Abstract

Modelers use automatic differentiation (AD) of computation graphs to implement complex deep learning models without defining gradient computations. Stochastic AD extends AD to stochastic computation graphs with sampling steps, which arise when modelers handle the intractable expectations common in reinforcement learning and variational inference. However, current methods for stochastic AD are limited: They are either only applicable to continuous random variables and differentiable functions, or can only use simple but high variance score-function estimators. To overcome these limitations, we introduce Storchastic, a new framework for AD of stochastic computation graphs. Storchastic allows the modeler to choose from a wide variety of gradient estimation methods at each sampling step, to optimally reduce the variance of the gradient estimates. Furthermore, Storchastic is provably unbiased for estimation of any-order gradients, and generalizes variance reduction techniques to any-order derivative estimates. Finally, we implement Storchastic as a PyTorch library at github.com/HEmile/storchastic.

1 Introduction

One of the driving forces behind deep learning is automatic differentiation (AD) libraries of complex computation graphs. Deep learning modelers are relieved by accessible AD of the need to implement complex derivation expressions of the computation graph. However, modelers are currently limited in settings where the modeler uses intractable expectations over random variables [37, 8]. Two common examples are reinforcement learning methods using policy gradient optimization [49, 29, 36] and latent variable models, especially when inferred using amortized variational inference [34, 20, 41, 43]. Typically, modelers estimate these expectations using Monte Carlo methods, that is, sampling, and resort to gradient estimation techniques [37] to differentiate through the expectation.

A popular approach for stochastic AD is reparameterization [20], which is both unbiased and has low variance, but is limited to continuous random variables and differentiable functions. The other popular approach [49, 45, 13] analyzes the computation graph and then uses the score function estimator to create a surrogate loss that provides gradient estimates when differentiated. While this approach is more general as it can also be applied to discrete random variables and non-differentiable functions, naive applications of the score function will have high variance, which leads to unstable and slow convergence. Furthermore, this approach is often implemented incorrectly [13], which can introduce bias in gradients.

We therefore develop a new framework called Storchastic to support deep learning modelers. They can use Storchastic to focus on defining stochastic deep learning models without having to worry about complex gradient estimation implementations. Storchastic extends DiCE [13] to other gradient estimation techniques than basic applications of the score function. It defines a surrogate loss by decomposing gradient estimation methods into four components: The proposal distribution, weight-
In short, our contributions are the following:

1. We introduce Storchastic, a new framework for general stochastic AD that uses four gradient estimation components, in Section 3.1-3.3.
2. We prove Theorem I which provides conditions under which Storchastic gives unbiased any-order derivative estimates in Section 3.4. To this end, we introduce a mathematical formalization of forward-mode evaluation in AD libraries in Section 2.4.
3. We derive a technique for extending variance reduction using control variates to any-order derivative estimation in Section 3.5.
4. We implement Storchastic as an open source library for PyTorch, Section 3.7.

Our main contribution is a framework with a formalization and a proof that, if the components satisfy certain conditions, performing \( n \)-th order differentiation on the Storchastic surrogate loss gives unbiased estimates of the \( n \)-th order derivative of the stochastic computation graph. We show these conditions hold for a wide variety of gradient estimation methods for first order differentiation. For many score function-based methods like RELAX [16], MAPO [28] and the unordered set estimator [23], the conditions also hold for any-order differentiation. In Storchastic, we only have to prove these conditions locally. This means that modelers are free to choose the gradient estimation method that best suits each sampling step, while guaranteeing that the gradient remains unbiased. Storchastic is the first stochastic AD framework to incorporate the measure-valued derivative [40, 18, 37] and SPSA [46, 2], and the first to guarantee variance reduction of any-order derivative estimates through control variates.

In short, our contributions are the following:

1. We introduce Storchastic, a new framework for general stochastic AD that uses four gradient estimation components, in Section 3.1-3.3.
2. We prove Theorem I which provides conditions under which Storchastic gives unbiased any-order derivative estimates in Section 3.4. To this end, we introduce a mathematical formalization of forward-mode evaluation in AD libraries in Section 2.4.
3. We derive a technique for extending variance reduction using control variates to any-order derivative estimation in Section 3.5.
4. We implement Storchastic as an open source library for PyTorch, Section 3.7.

Figure 1: An illustration of the (parallelized) Storchastic loss computation. a. Assign the stochastic nodes of the input stochastic computation graph (SCG) into two topologically sorted partitions. b. Evaluate the SCG. We first sample the set of values \( X_1 \) from the proposal distribution. For each of the samples \( x_1 \in X_1 \), we then sample a set of samples \( X_2 \). The rows in the figure indicate different samples in \( X_1 \), while the columns indicate samples in \( X_2 \). The different samples are used to evaluate the cost function \( f \mid X_1 \mid \cdot \mid X_2 \mid \times \) times. c. Compute the weighting function, control variate and gradient function for all samples. d. Using those components and the cost function evaluation, compute the stochastic surrogate loss, mimicking Algorithm I. \( \odot \) refers to element-wise multiplication, \( \oplus \) to element-wise summation and \( \sum \) for summing the entries of a matrix.
The problem we are interested in is estimating the gradients of these expectations with respect to the parameters. Since \( x \) is not influenced by the parameters, we have \( \nabla_\theta \left( \mathbb{E}_x[\ell_{KLD}] \right) = 0 \)
and \( \nabla^{(n)}_{\phi} \mathbb{E}_x [\ell_{KL,D}] = \mathbb{E}_x [\nabla^{(n)}_{\phi} \ell_{KL,D}] \). The second term is more challenging. We can move the gradient with respect to \( \theta \) in, since \( z \) is not influenced by \( \theta \): \( \nabla^{(n)}_{\theta} \mathbb{E}_{x,z \sim q_{\phi}(z|x)} [\ell_{Rec}] = \mathbb{E}_{x,z \sim q_{\phi}(z|x)} [\nabla^{(n)}_{\theta} \ell_{Rec}] \). However, we cannot compute \( \nabla^{(n)}_{\phi} \mathbb{E}_{x,z \sim q_{\phi}(z|x)} [\ell_{Rec}] \) without gradient estimation methods. This is because sampling from \( q_{\phi}(z|x) \) is dependent on \( \phi \). Furthermore, since we are dealing with a discrete stochastic node, we cannot apply the reparameterization method here without introducing bias.

2.4 Formalizing AD libraries and DiCE

To be able to properly formalize and prove the propositions in this paper, we introduce the ‘forward-mode’ operator that simulates forward-mode evaluation using AD libraries. This operator properly handles the common ‘stop-grad’ operator, which ensures that its argument is only evaluated during forward-mode evaluations of the computation graph. It is implemented in Tensorflow and Jax with the name `stop_gradient` and in PyTorch as `detach` or `no_grad`. ‘stop-grad’ is necessary to define surrogate losses for gradient estimation, which is why it is essential to properly define it. For formal definitions of the following operators and proofs we refer the reader to Appendix A.

**Definition 1** (informal). The stop-grad operator \( \perp \) is a function such that \( \nabla_x \perp (x) = 0 \). The forward-mode operator \( \rightarrow \), which is denoted as an arrow above the argument it evaluates, acts as an identity function, except that \( \overrightarrow{\perp}(a) = \overrightarrow{a} \). Additionally, we define the MagicBox operator as \( \overrightarrow{\times}(x) = \exp(x - \perp(x)) \).

Importantly, the definition of \( \rightarrow \) implies that \( \nabla_x f(x) \rightarrow \) does not equal \( \nabla_x \overrightarrow{f(x)} \) if \( f \) contains a stop-grad operator. MagicBox, which was first introduced in [13], is particularly useful for creating surrogate losses that remain unbiased for any-order differentiation. It is defined such that \( \overrightarrow{(1)} = 1 \) and \( \nabla_x \overrightarrow{f(x)} = \overrightarrow{f(x)} \nabla_x f(x) \). This allows injecting multiplicative factors to the computation graph only when computing gradients.

Making use of MagicBox, DiCE [13] is an estimator for automatic \( n \)th-order derivative estimation that defines a surrogate loss using the score function:

\[
\nabla^{(n)}_{\theta} \mathbb{E} \left[ \sum_{C \in \mathcal{C}} C \right] = \mathbb{E} \left[ \nabla^{(n)}_{\theta} \sum_{C \in \mathcal{C}} \log \frac{p(x_S | x_{pa(S)})}{C} \right]. \tag{1}
\]

DiCE correctly handles the credit assignment problem: The score function is only applied to the stochastic nodes that influence a cost node. It also handles pathwise dependencies of the parameter through cost functions. However, it has high variance since it is based on a straightforward application of the score function.

3 The Storchastic Framework

In this section, we introduce Storchastic, a framework for general any-order gradient estimation in SCGs that gives modelers the freedom to choose a suitable gradient estimation method for each stochastic node. First, we present 5 requirements that we used to develop the framework in Section 3.1. Storchastic deconstructs gradient estimators into four components that we present in Section 3.2. We use these components to introduce the Storchastic surrogate loss in Section 3.3 and give conditions that need to hold for unbiased estimation in Section 3.4. In Section 3.5 we discuss variance reduction, in Section 3.6 we discuss several estimators that fit in Storchastic, and in Section 3.7 we discuss our PyTorch implementation. An overview of our approach is outlined in Figure 1.

3.1 Requirements of the Storchastic Framework

First, we introduce the set of requirements we used to develop Storchastic.

1. Modelers should be able to choose a different gradient estimation method for each stochastic node. This allows for choosing the method best suited for that stochastic node, or adding background knowledge in the estimator.
2. *Storchastic* should be flexible enough to allow implementing a wide range of reviewed gradient estimation methods, including score function-based methods with complex sampling techniques [25, 28] or control variates [16, 47], and other methods such as measure-valued derivatives [18, 40] and SPSA [46] which are missing AD implementations [37].

3. Storchastic should define a surrogate loss [25], which gives gradients of the SCG when differentiated using an AD library. This makes it easier to implement gradient estimation methods as modelers get the computation of derivatives for free.

4. Differentiating the surrogate loss \( n \) times should give estimates of the \( n \)-th order derivative, which are used in for example reinforcement learning [15, 14] and meta-learning [12, 27].

5. Variance reduction methods through better sampling and control variates should generalize in higher-order derivative estimation.

6. Storchastic should be provably unbiased. To reduce the effort of developing new methods, researchers should only have to prove a set of local conditions that generalize to any SCG.

