon; \theta) \right|_{\epsilon = T_p^{-1}(z; \theta)} + \nabla_\theta g_\phi, \theta(z) \nabla_\theta \log p_\theta(z) \right\} dz, \tag{A.17}
\]

which is identical to Eq. (A.3) and yields the GDREGs identity as explained above.

**B. Derivation of the GDREGs estimator for the IWAE objective**

In this section we apply the GDREGs identity derived above to derive the GDREGs estimator for the IWAE objective, Eq. (22) in the main paper.

**B.1. Preliminaries on the IWAE objective**

The importance weighted autoencoder (IWAE) objective is given by

\[
\mathcal{L}^{\text{IWAE}}_{\phi, \theta} = \mathbb{E}_{z \sim q_\phi(z_k|x)} \left[ \log \left( \frac{1}{K} \sum_{k=1}^{K} w_k \right) \right]. \tag{B.1}
\]

where \( w_k \) are the importance weights (Burda et al., 2016).

Due to the structure of the IWAE objective, any gradient w.r.t. any of its parameters can be written as

\[
\nabla_* \mathcal{L}^{\text{IWAE}}_{\phi, \theta} = \mathbb{E}_{\epsilon \sim q(\epsilon)} \left[ \sum_{k=1}^{K} \frac{w_k}{\bar{w}_k} \nabla_* \log w_k \right], \quad \bar{w}_k = \frac{w_k}{\sum_j w_j} \tag{B.2}
\]

using the chain rule and \( \nabla_* w_k = \bar{w}_k \nabla_* \log w_k \). \( \bar{w}_k \) are the normalized importance weights, and we have reparameterized \( z_k \) as \( T_\phi(\epsilon_k; \Phi) \). Typically, the derivatives we are interested in are w.r.t. the parameters \( \phi \) and \( \theta \).
We also note the following identity that we use in the derivation of the doubly reparameterized estimators,

\[ \nabla_{z} \tilde{w}_k = (\tilde{w}_k - \tilde{w}_k^2) \nabla_{z} \log w_k \]

(B.3)

which follows from applying the chain-rule and using \( \nabla_{z} w_k = w_k \nabla_{z} \log w_k \).

Tucker et al. (2019) derive the DREGs identity (Eq. (9)) and use it to derive the following doubly-reparameterized gradient estimator (DREGs) w.r.t. the approximate posterior parameters \( \phi \) as:

\[
\hat{\nabla}_{\phi}^{DREGs} L_{IWAE} = \sum_{k=1}^{K} \tilde{w}_k \nabla_{z} \log w_k \nabla_{\phi} T_{q}(\epsilon_k; \phi), \quad \epsilon_{1:K} \sim q(\epsilon) \tag{B.4}
\]

B.2. Derivation of the GDREGs estimator

Similarly, we can derive a generalized doubly-reparameterized gradient (GDREGs) estimator w.r.t. the prior parameters \( \theta \). We use the GDREGs identity (Eq. (16)) derived above with \( g_{\phi}(z) = \tilde{w}_k \) and note that the reweighting term \( \log \frac{q_{\phi}(z)}{p_{\theta}(z)} \) looks like a log importance weight except for the missing likelihood:

\[
\nabla_{\theta}^{\phi} L_{IWAE} = E_{z_{1:K} \sim q_{\phi}(z_{1:K}|x)} \left[ \sum_{k=1}^{K} \tilde{w}_k \nabla_{\theta} \log w_k \right] = E_{z_{1:K} \sim q_{\phi}(z_{1:K}|x)} \left[ \sum_{k=1}^{K} \tilde{w}_k \nabla_{\theta} \log p_{\theta}(z) \right] \tag{B.5}
\]

\[
= E_{z_{1:K} \sim q_{\phi}(z_{1:K}|x)} \left[ \sum_{k=1}^{K} \left( \tilde{w}_k \nabla_{z} \log \frac{q_{\phi}(z_{k}|x)}{p_{\theta}(z_{k})} + \tilde{w}_k^{2} \nabla_{z} \log w_k \right) \right] \tag{B.6}
\]

\[
= E_{z_{1:K} \sim q_{\phi}(z_{1:K}|x)} \left[ \sum_{k=1}^{K} \left( \tilde{w}_k \nabla_{z} \log p(x|z_{k}) - \tilde{w}_k^{2} \nabla_{z} \log w_k \right) \right] \tag{B.7}
\]

Thus, the GDREGs estimator is given by:

\[
\hat{\nabla}_{\theta}^{GDREGs} L_{IWAE} = \sum_{k=1}^{K} \left( \tilde{w}_k \nabla_{z} \log p(x|z_{k}) - \tilde{w}_k^{2} \nabla_{z} \log w_k \right) \nabla_{\theta} T_{p}(\tilde{\epsilon}_{k}; \theta)|_{\tilde{\epsilon}_{k} = \tau_{p}^{-1}(z_{k}; \theta)} \quad z_{1:K} \sim q_{\phi}(z_{1:K}|x). \tag{22}
\]

Note that the \( z_{k} \) are sampled from \( q_{\phi}(z_{k}|x) \) but re-expressed as if they came from \( p_{\theta}(z) \).

We can rewrite the importance weights as

\[
w_k = \frac{p_{\theta}(z_{k})p(x|z_{k})}{q_{\phi}(z_{k}|x)} = \frac{q_{\phi}(z_{k}|x)}{q_{\phi}(z_{k}|x)}, \tag{B.9}
\]

Thus, if the variational posterior \( q_{\phi}(z_{k}|x) \) is equal to the true posterior \( p_{\theta}(z_{k}|x) \), all weights \( w_k \) become equal to \( p_{\theta}(z) \) and thus constant w.r.t. \( z_{k} \). In that case the second term in the GDREGs estimator Eq. (22) vanishes and the overall expression simplifies to

\[
\hat{\nabla}_{\theta}^{GDREGs} L_{IWAE} = \sum_{k=1}^{K} \tilde{w}_k \nabla_{\theta} T_{p}(\tilde{\epsilon}_{k}; \theta)|_{\tilde{\epsilon}_{k} = \tau_{p}^{-1}(z_{k}; \theta)}, \quad z_{1:K} \sim q_{\phi}(z_{k}|x) \tag{B.10}
\]

In contrast, the usual IWAE gradient involves the score function for \( p_{\theta}(z_{k}) \):

\[
\hat{\nabla}_{\theta}^{\text{h ave}} L_{IWAE} = \sum_{i=1}^{K} \tilde{w}_k \nabla_{\theta} \log p_{\theta}(z_{k}), \quad z_{1:K} \sim q_{\phi}(z_{k}|x). \tag{B.11}
\]
C. Derivation of the DREGs and GDREGs estimator for IWAE objectives of hierarchical VAEs

In this section we derivations of and further details on the extension of DREGs and GDREGs to hierarchical VAEs with the IWAE objective.

C.1. Preliminaries and notation for the hierarchical IWAE objective

For a hierarchically structured model with $L$ stochastic layers the IWAE objective is still given by Eq. (B.1) but with importance weights $w_k$ given by

$$w_k = p_k(x|z_k;...)p_\theta(z_k;...) \frac{q_\phi(z_{k1};...,z_{KL})}{q_\phi(z_k;...)}. \quad \text{(C.1)}$$

Here, $z_{kl}$ denotes the $k$th importance sample ($k \in \{1,\ldots,K\}$) for the $l$th layer ($l \in \{1,\ldots,L\}$). Both the variational posterior and the prior distribution factorize according to their respective hierarchical structure. While the prior factorizes top-down in most cases, the variational posterior can have many different structures. In order for the distributions to be valid in the context of a VAE, we require the individual dependency graphs for the prior (generative path) and the variational posterior (inference path) to be directed acyclic graphs. Cycles would mean that a latent variable conditionally dependent on itself. To keep the dependency structure general, we write the factorization of the variational posterior and prior as follows:

$$q_\phi(z_{k1};...,z_{KL}|x) = \prod_{l=1}^{L} q_{\phi_l}(z_{kl}|\text{pa}_\alpha(l),x) = \prod_{l=1}^{L} q_{\phi_l}(\text{pa}_\alpha(l);\phi_l)(z_{kl}) \quad \text{(C.2)}$$

$$p_\theta(z_{k1};...,z_{KL}) = \prod_{l=1}^{L} p_{\theta_l}(z_{kl}|\text{pa}_\beta(l)) = \prod_{l=1}^{L} p_{\theta_l}(\text{pa}_\beta(l);\theta_l)(z_{kl}) \quad \text{(C.3)}$$

Here, $\alpha_l(\cdot;\phi_l)$ and $\beta_l(\cdot;\theta_l)$ are the distribution parameters of the variational posterior and prior distribution in the $l$th layer, respectively, and we have made the dependencies of the conditional distributions explicit; $\text{pa}_\alpha(l)$ denotes the “parents” of the latent variable $z_{kl}$ according to the dependency graph of the inference path (the factorization of the posterior); similarly, $\text{pa}_\beta(l)$ denotes the latent variables that $z_{kl}$ directly depends on according to the factorization of the prior $p_\theta$. Typically, the prior is assumed to factorize top-down, such that $\text{pa}_\beta(l) = z_{k(l+1)}$ for all but the top-most layer.

The samples $z_{kl}$ are drawn from the variational posterior and can be expressed through reparameterization as $z_{kl} = \mathcal{T}_q(\epsilon_{kl};\alpha_l(\text{pa}_\alpha(l),\phi_l))$, where $\epsilon_{kl}$ is an independent noise variable per importance sample and layer.

We note that it is these dependencies of the distribution parameters $\alpha_l$ and $\beta_l$ on $\text{pa}_\alpha(l)$ and $\text{pa}_\beta(l)$, respectively, that give rise to the indirect score functions as discussed in Sec. 3.

C.2. Derivation of the hierarchical DREGs estimator for IWAE

With notation fully set up we consider the reparameterized gradients of the IWAE objective w.r.t. the variational parameters in a particular stochastic layer $\phi_l$:

$$\nabla_{\phi_l}^\text{TD}_{\text{IWAE}} = \mathbb{E}_{e_1,k\sim q(e)} \left[ \sum_{k=1}^{K} \bar{w}_k \nabla_{\phi_l}^\text{TD} \log w_k \right] \quad \text{(C.4)}$$

$$= \mathbb{E}_{e_1,k\sim q(e)} \left[ \sum_{k=1}^{K} \bar{w}_k \left( \nabla_{z_{kl}}^\text{TD} \log w_k \nabla_{\phi_l} \mathcal{T}_q(\epsilon_{kl};\alpha_l(\text{pa}_\alpha(l),\phi_l)) + \nabla_{\phi_l} \log w_k \right) \right] \quad \text{(C.5)}$$

where we have used the chain-rule to arrive at Eq. (C.5); the first term contains both the (true) pathwise gradients as well as the indirect score functions; the second term only contains a direct score function as we only take the partial derivative w.r.t. $\phi_l$.

We can rewrite this direct score function gradient because only one term in the (log-)importance weight directly depends on $\phi_l$,

$$\nabla_{\phi_l} \log w_k = -\nabla_{\phi_l} \log q_{\alpha_l(\text{pa}_\alpha(l);\phi_l)}(z_{kl}). \quad \text{(C.6)}$$
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Applying the DREGs identity to this term and using Eq. (B.3) yields:

\[
E_{\epsilon_1:K \sim q(\epsilon)} \left[ \sum_{k=1}^{K} \tilde{w}_k \nabla_{\phi_l} \log w_k \right] = -E_{\epsilon_1:K \sim q(\epsilon)} \left[ \sum_{k=1}^{K} (\tilde{w}_k - \bar{w}_k) \nabla_{\phi_l} \log w_k \nabla_{\phi_l} T_{q_l} (\epsilon_{kl}; \alpha_l(pa_{\alpha_l}(l), \phi_l)) \right] \tag{C.7}
\]

which agrees with the first term in Eq. (C.5) up to the prefactor. Thus, both the true pathwise gradients as well as the indirect score functions appear twice and the prefactors partly cancel to give rise to the DREGs estimator for hierarchical IWAE objectives:

\[
\hat{\psi}_{\phi_l}^{\text{DREGs for hierarchical IWAE objectives}} = \sum_{k=1}^{K} \tilde{w}_k \nabla_{\phi_l} \log w_k \nabla_{\phi_l} T_{q_l} (\epsilon_{kl}; \alpha_l(pa_{\alpha_l}(l), \phi_l)) \quad \epsilon_1:K \sim q(\epsilon) \tag{C.8}
\]

where \( z_{kl} = T_{q_l}(\epsilon_{kl}; \alpha_l(pa_{\alpha_l}(l), \phi_l)) \), \( \forall l \in \{1, \ldots, L\}, \forall k \in \{1, \ldots, K\} \) through reparameterization.

We emphasize that the total derivative w.r.t. \( z_{kl} \) contains pathwise gradients as well as indirect score functions for both the variational posterior as well as for the prior. The hierarchical DREGs estimator otherwise looks very similar to the DREGs estimator in the single layer case (Tucker et al., 2019).

In App. E.1 we explain how to implement this estimator effectively and in a structure-agnostic way. That is, we do not have to derive a new estimator for each new dependency graph of the variational posterior or the prior.

C.3. Derivation of the hierarchical GDREGs estimator for IWAE

Next, we derive the expression for the GDREGs estimator for hierarchical VAEs with IWAE objective.

Applying the DREGs identity entails re-expressing the samples \( z_{kl} \) from the variational posterior as if they were sampled from the prior. Starting form a sample \( (z_{k1}, \ldots, z_{KL}) \sim q_\phi(z_1, \ldots, z_L|x) \), we use the inverse flow of \( \rho_\theta \) to obtain new noise variables for each layer, \( (\epsilon_{k1}, \ldots, \epsilon_{KL}) \). We then use the forward flow of \( \rho_\theta \) to obtain back \( (z_{k1}, \ldots, z_{KL}) \) but with the gradient path now depending on \( \theta \) as discussed in App. A and Sec. 4.