### 3.2 Gradient Estimators in Storchastic

Next, we introduce each of the four components and motivate why each is needed to ensure Requirement [2] is satisfied. First, we note that several recent gradient estimators, like MAPO [29], unordered set estimator [25] and self-critical baselines [21, 42] act on sequences of stochastic nodes instead of on a single stochastic node. Therefore, we create a partition \( S_1, \ldots, S_k \) of \( S_{\prec C} \) topologically ordered by the influence relation, and define the shorthand \( x_i := x_{S_i} \). For each partition \( S_i \), we choose a gradient estimator, which is a 4-tuple \( (q_i, w_i, l_i, a_i) \). Here, \( q_i(x_i) \) is the proposal distribution, \( w_i(x_i) \) is the weighting function, \( l_i(x_i) \) is the gradient function and \( a_i \) is the control variate.

#### 3.2.1 Proposal distribution

Many gradient estimation methods in the literature do not sample a single value \( x_i \sim p(x_i | x_{\prec i}) \), but sample, often multiple, values from possibly a different distribution. Some instances of sampling schemes are taking multiple i.i.d. samples, importance sampling [32] which is very common in off-policy reinforcement learning, sampling without replacement [25], memory-augmented sampling [28] and antithetic sampling [51]. Furthermore, measure-valued derivatives [18, 40] and SPSA [46] also sample from different distributions by comparing the performance of two related distributions. To capture this, the proposal distribution \( q_i(x_i | x_{\prec i}) \) samples a set of values \( X_i = \{x_{i,1}, \ldots, x_{i,m}\} \) where each \( x_{i,j} \in \Omega_{S_i} \). The sample is conditioned on \( x_{\prec i} = \bigcup_{S \in S_i} x_{\text{pa}(S)} \), the values of the parent nodes of the stochastic nodes in \( S_i \). This is illustrated in Figure 1.b.

#### 3.2.2 Weighting function

When a gradient estimator uses a different sampling scheme, we have to weight each individual sample to ensure it remains a valid estimate of the expectation. For this, we use a nonnegative weighting function \( w_i : \Omega_{S_i} \rightarrow \mathbb{R}^+ \). Usually, this function is going to be detached from the computation graph, but we allow it to receive gradients as well to support implementing expectations and gradient estimation methods that compute the expectation over (a subset of) values [25, 28, 30].

#### 3.2.3 Gradient function

The gradient function is an unbiased gradient estimator together with the weighting function. It distributes the empirical cost evaluation to the parameters of the distribution. In the case of score function methods, this is the log-probability. For measure-valued derivatives and SPSA we can use the parameters of the distribution itself.

#### 3.2.4 Control variate

Modelers can use control variates to reduce the variance of gradient estimates [17, 37]. It is a function that has zero-mean when differentiated. Within the context of score functions, a common control variate is a baseline, which is a function that is independent of the sampled value. We also found that LAX, RELAX, and REBAR (Appendix D.2.4), and the GO gradient [7] (Appendix D.2.6) have natural implementations using a control variate. We discuss how we implement control variates in *Storchastic* in Section 3.5.
3.2.5 Example: Leave-one-out baseline

As an example, we show how to formulate the score function with the leave-one-out baseline \([35, 22]\) in *Storchastic*. This method samples \(m\) values with replacement and uses the average of the other values as a baseline.

- **Proposal distribution**: We use \(m\) samples with replacement, which can be formulated as
  \[
  q(\mathcal{X}_i|\mathcal{X}_{<i}) = \prod_{j=1}^m p(\mathbf{x}_{i,j}|\mathbf{x}_{<i}).
  \]
- **Weighting function**: Since samples are independent, we use \(w_i(\mathbf{x}_i) = \frac{1}{m}\).
- **Gradient function**: The score-function uses the log-probability \(l_i(\mathbf{x}_i) = \log p(\mathbf{x}_i|\mathbf{x}_{<i})\).
- **Control variate**: We use \(a_{i,j}(\mathbf{x}_{<i}, \mathcal{X}_i) = (1 - \frac{1}{m} \sum_{j' \neq j} f_C(\mathbf{x}_{<i}, \mathbf{x}_{i,j'}))\) where \(\frac{1}{m} \sum_{j' \neq j} f_C(\mathbf{x}_{<i}, \mathbf{x}_{i,j'})\) is the leave-one-out baseline. \((1 - \frac{1}{m} \sum_{j' \neq j} f_C(\mathbf{x}_{<i}, \mathbf{x}_{i,j'}))\) is used to ensure the baseline will be subtracted from the cost before multiplication with the gradient function. It will not affect the forward evaluation since \(1 - \frac{1}{m} \sum_{j' \neq j} f_C(\mathbf{x}_{<i}, \mathbf{x}_{i,j'})\) evaluates to 0.

3.3 The Storchastic Surrogate Loss

As mentioned in Requirement [3] we would like to define a *surrogate loss*, which we will introduce next. Differentiating this loss \(n\) times, and then evaluating the result using an AD library, will give unbiased estimates of the \(n\)-th order derivative of the parameter \(\theta\) with respect to the cost \(C\). Furthermore, according to Requirement[1] we assume the modeler has chosen a gradient estimator \((\hat{q}_i, \hat{w}_i, \hat{l}_i, \hat{a}_i)\) for each partition \(S_i\), which can all be different. Then the Storchastic surrogate loss is

\[
SL_{\text{Storch}} = \sum_{\mathbf{x}_1 \in \mathcal{X}_1} w_1(\mathbf{x}_1) \left[ a_1(\mathbf{x}_1, \mathcal{X}_1) + \sum_{\mathbf{x}_2 \in \mathcal{X}_2} w_2(\mathbf{x}_2) \left[ \sum_{j=1}^{k-1} \left( \sum_{i=1}^k \hat{f}_C(\mathbf{x}_{<i}, \mathbf{x}_{i,j}) a_k(\mathbf{x}_{<k}, \mathcal{X}_i) + \left( \sum_{i=1}^k \hat{f}_C(\mathbf{x}_{<i}, \mathcal{X}_i) \hat{C} \right) \right] \right] \]

where \(\overline{C}_{\mathbf{x}_{<k}}\) is used to distribute cost. It will not affect the forward evaluation since \(1 - \overline{C}_{\mathbf{x}_{<k}}\) evaluates to 0.

When this loss is differentiated \(n\) times using AD libraries, it will produce unbiased estimates of the \(n\)-th derivative, as we will show later. To help understand the Storchastic surrogate loss and why it satisfies the requirements, we will break it down using Algorithm[1]. The `ESTIMATE_GRADIENT` function computes the surrogate loss for the SCG, and then differentiates it \(n \geq 0\) times using the AD library to return an estimate of the \(n\)-th order gradient, which should be unbiased according to Requirement[1] if \(n\) is set to zero, this returns an estimate of the expected cost.
The SURROGATE_LOSS function computes the equation using a recursive computation, which is illustrated in Figure 1b-d. It iterates through the partitions and uses the gradient estimator to sample and compute the output of each component. It receives three inputs: The first input $i$ indexes the partitions and gradient estimators, the second input $x_{<i}$ is the set of previously sampled values for partitions $S_{<i}$, and $L$ is the sum of gradient functions of those previously sampled values. In line 8, we sample a set of values $\mathcal{X}_i$ for partition $i$ from $q(\mathcal{X}_i|x_{<i})$. In lines 9 to 14, we compute the sum over values $x_i$ in $\mathcal{X}_i$, which reflects the $i$-th sum of the equation. Within this summation, in lines 11 and 12, we compute the gradient function and control variate for each value $x_i$. We will explain in Section 3.5 why we multiply the control variate with the MagicBox of the sum of the previous gradient function.

In line 13, we go into recursion by moving to the next partition. We condition the surrogate loss on the previous samples $x_{<i}$ together with the newly sampled value $x_i$. We pass the sum of gradient functions for later usage in the recursion. Finally, in line 14, the sample performance and the control variate are added in a weighted sum. The recursion call happens for each $x_i \in \mathcal{X}_i$, meaning that this computation is exponential in the size of the sampled sets of values $\mathcal{X}_i$. For example, the surrogate loss samples $|\mathcal{X}_i|$ times from $q_2$, one for each value $x_i \in \mathcal{X}_i$. However, this computation can be trivially parallelized by using tensor operations in AD libraries. An illustration of this parallelized computation is given in Figure 1.

Finally, in line 7 after having sampled values for all $k$ partitions, we compute the cost, and multiply it with the MagicBox of the sum of gradient functions. This is similar to what happens in the DiCE estimator in Equation (1). Storchastic can be extended to multiple cost nodes by computing surrogate losses for each cost node, and adding these together before differentiation. For stochastic nodes that influence multiple cost nodes, the algorithm can share samples and gradient estimation methods to reduce overhead.

### 3.4 Conditions for Unbiased Estimation

We next introduce our main result that shows Storchastic satisfies Requirements 4 and 6, namely the conditions the gradient estimators should satisfy such that the Storchastic surrogate loss gives estimates of the $n$-th order gradient of the SCG. A useful part of our result is that, in line with Requirement 6, only local conditions of gradient estimators have to be proven to ensure estimates are unbiased. Our result gives immediate generalization of these local proofs to any SCG.

**Theorem 1.** Evaluating the $n$-th order derivative of the Storchastic surrogate loss in Equation (2) using an AD library is an unbiased estimate of $\nabla^m \mathbb{E}[C]$ under the following conditions. First, all functions $f_E$ corresponding to deterministic nodes $F$ and all probability measures $P_S$ corresponding to stochastic nodes $S$ are identical under evaluation. Second, for each gradient estimator $(q_i, w_i, l_i, a_i)$, $i = 1, ..., k$, all the following hold for $m = 0, ..., n$:

1.  $\mathbb{E}_{q_1}(\mathcal{X}_i|x_{<i}) \left[ \sum_{x_i \in \mathcal{X}_i} \nabla^m_{\theta} w_i(x_i) \mathcal{E}(l_i(x_i)) f(x_i) \right] = \nabla^m_{\theta} \mathbb{E}_{q_1}(f(x_i))$ for any deterministic function $f$;

2.  $\mathbb{E}_{q_1}(\mathcal{X}_i|x_{<i}) \left[ \sum_{x_i \in \mathcal{X}_i} \nabla^m_{\theta} w_i(x_i) a_i(x_{<i}, \mathcal{X}_i) \right] = 0$;

3.  for $n \geq m > 0$, $\mathbb{E}_{q_1}(\mathcal{X}_i|x_{<i}) \left[ \sum_{x_i \in \mathcal{X}_i} \nabla^m_{\theta} w_i(x_i) \right] = 0$;

4.  $q(\mathcal{X}_i|x_{<i}) = q(\mathcal{X}_i|x_{<i})$, for all permissible $\mathcal{X}_i$.

The first condition defines a local surrogate loss for single expectations of any function under the proposal distribution. The condition then says that this surrogate loss should give an unbiased estimate of the gradient for all orders of differentiation $m = 0, ..., n$. Note that since 0 is included, the forward evaluation should also be unbiased. This is the main condition used to prove unbiasedness of the Storchastic framework, and can be proven for the score function and expectation, and for measure-valued derivatives and SPSA for zeroth and first-order differentiation.

The second condition says that the control variate should be 0 in expectation under the proposal distribution for all orders of differentiation. This is how control variates are defined in previous work [34], and should usually not restrict the choice. The third condition constrains the weighting
function to be 0 in expectation for orders of differentiation larger than 0. Usually, this is satisfied by the fact that weighting functions are detached from the computation graph, but when enumerating expectations, this can be shown by using that the sum of weights is constant. The final condition is a regularity condition that says proposal distributions should not be different under forward mode.

We also assume that the SCG is identical under evaluation. This means that all functions and probability densities evaluate to the same value with and without the forward-mode operator, even when differentiated. This concept is formally introduced in Appendix A.

A full formalization and the proof of Theorem 1 are given in Appendix B.1. The general idea is to rewrite each sampling step as an expectation, and then inductively show that the inner expectation over the proposal distribution \( q_i \) is an unbiased estimate of the \( n \)-th order derivative over \( S_i \) conditional on the previous samples. To reduce the multiple sums over gradient functions inside MagicBox, we make use of a property of MagicBox, we formulate enumerating the arguments in individual MagicBoxes, ie:

\[
\nabla l(x) f(x) \equiv \nabla l(x) l(x) f(x).
\]

Equivalence under evaluation, denoted \( \equiv \), formally means that, under evaluation of \( \rightarrow \), the two expressions and their derivatives are equal. This equivalence is closely related to \( e^{a+b} = e^a e^b \).

3.5 Any-order variance reduction using control variates

To satisfy Requirement 5 we investigate implementing control variates such that the variance of any-order derivatives is properly decreased. This is challenging in general SCG's [33], since in higher orders of differentiation, derivatives of gradient functions will interact, but naive implementations of control variates only reduce the variance of the gradient function corresponding to a single stochastic node. *Storchastic* solves this problem similarly to the method introduced in [33]. In line 11 of the algorithm, we multiply the control variate with the sum of preceding gradient functions \( \nabla x_j \). We prove that this ensures every term of the any-order derivative will be affected by a control variate in Appendix C. This proof is new, since [33] only showed this for first and second order differentiation, not for general control variates, and uses a slightly different formulation that we show misses some terms.

**Theorem 2 (informal).** Let \( L_i = \sum_j^i l_i \). The Stochastic surrogate loss of \( \text{2} \) can equivalently be computed as

\[
SL_{Storch} \equiv \sum_{x_1 \in X_1} \cdots \sum_{x_k \in X_k} \prod_{i=1}^k w_i(x_i) \sum_{i=1}^k \nabla(l_{i-1}) \left( a_i(x_{<i}, X_i) + (\nabla(l_i) - 1)C \right) + C.
\]

This gives insight into how control variates are used in *Storchastic*. They are added to the gradient function, but only during differentiation since \( \nabla l_i = 1 \). Furthermore, since both terms are multiplied with \( \nabla l_i \) (see line 11 of Algorithm 1), both terms correctly distribute over the same any-order derivative terms. By choosing a control variate of the form \( a_i(x_{<i}, X_i) = (1 - \nabla l_i) \cdot b_i \), we recover baselines which are common in the context of score functions [13] [37]. For the proof, we use the following proposition also proven in Appendix C:

**Proposition 4.** For orders of differentiation \( n > 0 \),

\[
\nabla_N^{(n)} \sum_k \nabla_N^{(n)}(l_i) = \nabla_N^{(n)} \sum_{i=1}^k (\nabla(l_i) - 1)\nabla(l_{i-1}).
\]

3.6 Gradient Estimation Methods

In Appendix D we show how several prominent examples of gradient estimation methods in the literature can be formulated using *Storchastic*, and prove for what orders of differentiation the conditions hold. Starting off, we show that for finite discrete random variables, we can formulate enumerating over all possible options using *Storchastic*. The score function fits by mimicking DiCE [13]. We extend it to multiple samples with replacement to allow using the leave-one-out baseline [33] [22].
class ScoreFunctionLOO(storch.method.Method):
    def proposal_dist(self, distribution, amt_samples):
        return dist.sample((amt_samples,))

    def weighting_function(self, distribution, amt_samples):
        return torch.full(amt_samples, 1/amt_samples)

    def estimator(self, sample, cost):
        # Compute gradient function (log-probability)
        log_prob = sample.distribution.log_prob(tensor)
        sum_costs = storch.sum(costs.detach(), sample.name)
        # Compute control variate
        baseline = (sum_costs - costs) / (sample.n - 1)
        return log_prob, (1.0 - magic_box(log_prob)) * baseline

Figure 3: Implementing the score function with the leave-one-out baseline in the Storchastic library.

Furthermore, we show how importance sampling, sum-and-sample estimators such as MAPO [28],
the unordered set estimator [25] and RELAX and REBAR [16,47] fit in Storchastic. We also discuss
the antithetic sampling estimator ARM [51]. Unfortunately, condition 2 only holds for this estimator
for $n \leq 1$ since it relies on a particular property of the score function that holds only for first-order
gradient estimation. In addition to score function based methods, we discuss the GO gradient, SPSA
[44] and Measure-Valued Derivative [18], and show that the last two will only be unbiased for $n \leq 1.$
Finally, we note that reparameterization [20] can be implemented by transforming the SCG such
that the sampling step is outside the path from the parameter to the cost [45].

3.7 Implementation

We implemented Storchastic as an open source PyTorch [39] library. To ensure modelers can eas-
ily use this library, it automatically handles sets of samples as extra dimensions to PyTorch tensors
which allows running multiple sample evaluations in parallel. This approach is illustrated in Fig-
ure 1. By making use of PyTorch broadcasting semantics, this allows defining models for simple
single-sample computations that are automatically parallelized using Storchastic when using mul-
tiple samples. The Storchastic library has implemented most of the gradient estimation methods
mentioned in Section 3.6. Furthermore, new gradient estimation methods can seamlessly be added.

3.7.1 Example: Leave-one-out baseline in Discrete Variational Autoencoder

As a small case study, we show how to implement the score function with the leave-one-out baseline
introduced in Section 3.2.5 for the discrete variational autoencoder introduced in Section 2.3 in
PyTorch using Storchastic. While the code listed is simplified, it shows the flexibility with which
one can compute gradients in SCGs.

We list in Figure 3 how to implement the score function with the leave-one-out baseline. Line 3
implements the proposal distribution, line 6 the weighting function, line 10 the gradient function and
line 14 the control variate. Gradient estimation methods in Storchastic all extend a common
base class storch.method.Method to allow easy interoperability between different methods.

In Figure 4 we show how to implement the discrete VAE. The implementation directly follows the
SCG shown in Figure 2. In line 2, we create the ScoreFunctionLOO method defined in Figure 3.
Then, we run the training loop: In line 6 we create the stochastic node $\alpha$ by denoting the minibatch
dimension as an independent dimension. In line 8 we run the encoder with parameters $\phi$ to find the

\textit{new gradient estimation methods can seamlessly be added.}

\textit{3.7.1 Example: Leave-one-out baseline in Discrete Variational Autoencoder}

As a small case study, we show how to implement the score function with the leave-one-out baseline
introduced in Section 3.2.5 for the discrete variational autoencoder introduced in Section 2.3 in
PyTorch using Storchastic. While the code listed is simplified, it shows the flexibility with which
one can compute gradients in SCGs.

We list in Figure 3 how to implement the score function with the leave-one-out baseline. Line 3
implements the proposal distribution, line 6 the weighting function, line 10 the gradient function and
line 14 the control variate. Gradient estimation methods in Storchastic all extend a common
base class storch.method.Method to allow easy interoperability between different methods.

In Figure 4 we show how to implement the discrete VAE. The implementation directly follows the
SCG shown in Figure 2. In line 2, we create the ScoreFunctionLOO method defined in Figure 3.
Then, we run the training loop: In line 6 we create the stochastic node $\alpha$ by denoting the minibatch
dimension as an independent dimension. In line 8 we run the encoder with parameters $\phi$ to find the
variational posterior $q_z$. We call the gradient estimation method in line 9 to get a sample of $z$. Note
that this interface is independent of gradient estimation method chosen, meaning that if we wanted
to compare our implemented method with a baseline, all that is needed is to change line 2. After the
decoder, we compute the two costs in lines 12 and 13. Finally, we call Storchastic main algorithm
in line 15 and run the optimizer.

\footnote{Code is available at \url{github.com/HEmile/storchastic}}
from vae import minibatches, encode, decode, KLD, binary_cross_entropy
method = ScoreFunctionLOO("z", 8)
for data in minibatches():
    optimizer.zero_grad()
    # Denote minibatch dimension as independent plate dimension
    data = storch.denoise_independent(data.view(-1, 784), 0, "data")
    # Compute variational distribution given data, sample z
    q = torch.distributions.OneHotCategorical(logits=encode(data))
    z = method(q)
    # Compute costs, form the ELBO
    reconstruction = decode(z)
    storch.add_cost(KLD(q))
    storch.add_cost(binary_cross_entropy(reconstruction, data))
    # Stochastic backward pass, optimize
    ELBO = storch.backward()
    optimizer.step()

Figure 4: Simplified implementation of the discrete VAE using Storchastic.

We run this model on our currently implemented set of gradient estimation methods for discrete variables in Appendix E and report the results, which are meant purely to illustrate the case study.

4 Related Work

The literature on gradient estimation is rich, with papers focusing on general methods that can be implemented in Storchastic [46, 18, 16, 51, 28, 30, 7], see Appendix D, and works focused on Reinforcement Learning [49, 29, 36] or Variational Inference [35]. For a recent overview, see [37].

The literature focused on SCGs is split into methods using reparameterization [43, 20, 11, 31, 19] and those using the score function [45]. Of those, DiCE [13] is most similar to Storchastic, and can do any-order estimation on general SCGs. DiCE is used in the probabilistic programming library Pyro [3]. We extend DiCE to allow for incorporating many other gradient estimation methods than just basic score function. We also derive and prove correctness of a general implementation for control variates for any-order estimation which is similar to the one conjectured for DiCE in [33].