More precisely, we find that

\[
z_{k1}^{(q)} = T_{q_{kl}} (\epsilon_{kl}; \alpha_l(pa_{\alpha_l}(l), \phi_l)) \quad \text{original sampling of } (z_{k1}, \ldots, z_{KL}) \sim q_\phi(z_1, \ldots, z_L|x) \tag{C.9}
\]

\[
\epsilon_{kl} = T_{\rho_\theta^{-1}} \left( z_{k1}^{(q)} ; \beta_l(pa_\beta(l), \theta_l) \right) \quad \text{inverse prior flow to obtain new "noise" variables} \tag{C.10}
\]

\[
z_{kl} = T_{\rho_\theta} (\epsilon_{kl}; \beta_l(pa_\beta(l), \theta_l)) \quad \text{forward prior flow to re-express the } z_{kl} \tag{C.11}
\]

where \( \epsilon_{kl} \sim q(\epsilon) \) follows a simple distribution that is different from the more complicated distribution of \( \epsilon_{kl} \). Note how the initial reparameterization of a sample \( z_{kl} \) depends on the dependency structure of the variational posterior (through \( pa_{\alpha_l}(\cdot) \)), while the other transformations depend on the dependency structure of the prior (\( pa_\beta(\cdot) \)).

As for DREGs, we note that only one term in the log importance weight directly depends on the variable \( \theta_l \),

\[
\nabla_{\theta_l} \log w_k = \nabla_{\theta_l} \log p_{\beta_l(pa_{\beta_l}(l); \theta_l)}(z_{kl}). \tag{C.12}
\]

With these prerequisites, we can compute the GDREGs estimator for parameters \( \theta_l \) of the \( l \)th stochastic layer.

\[
\nabla_{\theta_l} \psi_{\phi_l}^{\text{DREGs for hierarchical IWAE objectives}} = E_{z_{1:K} \sim q_\phi(z|x)} \left[ \sum_{k=1}^{K} \tilde{w}_k \nabla_{\theta_l} \log w_k \right] \tag{C.13}
\]

\[
\overset{C.12}{=} E_{z_{1:K} \sim q_\phi(z|x)} \left[ \sum_{k=1}^{K} \tilde{w}_k \nabla_{\theta_l} \log p_{\beta_l(pa_{\beta_l}(l); \theta_l)}(z_{kl}) \right] \tag{C.14}
\]

\[
\overset{16}{=} E_{z_{1:K} \sim q_\phi(z|x)} \left[ \sum_{k=1}^{K} \left( \tilde{w}_k \nabla_{z_{kl}} \log q_\phi(z_{k1}, \ldots, z_{KL}|x) \cdot \frac{p_\theta(z_{k1}, \ldots, z_{KL})}{p_\theta(z_{k1}, \ldots, z_{KL})} \right) + (\tilde{w}_k - \bar{w}_k) \nabla_{z_{kl}} \log w_k \nabla_{\theta_l} T_{\rho_\theta} (\epsilon_{kl}; \theta_l) |_{\epsilon_{kl} = T_{\rho_\theta^{-1}}(z_{kl}; \theta_l)}} \right] \tag{C.15}
\]
where we suppressed dependencies on \( p_{\alpha^*}(l) \) where they are not necessary to simplify notation.

The estimator looks very similar to the GDREgs estimator for a single layer IWAE model Eq. (22). Note that just like above for hierarchical DREgs, the total gradients w.r.t. \( z_{kl} \) give rise to both (true) pathwise gradients as well as indirect score functions through the hierarchical dependencies of the variational posterior and prior.

In App. E.2 we show how to implement the hierarchical GDREgs estimator Eq. (C.16) effectively and in a way that is agnostic to the structure of the model. That is, we do not have to derive a separate estimator for every dependency graph of the variational posterior and prior.

### C.4. Double reparameterization and indirect score functions

In principle, we could apply double-reparameterization to the indirect score functions as well. However, as we explain now, we often cannot doubly-reparameterize all indirect score functions; moreover, even in cases where this is possible, it is still impractical, as the corresponding estimator depends on the exact model structure and would require adaptation to each dependency graph of the prior and variational posterior.

Double reparameterization of indirect score functions works in the same way as for the direct score functions except that \( g_{\phi, \theta}(z) \) is given by \( \tilde{w}_k^2 \) instead of \( \tilde{w}_k \) in this case. The derivatives of \( \tilde{w}_k^2 \) have a similar reproducing property as we observed in Eq. (B.3):

\[
\nabla_{z} \tilde{w}_k^2 = 2(\tilde{w}_k^2 - \tilde{w}_k^3) \nabla_{z} \log w_k.
\]

Thus, double reparameterization of the indirect score functions similarly gives rise to further indirect score functions. We note that these indirect score functions only appear for the “children” of the current stochastic layer, that is, stochastic variables in those layers that depend on the current layer. In this context, “children” refers to all children w.r.t. the dependency structure of both, the variational posterior and the prior. For a particular layer \( l \) we obtain indirect score functions from double reparameterization of all of its (direct or indirect) parent nodes. Following the dependency structure, we could collect all of these terms and reparameterize them to obtain pathwise gradients only.

However, a problem arises, because we need to account for dependencies of both the variational posterior and the prior. Reparameterization of a score function gives rise to indirect score functions in all its “children” layers for both the variational posterior and the prior. For general hierarchical structures, this leads to cycles, in that some of the children of one dependency tree (the variational posterior) are the parents in the other (the prior) and/or vice versa. In this case we are never able to collect all the terms and fully reparameterize all the score functions.

Moreover, even if the joint dependency graph of the variational posterior and the prior were acyclic, this derivation would be structure-specific and would need to be repeated for each hierarchical structure. We therefore do not doubly reparameterize the indirect score functions.
D. Worked example for a 2-layer hierarchical VAE

In this section we show an example of using the IWAЕ objective with a 2-layer VAE model consisting of a prior \(p_{\theta_1}(z_2)p_{\theta_2}(z_1|x_2)\) and likelihood \(p_{x}(x|z_1, z_2)\). The inference network is bottom-up: \(q_{\phi_1}(z_1|x)p_{\phi_2}(z_2|x, z_1)\). Therefore \(p_{\phi}(2) = z_1\) and \(p_{\phi}(1) = z_2\).

We hierarchically sample \(z_{k1}\) and \(z_{k2}\) from the approximate posterior and abbreviate:

\[
\begin{align*}
\tilde{z}_{k1}(\phi_1) &\equiv T_{q_1}(e_{k1}; \alpha_1(\phi_1)) \\
\tilde{z}_{k2}(\phi_1, \phi_2) &\equiv T_{q_{21}}(e_{k1}; \alpha_{21}(x, \tilde{z}_{k1}(\phi_1), \phi_2)).
\end{align*}
\]

We also explicitly distinguish between the distribution parameters \(\alpha_k\) and the network parameters \(\phi_k\) for the posterior as well as the distribution parameters \(\beta_k\) and the network parameters \(\theta_k\) for the prior. A single importance sample \(w_k\) with all of its functional dependencies is given by:

\[
w_k = \frac{p_{x}(x|z_{k1}(\phi_1), z_{k2}(\phi_1, \phi_2)) p_{\beta_{k1:2}(z_{k2}(\phi_1, \phi_2), \theta_1)}(z_{k1}(\phi_1))}{q_{\alpha_{k1}(x, \phi_1)}(z_{k1}(\phi_1)) q_{\alpha_{21}(x, \tilde{z}_{k1}(\phi_1), \phi_2)}(z_{k2}(\phi_1, \phi_2))}.
\]

The DREGs estimator for the variational parameters of the lower latent layer, \(\phi_1\), is then given by:

\[
\begin{align*}
\nabla^{\text{DREGs}}_{\phi_1} \mathcal{L}^{\text{IWAE}}_{\phi, \theta} &\equiv \sum_{k=1}^{K} \nabla_{\phi_1} \log w_k - \nabla_{\alpha_{21}} \log q_{\alpha_{21}(x, \tilde{z}_{k1}(\phi_1), \phi_2)}(z_{k2}(\phi_1, \phi_2)) \nabla_{z_{k1}} \alpha_{21}(x, \tilde{z}_{k1}(\phi_1), \phi_2) \\
&+ \nabla_{\beta_{k1:2}} \log p_{\beta_{k1:2}(z_{k2}(\phi_1, \phi_2), \theta_1)}(z_{k1}(\phi_1)) \nabla_{z_{k1}} \beta_{k1:2}(z_{k2}(\phi_1, \phi_2), \theta_1)
\end{align*}
\]

where we have expanded the total derivative w.r.t. \(z_{k1}\) into the (true) pathwise gradients and two indirect score functions.

Similarly, we can compute the DREGs estimator for the variational parameters of the upper level, \(\phi_2\):

\[
\begin{align*}
\nabla^{\text{DREGs}}_{\phi_2} \mathcal{L}^{\text{IWAE}}_{\phi, \theta} &\equiv \sum_{k=1}^{K} \nabla_{\phi_2} \log w_k - \nabla_{\alpha_{21}} \log q_{\alpha_{21}(x, \tilde{z}_{k1}(\phi_1), \phi_2)}(z_{k2}(\phi_1, \phi_2)) \nabla_{z_{k2}} \alpha_{21}(x, \tilde{z}_{k1}(\phi_1), \phi_2) \\
&+ \nabla_{\beta_{k1:2}} \log p_{\beta_{k1:2}(z_{k2}(\phi_1, \phi_2), \theta_1)}(z_{k1}(\phi_1)) \nabla_{z_{k2}} \beta_{k1:2}(z_{k2}(\phi_1, \phi_2), \theta_1)
\end{align*}
\]

For this model structure of the prior and variational posterior, there is only one indirect score function for this gradient. Note that the indirect score functions are computed automatically in our surrogate losses that we introduce in the following section, such that we do not need to compute them manually; the hierarchical DREGs estimator can be implemented without having to trace the dependency structure of the model manually.

To compute the GDREGs estimator, we first have to re-express the samples \(z_1\) and \(z_2\) as if they were sampled from \(p_{\theta_1, \theta_2}(z_1, z_2)\). We write this reparameterization as

\[
\begin{align*}
z_{k2}(\theta_2) &\equiv T_{p_2}(e_{k2}; \beta_2(\theta_2)) \\
z_{k1}(\theta_1, \theta_2) &\equiv T_{p_{21}}(e_{k1}; \beta_{12}(z_{k2}(\theta_2), \theta_1))
\end{align*}
\]

where \(e_1\) and \(e_2\) are noise variables drawn from \(\tilde{q}(\epsilon)\), which is given by the inverse prior flow of the samples drawn from \(q_{\phi_1, \phi_2}(x, x_2|x)\). The full functional dependency of a single importance sample is given by:

\[
w_k = \frac{p_{x}(x|z_{k1}(\theta_1, \theta_2), z_{k2}(\theta_2)) p_{\beta_{k1:2}(z_{k2}(\theta_2), \theta_1)}(z_{k1}(\theta_1, \theta_2))}{q_{\alpha_{k1}(x, \phi_1)}(z_{k1}(\theta_1, \theta_2)) q_{\alpha_{21}(x, \tilde{z}_{k1}(\theta_1, \theta_2), \phi_2)}(z_{k2}(\theta_2))}.
\]

The GDREGs estimator w.r.t. the prior parameters of the lower stochastic layer, \(\theta_1\), is given by:

\[
\begin{align*}
\nabla^{\text{GDREGs}}_{\theta_1} \mathcal{L}^{\text{IWAE}}_{\phi, \theta} &\equiv \sum_{k=1}^{K} \nabla_{\theta_1} \log p_{x}(x|z_{k1}, z_{k2}) - \nabla_{\theta_1} \log w_k \nabla_{\theta_1} T_{p_1}(e_{k1}; \theta_1)|_{e_{k1} = T_{p_1}^{-1}(z_{k1}, \theta_1)}; \\
z_{1:K} &\sim q_{\phi}(z_{k}|x)
\end{align*}
\]
As we discussed in Sec. 4.1 and similar to Tucker et al. (2019), we use surrogate loss functions to compute the gradients. To practically implement this surrogate loss, we use two copies of the variational posterior distribution. An unaltered one

\[ \nabla_{z_k} \log w_k = \nabla_{z_{k+1}} \log w_k - \nabla_{\alpha_{2:k}} \log q_{\alpha_{2:k}}(x, z_{k+1}(\theta_1, \theta_2), \phi_k) \nabla_{z_{k+1}} \alpha_{2:k} \nabla_{x_1} \alpha_{2:1}(x, z_{k+1}(\theta_1, \theta_2), \phi_k) \] 

The GDREGs estimator w.r.t. the prior parameters of the upper stochastic layer, \( \theta_2 \), is given by:

\[ \hat{\nabla}_{\theta_2} L_{\text{DREG}s}^{\text{IWAE}} = \sum_{k=1}^{K} \left( \tilde{w}_{k} \nabla_{z_k} \log p_{\lambda}(x \mid z_1, z_2) - \tilde{w}_{k} \nabla_{z_k} \log w_k \right) \nabla_{\theta_2} \mathcal{T}_p \left( \epsilon_{k+2} \mid \theta_2 \right) |_{\epsilon_{k+2} = \mathcal{T}_p^{-1}(z_{k+2})} \]

\[ \nabla_{z_k} \log w_k = \nabla_{z_{k+2}} \log w_k - \nabla_{\alpha_{2:k}} \log q_{\alpha_{2:k}}(x, z_{k+1}(\theta_1, \theta_2), \phi_k) \nabla_{z_{k+1}} \alpha_{2:k} \nabla_{x_1} \alpha_{2:1}(x, z_{k+1}(\theta_1, \theta_2), \phi_k) + \nabla_{\beta_{1:k}} \log p_{\beta_{1:k}}(z_{k+2}(\theta_1), \theta_1) \nabla_{z_{k+2}} \beta_{1:k} \nabla_{z_{k+1}} \beta_{1:1}(z_{k+2}(\theta_2), \theta_1) \] 

Note how the GDREGs estimator for \( \theta_2 \) has two indirect score functions for the upper layer where the DREGs estimator for \( \phi_2 \) only has one. This is due to the opposite factorization (opposite hierarchical dependency structure) of the variational posterior and the prior. This cyclic dependence is also the reason why we cannot replace all indirect score functions with DREGs and GDREGs gradients. Double reparameterization of one of the indirect score functions, leads to another indirect score function, whose double-reparameterization in turn leads back to the first indirect score function but with a different pre-factor.

Again, note that the indirect score functions are computed automatically in our surrogate losses, App. E, and we do not need to manually trace the dependency structure or derive them.