[38, 50] and [38] study actor-critic-like techniques and bootstrapping for SCGs to incorporate reparameterization using methods inspired by deterministic policy gradients [29]. By using models to differentiate through, these methods are biased through model inaccuracies and thus do not directly fit into Storchastic. However, combining these ideas with the automatic nature of Storchastic could be interesting future work.

5 Conclusion

We investigated general automatic differentiation for stochastic computation graphs. We developed the Storchastic framework, and introduced an algorithm for unbiased any-order gradient estimation that allows using a large variety of gradient estimation methods from the literature. We also investigated variance reduction and showed how to properly implement control variates such that it affects any-order gradient estimates. The framework satisfies the requirements introduced in Section 3.1.

For future work, we are interested in extending the analysis of Storchastic to how variance compounds when using different gradient estimation methods. Furthermore, Storchastic could be extended to allow for biased methods. We are also interested in closely analyzing the different components of gradient estimators, both from a theoretical and empirical point of view, to develop new estimators that combine the strengths of estimators in the literature.

References

[1] M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. S. Corrado, A. Davis, J. Dean, M. Devin, S. Ghemawat, I. Goodfellow, A. Harp, G. Irving, M. Isard, Y. Jia, R. Joze-
fowicz, L. Kaiser, M. Kudlur, J. Levenberg, D. Mané, R. Monga, S. Moore, D. Murray, C. Olah, M. Schuster, J. Shlens, B. Steiner, I. Sutskever, K. Talwar, P. Tucker, V. Vanhoucke, V. Vasudevan, F. Viégas, O. Vinyals, P. Warden, M. Wattenberg, M. Wicke, Y. Yu, and X. Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems. 2015.

[2] S. Bhatnagar, H. Prasad, and L. Prashanth. Stochastic Recursive Algorithms for Optimization, volume 434 of Lecture Notes in Control and Information Sciences. Springer London, London, 2013. ISBN 978-1-4471-4284-3 978-1-4471-4285-0. doi: 10.1007/978-1-4471-4285-0.

[3] E. Bingham, J. P. Chen, M. Jankowiak, F. Obermeyer, N. Pradhan, T. Karaletsos, R. Singh, P. A. Szerlip, P. Horsfall, and N. D. Goodman. Pyro: Deep universal probabilistic programming. Journal of Machine Learning Research, 20:28:1–28:6, 2019.

[4] J. Bradbury, R. Frostig, P. Hawkins, M. J. Johnson, C. Leary, D. Maclaurin, G. Necula, A. Paszke, J. VanderPlas, S. Wanderman-Milne, and Q. Zhang. JAX: Composable transformations of Python+NumPy programs, 2018.

[5] L. Buesing, T. Weber, and S. Mohamed. Stochastic gradient estimation with finite differences. page 4, 2016.

[6] G. Casella and C. P. Robert. Rao-blackwellisation of sampling schemes. Biometrika, 83(1): 81–94, 1996. ISSN 00063444.

[7] Y. Cong, M. Zhao, K. Bai, and L. Carin. GO gradient for expectation-based objectives. page 30, 2019.

[8] G. Correia, V. Niculae, W. Aziz, and A. Martins. Efficient marginalization of discrete and structured latent variables via sparsity. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, Advances in Neural Information Processing Systems, volume 33, pages 11789–11802. Curran Associates, Inc., 2020.

[9] Z. Dong, A. Mnih, and G. Tucker. DisARM: An antithetic gradient estimator for binary latent variables. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, Advances in Neural Information Processing Systems, volume 33, pages 18637–18647. Curran Associates, Inc., 2020.

[10] G. Farquhar, S. Whiteson, and J. N. Foerster. Loaded DiCE: Trading off bias and variance in any-order score function gradient estimators for reinforcement learning. In H. M. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. B. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada, pages 8149–8160, 2019.

[11] M. Figurnov, S. Mohamed, and A. Mnih. Implicit reparameterization gradients. In S. Bengio, H. M. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada, pages 439–450, 2018.

[12] C. Finn, P. Abbeel, and S. Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In D. Precup and Y. W. Teh, editors, Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017, volume 70 of Proceedings of Machine Learning Research, pages 1126–1135. PMLR, 2017.

[13] J. Foerster, G. Farquhar, M. Al-Shedivat, T. Rocktäschel, E. Xing, and S. Whiteson. DiCE: The infinitely differentiable monte carlo estimator. In International Conference on Machine Learning, pages 1529–1538, 2018.

[14] J. N. Foerster, R. Y. Chen, M. Al-Shedivat, S. Whiteson, P. Abbeel, and I. Mordatch. Learning with opponent-learning awareness. In E. André, S. Koenig, M. Dastani, and G. Sukthankar, editors, Proceedings of the 17th International Conference on Autonomous Agents and MultiAgent Systems, AAMAS 2018, Stockholm, Sweden, July 10-15, 2018, pages 122–130. International Foundation for Autonomous Agents and Multiagent Systems Richland, SC, USA / ACM, 2018.

[15] T. Furmston, G. Lever, and D. Barber. Approximate newton methods for policy search in markov decision processes. Journal of Machine Learning Research, 17:227:1–227:51, 2016.
[16] W. Grathwohl, D. Choi, Y. Wu, G. Roeder, and D. Duvenaud. Backpropagation through the void: Optimizing control variates for black-box gradient estimation. In 6th International Conference on Learning Representations, ICLR 2018 - Conference Track Proceedings, 2018.

[17] E. Greensmith, P. L. Bartlett, and J. Baxter. Variance reduction techniques for gradient estimates in reinforcement learning. Journal of Machine Learning Research, 5(9), 2004.

[18] B. Heidergott and F. Vázquez-Abad. Measure-valued differentiation for Markov chains. Journal of Optimization Theory and Applications, 136(2):187–209, 2008.

[19] E. Jang, S. Gu, and B. Poole. Categorical reparameterization with gumbel-softmax. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings, 2017.

[20] D. P. Kingma and M. Welling. Auto-encoding variational bayes. In 2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Conference Track Proceedings, 2014.

[21] W. Kool, H. van Hoof, and M. Welling. Attention, learn to solve routing problems! In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019. OpenReview.net, 2019.

[22] W. Kool, H. van Hoof, and M. Welling. Buy 4 REINFORCE samples, get a baseline for free! page 14, 2019.

[23] W. Kool, H. van Hoof, and M. Welling. Stochastic beams and where to find them: The gumbel-top-k trick for sampling sequences without replacement. In K. Chaudhuri and R. Salakhutdinov, editors, Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA, volume 97 of Proceedings of Machine Learning Research, pages 3499–3508. PMLR, 2019.

[24] W. Kool, H. van Hoof, and M. Welling. Ancestral gumbel-top-k sampling for sampling without replacement. Journal of Machine Learning Research, 21(47):1–36, 2020.

[25] W. Kool, H. van Hoof, and M. Welling. Estimating gradients for discrete random variables by sampling without replacement. page 28, 2020.

[26] Y. LeCun and C. Cortes. MNIST handwritten digit database. 2010.

[27] Z. Li, F. Zhou, F. Chen, and H. Li. Meta-SGD: Learning to Learn Quickly for Few-Shot Learning. arXiv:1707.09835 [cs], Sept. 2017.

[28] C. Liang, M. Norouzi, J. Berant, Q. Le, and N. Lao. Memory Augmented Policy Optimization for Program Synthesis and Semantic Parsing. arXiv:1807.02322 [cs, stat], Jan. 2019.

[29] T. P. Lillicrap, J. J. Hunt, A. Pritzel, N. Heess, T. Erez, Y. Tassa, D. Silver, and D. Wierstra. Continuous control with deep reinforcement learning. In 4th International Conference on Learning Representations, ICLR 2016, San Juan, Puerto Rico, May 2-4, 2016, Conference Track Proceedings, 2016.

[30] R. Liu, J. Regier, N. Tripuraneni, M. I. Jordan, and J. D. McAuliffe. Rao-blackwellized stochastic gradients for discrete distributions. In K. Chaudhuri and R. Salakhutdinov, editors, Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA, volume 97 of Proceedings of Machine Learning Research, pages 4023–4031. PMLR, 2019.

[31] C. J. Maddison, A. Mnih, and Y. W. Teh. The concrete distribution: A continuous relaxation of discrete random variables. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings, 2017.

[32] A. R. Mahmood, H. Van Hasselt, and R. S. Sutton. Weighted importance sampling for off-policy learning with linear function approximation. In NIPS, pages 3014–3022, 2014.

[33] J. Mao, J. Foerster, T. Rocktäschel, M. Al-Shedivat, G. Farquhar, and S. Whiteson. A baseline for any order gradient estimation in stochastic computation graphs. In K. Chaudhuri and R. Salakhutdinov, editors, Proceedings of the 36th International Conference on Machine Learning, volume 97 of Proceedings of Machine Learning Research, pages 4343–4351, Long Beach, California, USA, June 2019. PMLR.
A. Mnih and K. Gregor. Neural variational inference and learning in belief networks. In E. P. Xing and T. Jebara, editors, Proceedings of the 31st International Conference on Machine Learning, volume 32 of Proceedings of Machine Learning Research, pages 1791–1799, Beijing, China, June 2014. PMLR.

A. Mnih and D. J. Rezende. Variational inference for monte carlo objectives. In 33rd International Conference on Machine Learning, ICML 2016, 2016. ISBN 978-1-5108-2900-8.

V. Mnih, A. P. Badia, M. Mirza, A. Graves, T. P. Lillicrap, T. Harley, D. Silver, and K. Kavukcuoglu. Asynchronous methods for deep reinforcement learning. In Proceedings of the 33nd International Conference on Machine Learning, ICML 2016, New York City, NY, USA, June 19-24, 2016, pages 1928–1937, 2016.

S. Mohamed, M. Rosca, M. Figurnov, and A. Mnih. Monte carlo gradient estimation in machine learning. Journal of Machine Learning Research, 21:132:1–132:62, 2020.

P. Parmas. Total stochastic gradient algorithms and applications in reinforcement learning. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 31. Curran Associates, Inc., 2018.

A. Paszke, S. Gross, F. Massa, A. Lerer, J. Bradbury, G. Chanan, T. Killeen, Z. Lin, N. Gimelshein, L. Antiga, A. Desmaison, A. Kopf, E. Yang, Z. DeVito, M. Raison, A. Tejani, S. Chilamkurthy, B. Steiner, L. Fang, J. Bai, and S. Chintala. PyTorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d\textquotesingle Alch´e-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 8024–8035. Curran Associates, Inc., 2019.

G. C. Pflug. Sampling derivatives of probabilities. Computing, 1989. ISSN 0010-485X. doi: 10.1007/BF02243227.

R. Ranganath, S. Gerrish, and D. M. Blei. Black box variational inference. In Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics, AISTATS 2014, Reykjavik, Iceland, April 22-25, 2014, volume 33 of JMLR Workshop and Conference Proceedings, pages 814–822. JMLR.org, 2014.

S. J. Rennie, E. Marcheret, Y. Mroueh, J. Ross, and V. Goel. Self-Critical Sequence Training for Image Captioning. In 2017 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), pages 1179–1195, Honolulu, HI, July 2017. IEEE. ISBN 978-1-5386-0457-1. doi: 10.1109/CVPR.2017.131.

J. Schulman, N. Heess, T. Weber, and P. Abbeel. Gradient estimation using stochastic computation graphs. In Advances in Neural Information Processing Systems, 2015.

J. C. Spall et al. Multivariate stochastic approximation using a simultaneous perturbation gradient approximation. IEEE transactions on automatic control, 37(3):332–341, 1992.

G. Tucker, A. Mnih, C. J. Maddison, D. Lawson, and J. Sohl-Dickstein. REBAR: Low-variance, unbiased gradient estimates for discrete latent variable models. In Advances in Neural Information Processing Systems, 2017.

T. Weber, N. Heess, L. Buesing, and D. Silver. Credit assignment techniques in stochastic computation graphs. In K. Chaudhuri and M. Sugiyama, editors, The 22nd International Conference on Artificial Intelligence and Statistics, AISTATS 2019, 16-18 April 2019, Naha, Okinawa, Japan, volume 89 of Proceedings of Machine Learning Research, pages 2650–2660. PMLR, 2019.

R. J. Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. Machine Learning, 1992. ISSN 0885-6125. doi: 10.1007/bf00992696.

X. Xu, S. Zu, Y. Zhang, H. Zhou, and W. Feng. Backprop-Q: Generalized Backpropagation for Stochastic Computation Graphs. arXiv:1807.09511 [cs, stat], Jan. 2019.
A Forward-mode evaluation

In this section, we define several operators that we will use to mathematically define operators used within deep learning to implement gradient estimators.

To define these, we will need to distinguish how deep learning libraries evaluate their functions. \[\text{\texttt{JAX}}\] handles this using a different kind of equality, denoted $\rightarrow$. Unfortunately, it is not formally introduced, making it unclear as to what rules are allowed with this equality. For instance, they define the DiCE operator as

\[1. \quad \nabla_x f(\theta) \rightarrow 1\]
\[2. \quad \nabla_x (f(\theta) \nabla_x f(\theta)) = \nabla_x (f(\theta)) \nabla_x f(\theta) \rightarrow \nabla_x f(\theta)\]

However, without a clearly defined meaning of ‘equality under evaluation’, it is unclear whether the following is allowed:

\[\nabla_x f(\theta) \rightarrow \nabla_x 1 = 0\]

This would lead to a contradiction, as by definition

\[\nabla_x f(\theta) \rightarrow \nabla_x f(\theta) \rightarrow \nabla_x f(\theta)\]

We first introduce an unambiguous formulation for forward mode evaluation that does not allow such inconsistencies.

Definition 2. The \textit{stop-grad} operator $\bot$ is a function such that $\nabla_x \bot(x) = 0$. The \textit{forward-mode} operator $\rightarrow$ is a function such that, for well formed formulas $a$ and $b$,

\[\begin{align*}
1. \quad & \nabla_x (\bot(a)) = \nabla_x a \\
2. \quad & \nabla_x (a + b) = \nabla_x a + \nabla_x b \\
3. \quad & \nabla_x (a \cdot b) = \nabla_x a \cdot \nabla_x b \\
4. \quad & \nabla_x (a^b) = \nabla_x a^b \\
5. \quad & \nabla_x c = \nabla_x c, \text{ if } c \text{ is a constant or a variable.} \\
6. \quad & \nabla_x \bot(a) = \nabla_x a
\end{align*}\]

Additionally, we define the DiCE operator $\nabla_x (x) = \exp(x - \bot(x))$

When computing the results of a function $f(x)$, Deep Learning libraries instead compute $\nabla_x f(x)$. Importantly, $\nabla_x f(x)$ does not always equal $\nabla_x \nabla_x f(x)$. For example, $\nabla_x \bot(f(x)) \rightarrow \nabla_x 1 = 0$, while $\nabla_x \nabla_x (f(x)) = \nabla_x f(x)$.

In the last example, the derivative will first have to be rewritten to find a closed-form formula that does not contain the $\rightarrow$ operator. Furthermore, $\nabla_x \bot(f(x))$ only evaluates to a closed-form formula if it is reduced using derivation, or if it is enclosed in $\rightarrow$.

We note that $\mathbb{E}_{p(x)}[f(x)] = \mathbb{E}_{p(x)}[\nabla_x f(x)]$ for both continuous and discrete distributions $p(x)$ if $p(x) = p(x)$. This is easy to see for discrete distributions since these are weighted sums over an amount of elements. For continuous distributions we can use the Riemann integral definition.

\[\mathbb{E}_{p(x)}[f(x)] = \int p(x) f(x)\]
Definition 3. We say a function \( f(x) \) is identical under evaluation if for all \( n \in \{0, 1, 2, \ldots\} \),
\[
\nabla_x f^{(n)}(x) = \nabla_x g^{(n)}(x).
\]
Furthermore, we say that two functions \( f, g \) are equivalent under evaluation, denoted \( f \equiv g \), if for all \( n \in \{0, 1, 2, \ldots\} \), \( \nabla_x f^{(n)}(x) = \nabla_x g^{(n)}(x) \).

Proposition 1. 1: \( \overline{\mathcal{E}}(f(x)) = 1 \) and 2: \( \nabla_x \overline{\mathcal{E}}(f(x)) = \overline{\mathcal{E}}(f(x)) \cdot \nabla_x f(x) \)

Proof. 1.\[
\overline{\mathcal{E}}(f(x)) = \exp(f(x) - \perp(f(x))) = \exp(f(x) - \perp(f(x))) = \exp(f(x) - f(x)) = 1
\]
2.\[
\nabla_x \overline{\mathcal{E}}(f(x)) = \nabla_x \exp(f(x) - \perp(f(x))) = \exp(f(x) - \perp(f(x))) \nabla_x (f(x) - \perp(f(x))) = \overline{\mathcal{E}}(f(x))\nabla_x f(x)
\]

Furthermore, unlike in the DiCE paper, with this notation \( \nabla_x \overline{\mathcal{E}}(f(x)) \) unambiguously evaluates to \( \nabla_x f(x) \), as \( \nabla_x \overline{\mathcal{E}}(f(x)) = \overline{\mathcal{E}}(f(x))\nabla_x f(x) = \overline{\mathcal{E}}(f(x)) \cdot \nabla_x f(x) = \nabla_x f(x) \). Note that, although this is not a closed-form formula, by finding a closed-form formula for \( \nabla_x f(x) \), this can be reduced to \( \nabla_x f(x) \).

Proposition 2. For any two functions \( f(x) \) and \( l(x) \), it holds that for all \( n \in \{0, 1, 2, \ldots\} \),
\[
\nabla_x \overline{\mathcal{E}}(l(x)f(x)) = g^{(n)}(x).
\]

where \( g^{(n)}(x) = \nabla_x g^{(n-1)}(x) + g^{(n-1)}(x) \nabla_x l(x) \) for \( n > 0 \), and \( g^{(0)}(x) = f(x) \).

For this proof, we use a similar argument as in [13].

Proof. First, we show that \( \overline{\mathcal{E}}(l(x))g^{(n)}(x) = \nabla_x \overline{\mathcal{E}}(l(x))f(x) \). We start off with the base case, \( n = 0 \). Then, \( \overline{\mathcal{E}}(l(x))g^{(0)}(x) = \overline{\mathcal{E}}(l(x))f(x) \).

Next, assume the proposition holds for \( n \), that is, \( \overline{\mathcal{E}}(l(x))g^{(n)}(x) = \nabla_x \overline{\mathcal{E}}(l(x))f(x) \). Consider \( n + 1 \).
\[
\overline{\mathcal{E}}(l(x))g^{(n+1)}(x) = \overline{\mathcal{E}}(l(x))(\nabla_x g^{(n)}(x) + g^{(n)}(x) \nabla_x l(x))
\]
\[
= \nabla_x \overline{\mathcal{E}}(l(x))g^{(n)}(x)
\]
\[
= \nabla_x (\nabla_x ^{(n)}(\overline{\mathcal{E}}(l(x))f(x)))
\]
\[
= \nabla_x ^{(n+1)}(\overline{\mathcal{E}}(l(x))f(x))
\]

Where from line 1 to 2 we use the DiCE proposition in the reversed direction. From 2 to 3 we use the inductive hypothesis.

We use this result, \( \overline{\mathcal{E}}(l(x))g^{(n)}(x) = \nabla_x \overline{\mathcal{E}}(l(x))f(x) \), to prove our proposition. Since \( \overrightarrow{a} = 1 \cdot \overrightarrow{a} = \overrightarrow{a} = \overrightarrow{a} \overrightarrow{a} \),
\[
\overrightarrow{g^{(n)}(x)} = \overrightarrow{\mathcal{E}(l(x))g^{(n)}(x)} = \nabla_x ^{(n)}\overrightarrow{\mathcal{E}(l(x))f(x)}
\]

Definition 3. We say a function \( f \) is identical under evaluation if for all \( n \in \{0, 1, 2, \ldots\} \),
\[
\nabla_x f^{(n)}(x) = \nabla_x g^{(n)}(x).\]
Every function that does not contain a stop-grad operator (⊥) is identical under evaluation, although functions that are identical under evaluation can have stop-grad operators (for example, consider \( f(x) = f(x) + \perp(f(x) - f(x)) \)). Note that \( f(x) = f(x) \) does not necessarily mean that \( f \) is identical under evaluation, since for instance the function \( f'(x) = 2x \) \( f(x) \) has \( f'(x) = f(x) \), but \( \nabla f'(x) = 2 \nabla f(x) + \perp = \nabla f(x) + 2 \neq \nabla f'(x) = 2 \nabla f(x) + 2 \).

**Proposition 3.** If \( f(x) \) and \( l(x) \) are identical under evaluation, then all \( g^{(n)}(x) \) from \( n = 0, \ldots, n \) as defined in Proposition 2 are also identical under evaluation.

**Proof.** Consider \( n = 0 \). Then \( g^{(0)}(x) = f(x) \). Since \( f(x) \) is identical under evaluation, \( g^{(0)}(x) \) is as well.