### E. Surrogate losses to implement the DREGs and GDREGs estimators for IWAE objectives

As we discussed in Sec. 4.1 and similar to Tucker et al. (2019), we use surrogate loss functions to compute the gradients w.r.t. the likelihood, proposal, and prior parameters. That is, we use different losses, such that backpropagation results in the respective gradient estimator. While Tucker et al. (2019) use a single surrogate loss to compute the gradient estimators for all parts of the objective, we choose to use separate surrogate losses for each of the three parameter groups (likelihood, variational posterior, prior). In principle, we could combine them into a single loss, but in order to keep presentation simple we keep them separate. Computationally this does not make a difference as modern deep learning frameworks avoid duplicate computation.

For the likelihood parameters, we use the regular (negative) IWAE objective Eq. (3) as a loss. That is, the gradient estimator for the likelihood parameters is given by the gradient of the negative IWAE objective.

To construct the other surrogate losses we need to stop the gradients at various points in the computation graph. In the following, we use the shorthand notation \( \nabla_{\text{stop}} \) to indicate that we stop gradients into the underlined parts of an expression. Where it might be ambiguous, or to highlight where we do not stop gradients, we use the shorthand \( \nabla_{\text{flow}} \) to indicate that gradients flow. For example, \( f(\phi, \theta) \) means that we backpropagate gradients into \( \phi \) but not into \( \theta \).

### E.1. DREGs for variational posterior parameters \( \phi \)

#### E.1.1. Single stochastic layer

Here we reproduce part of the surrogate loss for the variational parameters \( \phi \) by Tucker et al. (2019) for the single stochastic layer case:

\[ L_{\text{DREG}s}(\phi) = \sum_{k=1}^{K} \tilde{w}_{k} \left( \log p_{\lambda}(x \mid z_{k}) + \log p_{\beta}(\theta) \mid z_{k} \right) - \log q_{\alpha}(\phi \mid z_{k}) \]

\[ z_{k} = \mathcal{T}_q(\epsilon_{k}; \phi) \quad \epsilon_{k} \sim q(\epsilon_{k}) \]

That is, we sample \( z_{k} \sim q(\phi \mid x) \) as usual (by reparameterizing independent noise variables \( \epsilon_{k} \)) but stop the gradients of the parameters that parameterize the distributions when evaluating their densities, \( \log q_{\alpha}(\phi \mid z_{k}) \). In addition we stop the gradients around the normalized importance weights \( \tilde{w}_{k} \). Differentiating \( L_{\text{DREG}s} \) w.r.t. the proposal parameters \( \phi \) yields the DREGs estimator Eq. (11). Note that we do not explicitly stop gradients into \( \lambda \) or \( \theta \) because we use separate surrogate losses for those parameter groups. If we were to use a combined loss, we would potentially have to stop gradients into these parameters as well, depending on the estimator used.

To practically implement this surrogate loss, we use two copies of the variational posterior distribution. An unaltered one
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(no stopped gradients) to sample \( z \) and one with gradients into the proposal parameters stopped to evaluate the log densities. The stopped gradient makes sure that we do not obtain a direct score function as we have doubly-reparameterized it.

Note that for single-stochastic-layer models we could also stop the gradients of the distribution parameters \( \alpha \) instead as they only depend on \( \phi \). We emphasize that this is not possible for hierarchical models as this would eliminate the indirect score functions and thus produce potentially biased gradients.

E.1.2. MULTIPLE STOCHASTIC LAYERS

For multiple layers, the surrogate loss for the DREGs estimator Eq. (E.8) is given by:

\[
L_{\text{DREGs}}(\phi) = \sum_{k=1}^{K} \tilde{w}_k^2 \log w_k
\]

\[
\log w_k = \log p_\beta(\mathbf{x}|\mathbf{z}_k) + \sum_{l=1}^{L} \log p_{\beta_l}(\mathbf{z}_{kl}) - \sum_{l=1}^{L} \log q_{\alpha_l}(\mathbf{z}_{kl})
\]

\[
z_{kl} = T_{q_l}(\epsilon_{kl}; \alpha_l(p_{\alpha_l}(l)\phi_l)) \quad \epsilon_{kl} \sim q(\epsilon_{kl})
\]

Again, we do not explicitly stop gradients into \( \lambda \) or \( \theta_l \) as we only take gradients w.r.t. \( \phi_l \).

The indirect score functions arise due to the indirect dependence of the distribution parameters \( \alpha_l(p_{\alpha_l}(l)\phi_l) \) and \( \beta_l(p_{\beta_l}(l)\theta_l) \) on the parent latent variables \( p_{\alpha_l}(l) \) and \( p_{\beta_l}(l) \), respectively. Note how the former depends on the hierarchical structure of the variational posterior, whereas the latter depends on the hierarchical structure of the prior.

To implement this surrogate loss effectively, we again use two copies of the variational posterior distribution. One un-altered one (without stopped gradients) from which we sample the individual reparameterized functions and thus produce potentially biased gradients.

E.2. GDREGs for prior parameter \( \theta \)

E.2.1. SINGLE STOCHASTIC LAYER

\[
L_{\text{GDREGs}}(\theta) = \sum_{k=1}^{K} \tilde{w}_k \log p_\lambda(\mathbf{x}|\mathbf{z}_k) - \tilde{w}_k^2 \left( \log p_\lambda(\mathbf{x}|\mathbf{z}_k) + \log p_\beta(\mathbf{z}_k) - \log q_\alpha(\mathbf{z}_k) \right)
\]

\[
z_k = T_p(\epsilon_k; \theta) \quad \epsilon_k \sim q(\epsilon_k)
\]

Taking the derivative of Eq. (E.3) w.r.t. \( \theta \) gives rise to the GDREGs estimator for the single stochastic layer IWAE objective. As explained in Sec. 4, we need to re-express \( z_k \) such that its path depends on \( \theta \). In effect, we first sample \( z_k = T_\theta(\epsilon_k; \phi) \), then compute the new noise variable \( \tilde{\epsilon}_k = T_p^{-1}(z_k) \), and re-compute \( z_k = T_\theta(\tilde{\epsilon}_k; \theta) \). Note that we have to stop gradients into the noise variables \( \tilde{\epsilon}_k \) to obtain the correct gradient estimator. This explains the stop_grad in Fig. 2.

As above, we do not explicitly stop gradients into \( \lambda \) and \( \phi \) as we use separate losses for these parameter groups and only compute gradients of Eq. (E.3) w.r.t. \( \theta \).

To effectively implement this loss, we use two copies of the prior distribution. One that we implement as a normalizing flow and a second one with stopped gradients into the parameters. We then proceed as follows:

- Compute the new noise variables \( \tilde{\epsilon}_k \) by using the inverse flow \( T_p^{-1} \) on the samples \( z_k \) from the variational posterior.
- Stop the gradients into \( \tilde{\epsilon}_k \).
- Use the forward flow \( T_p(\tilde{\epsilon}_k; \theta) \) to re-compute \( z_k \) but with path dependent on \( \theta \). These samples when derived w.r.t. \( \theta \) will give rise to the pathwise gradients.
As before we use two copies of the prior distribution, one with regular gradients that is set up as a flow, and a second with stopped gradients into the parameters. This allows us to implement the GDR

\[
\alpha \mathbb{E} \log p(x, z_{k1}, \ldots, z_{kL}) - \mathbb{E} \log w_k \log p(x | z_{k1}, \ldots, z_{kL}) + \sum_{l=1}^{L} \log p_{\beta_l}(p_{\alpha_l}(l), \theta_l)(z_{kl}) - \sum_{l=1}^{L} \log q_{\epsilon_{kl}}(p_{\alpha_l}(l), \phi_l)(\tilde{z}_{kl})
\]

(E.4)

As the single layer case, we need to re-express variational posterior samples \( z_{kl} \) as if they were sampled from the prior. To obtain the correct gradients, we again have to stop gradients into the new noise variables \( \epsilon_{kl} \), also see Fig. 3.