Assume the proposition holds for \( n \), and consider \( n + 1 \). Let \( m \) be any positive number.

\[
\nabla^{(m)}_x g^{(n+1)}(x) = \nabla^{(m)}_x (\nabla_x g^{(n)}(x) + g^{(n)}(x) \nabla_x l(x)).
\]

Since \( g^{(n)}(x) \) is identical under evaluation by the inductive hypothesis, \( \nabla^{(m)}_x g^{(n)}(x) = \nabla^{(m+1)}_x g^{(n)}(x) = \nabla^{(m+1)}_x g^{(n)}(x) \).

Next, using the general Leibniz rule, we find that \( \nabla^{(m)}_x g^{(n)}(x) \nabla_x l(x) = \sum_{j=0}^{m} \left( \nabla^{(m-j)}_x g^{(n)}(x) \nabla^{(j+1)}_x l(x) \right) \). Since both \( g^{(n)}(x) \) and \( l(x) \) are identical under evaluation, this is equal to \( \sum_{j=0}^{m} \left( \nabla^{(m-j)}_x g^{(n)}(x) \nabla^{(j+1)}_x l(x) \right) = \nabla^{(m)}_x g^{(n)}(x) \nabla_x l(x) \).

Therefore, \( \nabla^{(m)}_x g^{(n+1)}(x) = \nabla^{(m)}_x (\nabla_x g^{(n)}(x) + g^{(n)}(x) \nabla_x l(x)) = \nabla^{(m)}_x g^{(n+1)}(x) \), which shows that \( g^{(n+1)}(x) \) is identical under evaluation.

We next introduce a very useful proposition that we will use to prove unbiasedness of the Stochastic framework. This result was first used without proof in [10].

**Proposition 4.** For any three functions \( l_1(x) \), \( l_2(x) \) and \( f(x) \), \( \nabla_\perp l_1(x) + l_2(x) f(x) \equiv \nabla_\perp (l_1(x)) \nabla_\perp (l_2(x)) f(x) \). That is, for all \( n \in (0, 1, 2, \ldots) \),

\[
\nabla^{(n)}_\perp (l_1(x) + l_2(x)) f(x) = \nabla^{(n)}_\perp (l_1(x)) \nabla^{(n)}_\perp (l_2(x)) f(x).
\]

**Proof.** Start with the base case \( n = 0 \). Then, \( \nabla_\perp (l_1(x) + l_2(x)) f(x) = f(x) = 1 \cdot 1 \cdot \nabla_\perp f(x) = \nabla_\perp (l_1(x)) \nabla_\perp (l_2(x)) f(x) \).

Next, assume the proposition holds for \( n \). Then consider \( n + 1 \):

\[
\nabla^{(n+1)}_\perp (l_1(x) + l_2(x)) f(x) = \nabla^{(n)}_\perp (l_1(x)) \nabla^{(n)}_\perp (l_2(x)) f(x).
\]

Define function \( h(x) = f(x) \nabla_\perp (l_1(x) + l_2(x)) + \nabla_\perp f(x) \). Since the proposition works for any function, we can apply the inductive hypothesis replacing \( f(x) \) by \( h(x) \):

\[
\nabla^{(n)}_\perp (l_1(x)) \nabla^{(n)}_\perp (l_2(x)) f(x) = \nabla^{(n+1)}_\perp (l_1(x) + l_2(x)) f(x).
\]

Finally, we use Proposition 2 with \( g^{(1)}(x) = h(x) \) and \( l(x) = l_1(x) + l_2(x) \):

\[
\nabla^{(n)}_\perp (l_1(x) + l_2(x)) f(x) \nabla_\perp (l_1(x) + l_2(x)) + \nabla_\perp f(x)
\]

\[
= \nabla^{(n+1)}_\perp (l_1(x) + l_2(x)) f(x) = \nabla^{(n+1)}_\perp (l_1(x) + l_2(x)) f(x)
\]

}\]
It should be noted that it cannot be proven that \( \nabla_{x}^{(n)} \sum_{i=1}^{k} l_{i}(x) f(x) = \nabla_{x}^{(n)} \sum_{i=1}^{k-1} l_{i}(x) \sum_{j=1}^{k} l_{j}(x) f(x) \) because the base-case cannot be proven without the \( \rightarrow \) operator interpreting the \( \sum \) operator.

Also note the parallels with the exponential function, where \( e^{l_{1}(x) + l_{2}(x)} = e^{l_{1}(x)} e^{l_{2}(x)} \).

**B The Stochastic framework (formal)**

In this section we formally introduce Stochastic to provide the mathematical machinery needed to prove our results. Let \( S_{1}, \ldots, S_{k} \) be a partition of \( S_{<F} \). Assume the sets \( S_{1}, \ldots, S_{k} \) are topologically sorted, that is, there is no \( i < j \) such that there exists a stochastic node \( S \in S_{j} \) that is also in \( S_{<i} = \bigcup_{j=1}^{i-1} S_{j} \). We use assignment \( x_{i} \) to denote a set that gives a value to each of the random variables \( S \in S_{i} \). That is, \( x_{i} \in \prod_{S \in S_{i}} \Omega_{S} \). We additionally use \( x_{<i} \) to denote a set that gives value to all random variables in \( S_{<i} \). In the same vein, \( X_{i} \) denotes a set of sets of values \( x_{i} \), that is \( X_{i} = \{ x_{i}, \ldots, x_{i} | x_{i} \} \).

**Definition 4.** For each partition \( S_{i} \) there is a gradient estimator \( (q_{i}, w_{i}, l_{i}, a_{i}) \) where \( q(X_{i} | x_{<i}) \) is a distribution over a set of values \( X_{i} \) conditioned on \( x_{<i} \), \( w_{i} : \prod_{S \in S_{i}} \Omega_{S} \rightarrow \mathbb{R}^{+} \) is the weighting function that weights different values \( x_{i} \), \( l_{i} : \prod_{S \in S_{i}} \Omega_{S} \rightarrow \mathbb{R} \) is the gradient function that provides the gradient produced by each \( x_{i} \), and the control variate \( a_{i} : \prod_{S \in S_{i}} \Omega_{S} \rightarrow \mathbb{R} \) is a function of both \( x_{i} \) and \( x_{<i} \).

\( q(X_{i} | x_{<i}) \) is factorized as follows: Order stochastic nodes \( S_{i,1}, \ldots, S_{i,m} \in S_{i} \) topologically, then

\[
q(X_{i} | x_{<i}) = \prod_{j=1}^{m} q(X_{i,j} | X_{i,j}, x_{<i}).
\]

In the rest of this appendix, we will define some shorthands to declutter the notation, as follows:

- \( w_{i} = w_{i}(x_{i}) \) and \( W_{i} = \prod_{j=1}^{i} w_{i} \)
- \( l_{i} = l_{i}(x_{i}) \) and \( L_{i} = \sum_{j=1}^{i} l_{i} \)
- \( a_{i} = a_{i}(x_{<i}, X_{i}) \)
- \( q_{1} = q(X_{1}) \) and \( q_{i} = q(X_{i} | x_{<i}) \) (for \( i > 1 \))

These interfere with the functions and distributions themselves, but it should be clear from context which of the two is meant.

**Proposition 5.** Given a topologically sorted partition \( S_{1}, \ldots, S_{k} \) of \( S_{<F} \) and corresponding gradient estimators \( (q_{i}, w_{i}, l_{i}, a_{i}) \) for each \( 1 \leq i \leq k \), the evaluation of the \( n \)-th order derivative of the Stochastic surrogate loss \( \nabla_{X}^{(n)} \sum_{X_{i} \in X_{i}} \nabla_{X}^{(n)} W_{k+1}(X_{i}) f(X_{i}) \) is equal in expectation to

\[
\mathbb{E}_{q_{1}} \left[ \sum_{X_{i} \in X_{i}} \nabla_{X}^{(n)} W_{k+1}(X_{i}) a_{1} + \ldots + \mathbb{E}_{q_{k}} \left[ \sum_{X_{i} \in X_{i}} \nabla_{X}^{(n)} W_{k+1}(X_{i}) a_{k} + \nabla_{X}^{(n)} W_{k+1}(X_{i}) f(X_{i}) + \ldots \right] \right] \quad (3)
\]

where the \( i \)-th term in the dots is \( \mathbb{E}_{q_{i}} \left[ \sum_{X_{i} \in X_{i}} \nabla_{X}^{(n)} W_{k+1}(X_{i}) a_{i} + \ldots \right] \)
Proof. By moving the weights inwards and using the $L_i$ notation,
\[
\nabla_N^{(n)} SL_{\text{Storch}} = \nabla_N^{(n)} \sum_{x_i \in X_i} w_i \left[ a_i + \cdots + \sum_{x_k \in X_k} w_k \left[ C(L_{k-1})a_k + C(L_k) \right] \right] \]
\[
= \nabla_N^{(n)} \sum_{x_i \in X_i} w_i a_i + \cdots + \sum_{x_k \in X_k} w_k \nabla_X^{(n)}(L_{k-1})a_k + \cdots 
\]
\[
+ \sum_{x_k \in X_k} W_k C(L_{k-1})a_k + W_k C(L_k)C 
\]
\[
= \sum_{x_i \in X_i} \nabla_N^{(n)} w_i a_i + \cdots + \sum_{x_k \in X_k} \nabla_N^{(n)} W_k C(L_{k-1})a_k + \cdots 
\]
\[
+ \sum_{x_k \in X_k} \nabla_N^{(n)} W_k C(L_{k-1})a_k + \nabla_N^{(n)} W_k C(L_k)C 
\]
This is all under sampling $X_1 \sim q(X_1), X_2 \sim q(X_2|X_1), \ldots, X_k \sim q(X_k|X_{<k})$. Taking expectations over these distributions before the respective summation over $X_i$ gives the result. \qedsymbol

In the Stochastic framework, we require that $\mathbb{E}[F]$ is identical under evaluation, that is, $\nabla_N^{(n)} \mathbb{E}[F] = \nabla_N^{(n)} \mathbb{E}[F]$. This in practice means that the probability distributions and functions in the stochastic computation graph contain no stop gradient operators ($\bot$).

Using Proposition 2, we give a recursive expression for $\nabla_N^{(n)} w_i (a_i + \nabla(l_i)f(x_i))$.