As for hierarchical DREgs, the indirect score functions stem from the second and third term of \( \log w_k \) and arise because the distribution parameters \( \alpha_l \) and \( \beta_l \) depend on the "parent" stochastic layers.

As before we use two copies of the prior distribution, one with regular gradients that is set up as a flow, and a second with stopped gradients into the parameters. This allows us to implement the GDREgs estimator regardless of the model structure.

**F. Implementation details**

In our implementations we use NumPy (Harris et al., 2020), JAX (Bradbury et al., 2018), Haiku (Hennigan et al., 2020), as well as tensorflow probability and tensorflow distributions (Dillon et al., 2017).

**Stopping gradients.** All major frameworks allow for gradients to be stopped or interrupted. For example, in TensorFlow (Abadi et al., 2016) we can use tf.stop_gradient and in JAX we can use jax.lax.stop_gradient. To implement stopped gradients w.r.t. the parameters of a distribution we use haiku.experimental.custom_getter contexts, which allow us to manipulate the parameters before they are used to construct the respective networks; in this case we use the context to stop gradients.

**Re-expressing samples.** To re-express variational posterior samples as if they came from the prior, we directly implement the computation flow as it is described in e.g. Figs. 2 and 3 and detailed in App. E.2.

In the code listings Listings 1 and 2 we provide (pseudo-)code for a simple implementation of the surrogate objectives. Listing 1 contains the import statements as well as the function and class definitions to create parameterized distributions that allow for

1. stopping the gradients into their parameters, and
2. re-expressing samples using the bijector interface in tensorflow probability.

In Listing 2 we implement surrogate objectives for the naive and the GDREgs estimators of the cross-entropy. More specifically, we wish to estimate:

\[
\nabla_{\theta}^{TD} L^{ce} = \nabla_{\theta}^{TD} \mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ \log p_{\theta}(z) \right].
\]

(F.1)

The naive estimator (using a single Monte Carlo sample) is given by

\[
\nabla_{\theta}^{\text{naive}} L^{ce} = \nabla_{\theta} \log p_{\theta}(z) \quad z \sim q_{\phi}(z).
\]

(F.2)
The corresponding GDREGs estimator (again using a single MC sample) is given by Eq. (21):

\[
\hat{\nabla}_\theta \mathcal{L}^{\text{DREGs}}_{\text{ce}} = \nabla_z \log \frac{q_\phi(z)}{p_\theta(z)} \nabla_\varphi \epsilon_{T_p^{-1}(z, \theta)} \bigg|_{\epsilon=\epsilon_{T_p^{-1}(z, \theta)}} \sim q_\phi(z). \tag{21}
\]

Listing 1: Function and class definitions necessary to define the surrogate objectives for the DREGs and GDREGs estimators.

```python
from typing import List
import haiku as hk
import jax
import jax.lax as lax
import jax.numpy as jnp
from tensorflow_probability.substrates import jax as jtfp
jtfd = jtfp.distributions

# A custom getter that stops gradients of parameters.
def stop_grad_getter(next_getter, value, _):
    return lax.stop_gradient(next_getter(value))

# Reparameterize samples z_q as if they were sampled from p.
def reparameterize_as_if_from(p: jtfd.TransformedDistribution, z_q: jnp.ndarray) -> jnp.ndarray:
    eps = p.bijector.inverse(z_q)
    eps = jax.lax.stop_gradient(eps)
    return p.bijector.forward(eps)

# A Normal distribution that is conditioned through an MLP.
class ConditionalNormal(hk.Module):
    def __init__(self, output_size: int, hidden_layer_sizes: List[int], name: str = "conditional_normal"):
        super(ConditionalNormal, self).__init__(name=name)
        self.name = name
        self.fcnet = hk.nets.MLP(output_sizes=hidden_layer_sizes + [2 * output_size],
                                  activation=jnp.tanh,
                                  activate_final=False,
                                  with_bias=True,
                                  name=name
                                  )
```

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```python
def condition(self, inputs):
    """Computes the parameters of a normal distribution based on the inputs."""
    outs = self.fcnet(inputs)
    mu, sigma = jnp.split(outs, 2, axis=-1)
    sigma = jax.nn.softplus(sigma)
    return mu, sigma

def __call__(self, inputs, **kwargs):
    """Creates a normal distribution conditioned on the inputs."""
    # Optional 'stop_gradient_params' argument stops the parameters
    # of the distribution.
    if kwargs.get("stop_gradient_params", False):
        with hk.experimental.custom_getter(stop_grad_getter):
            mu, sigma = self.condition(inputs)
    else:
        mu, sigma = self.condition(inputs)

    # Optional 'as_flow' argument parameterizes the distribution as a flow
    # to have access to 'Bijector.inverse' and 'Bijector.forward'
    # to use with the function 'reparameterize_as_if_from'
    if kwargs.get("as_flow", False):
        bijector = jtfp.bijectors.Chain(
            [jtfp.bijectors.Shift(shift=mu), jtfp.bijectors.Scale(scale=sigma)])
        base = jtfd.Normal(loc=jnp.zeros_like(mu), scale=jnp.ones_like(sigma))
        return jtfd.TransformedDistribution(
            distribution=base, bijector=bijector, name=self.name + "_flow")
    return jtfd.Normal(loc=mu, scale=sigma)
```

Listing 2: Code to implement the surrogate objective for the naive estimator of the cross-entropy as well as for the GDREGs estimator Eq. (21). Computing derivatives w.r.t. the parameters of the prior \( p \) using automatic differentiation gives rise to the correct expressions for the estimators.

```
# Create distributions
# Inputs 'x' and context 'c'
q = ConditionalNormal(x)
p = ConditionalNormal(c)
q_stop = ConditionalNormal(x, stop_gradient_params=True)
p_stop = ConditionalNormal(c, stop_gradient_params=True)
p_flow = ConditionalNormal(c, as_flow=True)