**Proposition 6.** For any gradient estimator $(q_i, w_i, l_i, a_i)$ it holds that
\[
\nabla_N^{(n)} w_i (\nabla(l_i)f(x_i)) = \nabla_N^{(n)} w_i (\nabla(l_i)f(x_i))
\]
where $g_i^{(n)}(x_i) = \nabla_N g_i^{(n-1)}(x_i) + g_i^{(n-1)} \nabla_N l_i$ for $n > 0$, and $g_i^{(0)}(x_i) = w_i f(x_i)$.

**Proof.** Using Proposition 2, we find that
\[
\nabla_N^{(n)} w_i (\nabla(l_i)f(x_i)) = \nabla_N^{(n)} w_i (\nabla(l_i)f(x_i)) = \nabla_N^{(n)} w_i (\nabla(l_i)f(x_i))
\]
\[
\]
Proposition 6 is useful because it gives a fairly simple recursion to proof unbiasedness of any-order estimators with, when the gradient estimator is implemented in Stochastic. Note that it doesn’t itself show that such gradient estimators are unbiased in any-order derivatives.

### B.1 Unbiasedness of the Stochastic framework

In this section, we use the equivalent expectation from Proposition 5.

**Theorem 1.** Let $(q_i, w_i, l_i, a_i)$ for $i = 1, \ldots, k$ be a sequence of gradient estimators. Let the stochastic computation graph $\mathbb{E}[F]$ be identical under evaluation. The evaluation of the nth-order derivative of the Stochastic surrogate loss is an unbiased estimate of $\nabla_N^{(n)} \mathbb{E}[F]$, that is
\[
\nabla_N^{(n)} \mathbb{E}[F] = \mathbb{E}_{q_1} \left[ \sum_{x_i \in X_i} \nabla_N^{(n)} w_i a_i + \cdots + \mathbb{E}_{q_k} \left[ \sum_{x_k \in X_k} \nabla_N^{(n)} W_k C(L_{k-1})a_k + \nabla_N^{(n)} W_k C(L_k)F \right] \right]
\]
if the following conditions hold for all estimators $i = 1, \ldots, k$ and all preceding orders of differentiation $n \geq m \geq 0$:

---

2In other words, all deterministic functions, and all probability measures associated with the stochastic nodes are identical under evaluation.
1. $\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla^m_N w_i \nabla^m_N (l_i) f(x_i)\right] = \nabla^m_N \mathbb{E}_q [f(x)]$ for any deterministic function $f$;

2. $\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla^m_N w_i a_i\right] = 0$;

3. for $n \geq m > 0$, $\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla^m_N w_i\right] = 0$;

4. $q(\mathcal{X}_i|x_{<i}) = q(\mathcal{X}_i|x_{<i})$.

**Proof.** In this proof, we make extensive use of the general Leibniz rule, which states that

$$\nabla^n x f(x) g(x) = \sum_{m=0}^{n} \binom{n}{m} \nabla^m x f(x) \nabla^{n-m} x g(x).$$

We consider the terms $\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla^m_N W^m_{j} (L_i) a_i\right]$ and the term $\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla_{N}^m W^m_{j} (L_k) F\right]$ separately, starting with the first.

**Lemma 1.1.** For any positive number $1 \leq j \leq k$,

$$\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \ldots \mathbb{E}_q \left[\sum_{x_j \in \mathcal{X}_j} \nabla^m_N W^m_{j} (L_j) a_j\right]\right] = 0.$$

**Proof.** We will prove the lemma using induction. First, let $j = 1$. Then, using condition 2,

$$\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla^m_N w_1 a_1\right] = 0$$

Next, assume the inductive hypothesis holds for $j$, and consider the inner expectation of $j + 1$:

$$= \mathbb{E}_{q_{j+1}}\left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \nabla^m_N W^m_{j+1} (L_j) a_{j+1} W_{j+1}\right] = \mathbb{E}_{q_{j+1}}\left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \nabla^m_N W^m_{j+1} a_{j+1} (L_j) W_{j+1}\right]$$

$$= \mathbb{E}_{q_{j+1}}\left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \sum_{m=0}^{n} \binom{n}{m} \nabla^m_N W^m_{j+1} a_{j+1} \nabla^{n-m} N (L_j) W_{j+1}\right]$$

Next, note that $W_j$ and $A_j$ are both independent of $x_{j+1}$. Therefore, they can be moved out of the expectation. To do this, we implicitly use condition 4 to move the $\rightarrow$ operator through the expectation.

$$\mathbb{E}_{q_{j+1}}\left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \sum_{m=0}^{n} \binom{n}{m} \nabla^m_N W^m_{j+1} a_{j+1} \nabla^{n-m} N (L_j) W_{j+1}\right]$$

$$= \sum_{m=0}^{n} \binom{n}{m} \nabla^m_N W^m_{j+1} a_{j+1} \mathbb{E}_{q_{j+1}}\left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \nabla^{n-m} N (L_j) W_{j+1}\right]$$

By condition 2 of the theorem, $\mathbb{E}_{q_{j+1}}\left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \nabla^{n-m} N (L_j) W_{j+1}\right] = 0$. Therefore, we can remove this term and conclude that

$$\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \ldots \mathbb{E}_{q_{j+1}} \left[\sum_{x_{j+1} \in \mathcal{X}_{j+1}} \nabla^m_N W^m_{j+1} (L_j) a_{j+1}\right]\right] = 0.$$

□

Next, we consider the term $\mathbb{E}_q\left[\sum_{x_i \in \mathcal{X}_i} \nabla^m_N W^m_{k} (L_k) F\right]$ and prove using induction that
**Lemma 1.2.** For any $1 \leq j \leq k$, it holds that

$$
\mathbb{E}_{q_1} \left[ \sum_{x_1 \in X_1} \ldots \mathbb{E}_{q_j} \left[ \sum_{x_j \in X_j} \nabla_{N}^{(n)} W_j \mathbb{C}(L_j) F' \right] \ldots \right] = \nabla_{N}^{(n)} \mathbb{E}[F']
$$

where $F' = \mathbb{E}_{S_j+1, \ldots, S_k}[F]$. Furthermore, for $1 < j \leq k$, it holds that

$$
\mathbb{E}_{q_1} \left[ \sum_{x_1 \in X_1} \ldots \mathbb{E}_{q_j} \left[ \sum_{x_j \in X_j} \nabla_{N}^{(n)} W_j \mathbb{C}(L_j) F' \right] \ldots \right] = \mathbb{E}_{q_1} \left[ \sum_{x_1 \in X_1} \ldots \mathbb{E}_{q_{j-1}} \left[ \sum_{x_{j-1} \in X_{j-1}} \nabla_{N}^{(n)} W_{j-1} \mathbb{C}(L_{j-1}) \mathbb{E}_{S_j}[F'] \right] \ldots \right]
$$

**Proof.** The base case $j = 1$ directly follows from condition 1:

$$
\mathbb{E}_{q_1} \left[ \sum_{x_1 \in X_1} \nabla_{N}^{(n)} W_1 \mathbb{C}(l_1) F' \right] = \nabla_{N}^{(n)} \mathbb{E}_{S_1}[F'] = \nabla_{N}^{(n)} \mathbb{E}[F],
$$

since $\mathbb{E}[F] = \mathbb{E}_{S_1, \ldots, S_k}[F]$ and by the assumption that $\mathbb{E}[F]$ is identical under evaluation.

Assume the lemma holds for $j < k$ and consider $j + 1$. First, we use Proposition 4 and reorder the terms:

$$
\mathbb{E}_{q_{j+1}} \left[ \sum_{x_{j+1} \in X_{j+1}} \nabla_{N}^{(n)} W_{j+1} \mathbb{C}(L_{j+1}) F' \right]
$$

Next, we again use the general Leibniz rule:

$$
\mathbb{E}_{q_{j+1}} \left[ \sum_{x_{j+1} \in X_{j+1}} \nabla_{N}^{(n)} W_{j+1} \mathbb{C}(L_{j+1}) w_{j+1} \mathbb{C}(l_{j+1}) F' \right]
$$

where we use for the general Leibniz rule $f = W_j \mathbb{C}(L_j)$ and $g = w_{j+1} \mathbb{C}(l_{j+1}) F'$. Note that $\nabla_{N}^{(n-m)} W_j \mathbb{C}(L_j)$ does not depend on $x_{j+1}$. Therefore,

$$
\mathbb{E}_{q_{j+1}} \left[ \sum_{x_{j+1} \in X_{j+1}} \nabla_{N}^{(n)} W_{j+1} \mathbb{C}(L_{j+1}) w_{j+1} \mathbb{C}(l_{j+1}) F' \right]
$$

$$
= \sum_{m=0}^{n} \binom{n}{m} \nabla_{N}^{(n-m)} W_j \mathbb{C}(L_j) \nabla_{N}^{(m)} w_{j+1} \mathbb{C}(l_{j+1}) F'
$$

$$
= \sum_{m=0}^{n} \binom{n}{m} \nabla_{N}^{(n-m)} W_j \mathbb{C}(L_j) \nabla_{N}^{(m)} \mathbb{E}_{S_{j+1}}[F']
$$

$$
= \nabla_{N}^{(n)} W_j \mathbb{C}(L_j) \mathbb{E}_{S_{j+1}}[F']
$$

From lines 2 to 3, we use condition 1 to reduce the expectation. In the last line, we use the general Leibniz rule in the other direction. We showed that

$$
\mathbb{E}_{q_1} \left[ \sum_{x_1 \in X_1} \ldots \mathbb{E}_{q_{j+1}} \left[ \sum_{x_{j+1} \in X_{j+1}} \nabla_{N}^{(n)} W_{j+1} \mathbb{C}(L_{j+1}) F' \right] \ldots \right]
$$

$$
= \mathbb{E}_{q_1} \left[ \sum_{x_1 \in X_1} \ldots \mathbb{E}_{q_j} \left[ \sum_{x_j \in X_j} \nabla_{N}^{(n)} W_j \mathbb{C}(L_j) \mathbb{E}_{S_{j+1}}[F'] \right] \ldots \right] = \nabla_{N}^{(n)} \mathbb{E}[F]
$$

where we use the inductive hypothesis from step 2 to 3, using that $\mathbb{E}_{S_{j+1}}[F'] = \mathbb{E}_{S_{j+1}, \ldots, S_k}[F]$. □
Using these two lemmas and condition 4, it is easy to show the theorem:

\[
\mathbb{E}_{q_i} \left[ \sum_{x_i \in X_i} \ldots \mathbb{E}_{q_k} \left[ \sum_{x_k \in X_k} \nabla^{(n)} W_k \left( A_k + \mathbb{E}_{L_k} (L_k) F \right) \right] \right] = 0 + \nabla^{(n)} \mathbb{E}[F] = \nabla^{(n)} \mathbb{E}[F]
\]

Note that we used in the proof that condition 1 implies that \( \nabla^{(n)} \mathbb{E}_{q_i} [\sum_{x_i \in X_i} \mathbb{E}_{w_i} (l_i)] = 0 \), which can be seen by taking \( f(x) = 1 \) and noting that \( \nabla^{(n)} \mathbb{E}_{l_i}[1] = 0 \) for \( n > 0 \).