# Sample from the variational posterior
z_q = q.sample(sample_shape=[num_samples], seed=hk.next_rng_key())  # [k, bs, z]

# Reparameterize the samples from q as if they were sampled from p
z_q_as_p = reparameterize_as_if_from(p_flow, z_q)

# Cross-entropy surrogate losses
cross_entropy_naive = p.log_prob(z_q)
cross_entropy_gdregs = q_stop.log_prob(z_q_as_p) - p_stop.log_prob(z_q_as_p)
```

G. Experimental details and additional results

In this section we provide additional experimental details as well as additional results.

G.1. Illustrative example

As discussed in the main text, we use a 2-layer linear VAE inspired by the single layer example of Rainforth et al. (2018); Tucker et al. (2019). We use a top-down generative model \( z_2 \to z_1 \to x \), with \( z_1, z_2, x \in \mathbb{R}^D \) and \( D = 5 \). The hierarchical prior is given by \( z_2 \sim \mathcal{N}(0, I) \), \( z_1 | z_2 \sim \mathcal{N}(\mu_{\theta}(z_2), \sigma_{\theta}^2(z_2)) \), and the likelihood is given by \( x | z_1 \sim \mathcal{N}(z_1, I) \).
We choose a bottom-up variational posterior that factorizes as: 

\[ q_{\phi_1}(z_1|x) = \mathcal{N}(\mu_{\phi_1}(x), \sigma^2_{\phi_1}(x)) \] 

and 

\[ q_{\phi_2}(z_2|z_1) = \mathcal{N}(\mu_{\phi_2}(z_1), \sigma^2_{\phi_2}(z_1)) \].

All functions \( \mu_* \) and \( \sigma_* \) are given by linear functions with weights and biases; the likelihood and the upper layer of the prior do not have any learnable parameters.

To generate data, we sample 512 datapoints from the model where we have set \( \mu_\theta(z_2) = z_2 \) and \( \sigma_\theta(z_2) = 1 \).

We then train the parameters \( \phi \) and \( \theta \) in all linear layers using SGD on the IWAE objective til convergence. We then evaluate the gradient variance and gradient signal-to-noise ratio for each estimator. For the proposal parameters \( \phi \) we compare DREGs to the naive score function (labelled as IWAE) and to STL; for the prior parameters \( \theta \) we compare GDRREGs to IWAE.

In Fig. 4 in the main paper we show the average gradient variance and gradient signal-to-noise ratio (SNR). The average is taken over all parameters of either the variational posterior or the prior. The gradient variance and gradient SNR for individual parameters exhibit the same qualitative behaviour.

G.2. Conditional and unconditional image modelling

For conditional and unconditional image modelling, we use VAEs with one or multiple stochastic layers, where the generative path is top-down and the inference path is bottom-up, as specified in Eq. (23), which we reproduce here for convenience:

\[
q_{\phi}(x|c) = q_{\phi_1}(z_1|x,c) \prod_{l=2}^{L} q_{\phi_l}(z_l|z_{l-1},x,c) \\
p_{\theta}(z|c) = p_{\theta_L}(z_L|c) \prod_{l=1}^{L-1} p_{\theta_l}(z_l|z_{l+1},c) \\
p_\lambda(x|z) = p_\lambda(x|z_1, \ldots, z_L).
\]

For conditional image modelling, we predict the bottom half of an image given its top half as in Tucker et al. (2019), providing the top half as an additional context input \( c \) to the prior and variational posterior. Given the above model structure, \( p_{\alpha}(l) = z_{k(l-1)} \) and \( p_{\beta}(l) = z_{k(l+1)} \).

Each conditional distribution in Eq. (23) is given by an MLP of 2 hidden layers of 300 \tanh units each. If a distribution has multiple inputs, we concatenate them along the feature dimension. The prior and variational posterior are all given by diagonal Gaussian distributions, whereas the likelihood is given by a Bernoulli distribution. The unconditional prior distribution in the uppermost layer \( p_{\theta_L}(z_L) \) is given by a standard Normal distribution, \( p_{\theta_L}(z_L) = \mathcal{N}(0, 1) \). All latents \( z_l \) are 50 dimensional.

To avoid overfitting, we use dynamically binarized versions of the datasets. We use the Adam optimizer with default learning rate \( 3 \cdot 10^{-4} \) and default parameters \( b_1 = 0.9 \), \( b_2 = 0.999 \), and \( \epsilon = 10^{-8} \). We use a batch size of 64 and \( K = 64 \) importance samples for training and evaluation. Note that for testing we report test objective values rather than an estimate of \( \log p(x) \) by using a large number of importance samples. We do this as we are interested in the relative behaviour of the estimators.

In Fig. G.1 we provide further plots that show the evolution of the test objective and the gradient variance of the prior, the variational posterior, as well as the likelihood throughout training on conditional modelling of MNIST and FashionMNIST (predict bottom half given top half). As in the main paper we find that using GDRREGs for the prior instead of the naive estimator (denoted as IWAE) always improves performance on the test objective regardless of the estimator for the variational posterior. We also note that GDRREGs always reduces gradient variance for the prior early in training and also typically throughout training, especially for deeper models and when combined with the DREGs estimator for the variational posterior.

Interestingly, using the GDRREGs estimator for the prior leads to an increase in the gradient variance for the variational posterior when we use the naive estimator but similar or even lower posterior gradient variance when combined with the DREGs estimator (third column in Fig. G.1). It always leads to a slight improvement in gradient variance for the likelihood parameters (fourth column in Fig. G.1). We hypothesize that this is the case because lower gradient variance in for one set of parameters makes it easier to estimate the gradients for another set as a secondary effect.

In Fig. G.2 we show that the training objective behaves qualitatively similar to the test objective in that the applying the DREGs or GDRREGs estimator results in improved objective values in the same way, regardless of whether we consider the training or test objective. That is, our hierarchical extension of DREGs results in a better training objective values for both
conditional and unconditional tasks. GDREGs is particularly helpful for conditional tasks.

Moreover, in the main text we had hypothesized that GDREGs performs better on conditional image modelling tasks than unconditional tasks because access to the context makes the variational posterior and the prior more similar. In the case of analytically computed cross-entropy in App. H, we derive that the GDREGs estimator outperforms a naive estimator of the score function in terms of gradient variance when the posterior and prior are similar. We hypothesize that this also holds more generally for the IWAE objective, where we cannot compute the gradient variance in closed form but only estimate it empirically. To investigate this, we computed the total average KL (rightmost column in Fig. G.2) over all latent variables and found that it is indeed lower for conditional than unconditional modelling, which indicates that the distributions are closer together in this case.

G.3. Offline evaluation of the DReg and GDRG estimator

In the image modelling experiments in Sec. 5.2 we discussed the gradient variance of the different estimators for the posterior and prior parameters. However, we only analyzed estimators online on their respective runs; that is, in Fig. 6 the prior and posterior gradient variance shown corresponds to the variance of the estimator also used during training.
Here, we provide an ablation study for conditional image modelling on MNIST with a 2-layer VAE where we evaluate the different estimators offline; that is, for each combination of estimators used for training we also show the gradient variance of the other estimators.

In Fig. G.3 we consider the gradient variance w.r.t. the variational posterior parameters $\phi$ and compare the naive (IWAE) estimator to the DREGs estimator. We find that regardless which combination of estimators has been used during training, the DREGs estimator always results in a better (lower) gradient variance than the naive estimator.

Similarly, in Fig. G.4 we consider the gradient variance w.r.t. the prior parameters $\theta$ and compare the naive (IWAE) estimator to the GDREGs estimator. We find that generally the GDREGs gradient estimates have lower variance than the naive (IWAE) estimates. However, when we use the naive estimator for the prior parameters during training, this reduction is smaller and may only be present in the beginning of training. However, consistently, the GDREGs gradient estimates have lower variance when we use the DREGs estimator during training to estimate the variational posterior parameters.
The naive estimator of this score function is given by:

$$\hat{\nabla}_{\theta} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2$$

Note that all operations are element-wise.

H. The cross-entropy for Gaussian distributions

Here, we investigate the properties of the GDR\textsubscript{gs} estimator compared to the naive estimator in a setting where all quantities of interest can be computed in closed form, the cross-entropy of two Gaussian distributions, \(q_\phi(z) = N(z; \mu_q, \sigma_q)\) and \(p_\theta(z) = N(z; \mu_p, \sigma_p)\).

The negative cross-entropy is given by

$$L_{\phi, \theta}^{ce} = \mathbb{E}_{z \sim q_\phi(z)} [\log p_\theta(z)] = \frac{1}{2} \log(2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2$$

Note that in this analytic case, we can compute the gradients without having to sample. However, in the following we want to compare the naive (score function) estimator to the GDR\textsubscript{gs} estimator.

The naive estimator of this score function is given by:

$$\hat{\nabla}_{\theta} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2$$

while the GDR\textsubscript{gs} estimator is given by (see Eq. (21)):

$$\hat{\nabla}_{\theta} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2$$

H.1. Gradient variance of the estimators

In the case under consideration, the parameters \(\theta\) are given by the mean and variance of the prior, \(\theta = \{\mu_p, \sigma_p\}\), and we can compute both the expectation as well as the variance of these gradient estimators in closed form.

Naive estimator

$$\mathbb{E}_{q_\phi(z)} \left[ \hat{\nabla}_{\theta} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2 \right] = \frac{\mu_q - \mu_p}{\sigma_p^2}$$

$$\mathrm{Var}_{q_\phi(z)} \left[ \hat{\nabla}_{\theta} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2 \right] = \frac{\sigma_q^2}{\sigma_p^4}$$

$$\mathbb{E}_{q_\phi(z)} \left[ \hat{\nabla}_{\sigma_p^2} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2 \right] = \frac{\sigma_q^2}{\sigma_p^4} + \frac{(\mu_q - \mu_p)^2}{\sigma_p^4}$$

$$\mathrm{Var}_{q_\phi(z)} \left[ \hat{\nabla}_{\sigma_p^2} \log (2\pi) + \log \sigma_p + \sigma_q^2 + (\mu_p - \mu_q)^2 \right] = 2 \frac{\sigma_q^4}{\sigma_p^6} + 4 \sigma_q^2 \frac{(\mu_q - \mu_p)^2}{\sigma_p^6}$$

Note that all operations are element-wise.
The proposed GDReGs estimator

\[
\mathbb{E}_{q_\phi(z)} \left[ \nabla_{\mu_p} \mathcal{L}_{\phi, \theta}^{ce} \right] = \frac{\mu_q - \mu_p}{\sigma_p^2} \tag{H.7}
\]

\[
\text{Var}_{q_\phi(z)} \left[ \nabla_{\mu_p} \mathcal{L}_{\phi, \theta}^{ce} \right] = \frac{\sigma_q^2 (\sigma_p^2 - \sigma_q^2)^2}{\sigma_p^4} \tag{H.8}
\]

\[
\mathbb{E}_{q_\phi(z)} \left[ \nabla_{\sigma_p} \mathcal{L}_{\phi, \theta}^{ce} \right] = \frac{\sigma_q^2 - \sigma_p^2}{\sigma_p^3} + \frac{(\mu_q - \mu_p)^2}{\sigma_p^2} \tag{H.9}
\]

\[
\text{Var}_{q_\phi(z)} \left[ \nabla_{\sigma_p} \mathcal{L}_{\phi, \theta}^{ce} \right] = 2 \left( \frac{\sigma_q^2 - \sigma_p^2}{\sigma_p^6} \right) + \frac{2 \sigma_q^4}{\sigma_p^6} (\mu_q - \mu_p)^2 \tag{H.10}
\]

Note that all operations are element-wise.

Both estimators have equal expectation; this is because GDReGs is an unbiased estimator.

Comparing the variances in Eq. (H.4) and Eq. (H.8) we note that the GDReGs estimator has a lower gradient variance than the naive estimator for the mean parameters \( \mu_p \) if

\[
\sigma_p^2 \leq 2 \sigma_q^2. \tag{H.11}
\]

Similarly, comparing Eq. (H.6) and Eq. (H.10), we find that the GDReGs estimator has lower variance than the naive estimator for the variance parameters \( \sigma_p \) if

\[
\sigma_p^2 \leq 4 \sigma_q^2 \left( 1 - \frac{\sigma_q^2}{(\mu_p - \mu_q)^2 + 2 \sigma_q^2} \right) \tag{H.12}
\]

In the case of \( \mu_p = \mu_q \) this also reduces to \( \sigma_p^2 \leq 2 \sigma_q^2 \).

Thus, we expect the GDReGs estimator to perform better than the naive estimator when \( p_\theta(z) \) and \( q_\phi(z) \) are close together.

**H.2. Constructing the optimal control variate**

Because the GDReGs estimators and the naive estimators have the same expectation, we can build a control variate out of their difference:

\[
\left[ \nabla_{\mu_p}^{\text{naive}} + \alpha \left( \nabla_{\mu_p}^{\text{GDReG}} - \nabla_{\mu_p}^{\text{naive}} \right) \right] \mathcal{L}_{\phi, \theta}^{ce}. \tag{H.13}
\]

We can then compute its optimal strength \( \alpha^* \), by minimizing its variance,

\[
\alpha^* = \arg \min_{\alpha} \text{Var}_{q_\phi(z)} \left[ \left[ \nabla_{\mu_p}^{\text{naive}} + \alpha \left( \nabla_{\mu_p}^{\text{GDReG}} - \nabla_{\mu_p}^{\text{naive}} \right) \right] \mathcal{L}_{\phi, \theta}^{ce} \right]. \tag{H.14}
\]

We find that:

\[
\alpha^*_\mu = \frac{\sigma_q^2}{\sigma_p^2} \tag{H.15}
\]

\[
\alpha^*_\sigma = \frac{2 \sigma_q^2 (\mu_p - \mu_q)^2 + \sigma_q^2}{\sigma_p^2 (\mu_p - \mu_q)^2 + 2 \sigma_q^2} \tag{H.16}
\]

\[
\text{Var}_{q_\phi(z)} \left[ \left[ \nabla_{\mu_p}^{\text{naive}} + \alpha^*_\mu \left( \nabla_{\mu_p}^{\text{GDReG}} - \nabla_{\mu_p}^{\text{naive}} \right) \right] \mathcal{L}_{\phi, \theta}^{ce} \right] = 0 \tag{H.17}
\]

\[
\text{Var}_{q_\phi(z)} \left[ \left[ \nabla_{\sigma_p}^{\text{naive}} + \alpha^*_\sigma \left( \nabla_{\sigma_p}^{\text{GDReG}} - \nabla_{\sigma_p}^{\text{naive}} \right) \right] \mathcal{L}_{\phi, \theta}^{ce} \right] = \frac{2 \sigma_q^4}{\sigma_p^6} (\mu_q - \mu_p)^2 \tag{H.18}
\]

Note that the expression for the optimal strength has different form for the mean \( \mu_p \) and variance \( \sigma_p \) parameters. Moreover, note that the analytic estimator has zero gradient variance whereas our estimator with control variate still has non-zero gradient variance for the variance parameters \( \sigma_p \).
This optimal estimator holds for a single layer VAE, where both the variational posterior as well as the prior are Gaussian. In a hierarchical model where both the prior and the posterior are factorized top-down, the same derivation holds for the lowest stochastic layer (similar to how semi-analytic approximations for the conditional KL can be derived in this case). Unfortunately, in this case the expectations cannot be computed in closed form anymore.