### C Any-order control variate

Many gradient estimators are combined with control variates to reduce variance. We consider control variates for any-order derivative estimation. \([33]\) introduces an any-order baseline in the context of score functions, but only provides proof that this is the baseline for the second-order gradient estimate. We use the Storchastic framework to prove that it is also the correct baseline for any-order derivatives\(^3\). Furthermore, we generalize the ideas behind this baseline to all control variates, instead of just score-function baselines.

The control variate that implements any-order baselines is:

\[
a_i(x_{<i}, X_i) = (1 - \mathbb{E}_{l_i}) b_i(x_{<i}, X_i \setminus \{ x_i \}).
\]

First, we show that baselines satisfy condition 2 of Theorem 1. We will assume here that we take only 1 sample with replacement, but the result generalizes to taking multiple samples in the same way as for the first-order baseline. For \( n = 0 \), the any-order baseline evaluates to zero which can be seen by considering \( 1 - \mathbb{E}_{l_i} \). If \( n > 0 \), then noting that \( b_i \) is independent of \( x_i \),

\[
\mathbb{E}_{q_i}[\nabla^{(n)} (1 - \mathbb{E}_{l_i}) b_i] = \mathbb{E}_{q_i}[-b_i \nabla^{(n)} - \mathbb{E}_{l_i}] = -b_i \nabla^{(n)} \mathbb{E}_{l_i}[1] = 0
\]

We next provide a proof for the validity of this baseline for variance reduction of any-order gradient estimation. To do this, we first prove a new general result on the \( \mathbb{E}_{l_i} \) operator:

**Proposition 7.** For any sequence of functions \( \{l_1, \ldots, l_k\} \), \( \mathbb{E}_{l_k} \) is equivalent under evaluation for orders of differentiation \( n > 0 \) to \( \sum_{i=1}^{k} (\mathbb{E}_{l_i} - 1) \mathbb{E}_{l_{i-1}}(L_{i-1}) \). That is, for all positive numbers \( n > 0 \),

\[
\nabla^{(n)} \mathbb{E}_{l_k}(L_k) = \nabla^{(n)} \sum_{i=1}^{k} (\mathbb{E}_{l_i} - 1) \mathbb{E}_{l_{i-1}}(L_{i-1})
\]

**Proof.** We will prove this using induction on \( k \), starting with the base case \( k = 1 \). Since \( n > 0 \),

\[
\nabla^{(n)} (\mathbb{E}_{l_1} - 1) \mathbb{E}_{l_0}(0) = \mathbb{E}_{l_0}(0) \nabla^{(n)} \mathbb{E}_{l_1}(l_1) = \nabla^{(n)} \mathbb{E}_{l_1}(l_1)
\]

Next, assume the proposition holds for \( k \) and consider \( k + 1 \). Then by splitting up the sum,

\[
\nabla^{(n)} \sum_{i=1}^{k+1} (\mathbb{E}_{l_i} - 1) \mathbb{E}_{l_{i-1}}(L_{i-1}) = \nabla^{(n)} (\mathbb{E}_{l_{k+1}} - 1) \mathbb{E}_{l_k}(L_k) + \nabla^{(n)} \sum_{i=1}^{k} (\mathbb{E}_{l_i} - 1) \mathbb{E}_{l_{i-1}}(L_{i-1})
\]

\[
= \nabla^{(n)} (\mathbb{E}_{l_{k+1}} - 1) \mathbb{E}_{l_k}(L_k) + \nabla^{(n)} \mathbb{E}_{l_k}(L_k)
\]

\(^3\)We use a slight variant of the baseline introduced in \([33]\) to solve an edge case. We will explain in the end of this section how they differ.
where in the second step we use the inductive hypothesis.

We will next consider the first term using the general Leibniz rule:

\[
\n^{(n)}N(l + 1) - 1)N(L_k) = \sum_{m=0}^{n} \binom{n}{m} \n^{(m)}N(l + 1) - 1)N^{(n-m)}N(L_k)
\]

We note that the term corresponding to \( m = 0 \) can be ignored, as \( \n(l + 1) - 1 = (1 - 1) = 0 \).

Furthermore, for \( m > 0, \n^{(m)}N(l + 1) - 1 = \n^{(m)}N(l + 1) \). Therefore,

\[
\n^{(n)}N(l + 1) - 1)N(L_k) = \sum_{m=1}^{n} \binom{n}{m} \n^{(m)}N(l + 1)N^{(n-m)}N(L_k)
\]

Finally, we add the other term \( \n^{(n)}N(L_k) \) again. Then using the general Leibniz rule in the other direction and Proposition 4,

\[
= \sum_{m=1}^{n} \binom{n}{m} \n^{(m)}N(l + 1)N^{(n-m)}N(L_k) + \n^{(n)}N(L_k)
\]

\[
= \sum_{m=0}^{n} \binom{n}{m} \n^{(m)}N(l + 1)N^{(n-m)}N(L_k) = \n^{(n)}N(l + 1)N(L_k) = \n^{(n)}N(L_{k+1})
\]

Next, we note that we can rewrite the expectation of the Stochastic surrogate loss in Equation (3) to

\[
\mathbb{E}_{q_k} \left[ \sum_{x_i \in X_1} \cdots \mathbb{E}_{q_k} \left[ \sum_{x_i \in X_k} \n^{(n)}W_k \left( A_k + \n(L_k)F \right) \right] \cdots \right]
\]

where \( A_k = \sum_{i=1}^{k} \n \left( \sum_{j=1}^{i-1} l_j \right) a_i \). This can be seen by using Condition 1 and 4 of Theorem 1 to iteratively move the \( \n \left( \sum_{j=1}^{i-1} l_j \right) a_i \) terms into the expectations, which is allowed since they don’t depend on \( S_{>i} \).

**Theorem 2.** Under the conditions of Theorem 1,

\[
A_k + \n(L_k)F \equiv \sum_{i=1}^{k} \n(L_{i-1}) (a_i + (\n(l_i) - 1) F) + F,
\]

where \( A_k = \sum_{i=1}^{k} \n \left( \sum_{j=1}^{i-1} l_j \right) a_i \).
Proof.

\[ \nabla_N^{(n)} (A_k + \mathbb{E}(L_k)F) = \nabla_N^{(n)} A_k + \sum_{m=0}^{n} \binom{n}{m} \nabla_N^{(m)} \mathbb{E}(L_k) \nabla_N^{(n-m)} F \]

From (4) to (5), we use that stochastic node. Consider the second-order gradient of the cost function using the recursion in setting \( m = 0 \) in the second term would evaluate to 0 as \( \mathbb{E}(l_i) = 1 \).

Next, consider the inner computation of the Stochastic framework in which all \( a_i \) use a baseline of the form in Equation C. Note that \( a_i = 0 \) is also in this form by setting \( b_i = 0 \). Assume \( n > 0 \) and without loss of generality, assume \( \nabla_N^{(m)} w_i = 0 \) for all \( m \) and \( i \). Then using Proposition 7

\[ \prod_{i=1}^{k} w_i \nabla_N^{(n)} \left( \sum_{i=1}^{k} (1 - \mathbb{E}(l_i)) \mathbb{E}(L_{i-1}) b_i + \mathbb{E}(L_k) F \right) \]

\[ = \prod_{i=1}^{k} w_i \nabla_N^{(n)} \left( - \sum_{i=1}^{k} (\mathbb{E}(l_i) - 1) \mathbb{E}(L_{i-1}) b_i + \sum_{i=1}^{k} (\mathbb{E}(l_i) - 1) \mathbb{E}(L_{i-1}) F \right) \]

The intuition behind the variance reduction of this any-order gradient estimate is that all terms of the gradient involving \( l_i \), possibly multiplied with other \( l_j \) such that \( j < i \), use the \( i \)-th baseline \( b_i \). This allows modelling baselines for each sampling step to effectively make use of background knowledge or known statistics of the corresponding set of random variables.

We note that our baseline is slightly different from [33], which instead of \( \mathbb{E}(L_{i-1}) = \mathbb{E}((\sum_{j=1}^{i-1} l_j) \mathbb{E}(\sum_{j} l_j)) \). Although this might initially seem more intuitive, we will show with a small counterexample why we should consider any stochastic nodes ordered topologically before \( i \) instead of just those that directly influence \( i \).

Consider the stochastic computation graph with stochastic nodes \( p(S_1 | N) \) and \( p(S_2 | N) \) and cost function \( f(x_1, x_2) \). For simplicity, assume we use single-sample score function estimators for each stochastic node. Consider the second-order gradient of the cost function using the recursion in

\footnote{This is assumed simply to make the notation clearer. If the weights are differentiable, the same thing can be shown using an application of the general Leibniz rule.}

23
While this is not an estimate but the true gradient, it fits in the Storchastic framework, focusing primarily on discrete gradient estimation methods.

In this section, we prove the validity of several gradient estimators within the Storchastic framework, focusing primarily on discrete gradient estimation methods.

### D Examples of Gradient Estimators

In this section, we prove the validity of several gradient estimators within the Storchastic framework, focusing primarily on discrete gradient estimation methods.

#### D.1 Expectation

Assume \( p(x_i) \) is a discrete (i.e., categorical) distribution with a finite amount of classes \( 1, ..., C_i \).

While this is not an estimate but the true gradient, it fits in the Storchastic framework as follows:

1. \( w_i(x_i) = p(x_i | x_{<i}) \)
2. \( q(X_i | x_{<i}) = \delta_{\{1, ..., C_i\}}(X_i) \) (that is, a dirac delta distribution with full mass on sampling exactly the sequence \( \{1, ..., C_i\} \))
3. \( l_i(x_i) = 0 \)
4. \( a_i(x_i) = 0 \)
Next, we prove the individual conditions to show that this method can be used within Stochastic, starting with condition 1:

\[
\mathbb{E}_q \left[ \sum_{x_i \in \mathcal{X}_i} \nabla_N^{(n)} w_i \nabla(l_i) f(x_i) \right] = \sum_{j=1}^{C_i} \nabla_N^{(n)} p(x_i = j | x_{<i}) \nabla(0) f(j) \\
= \sum_{j=1}^{C_i} \sum_{m=0}^{n} \nabla_N^{(n-m)} p(x_i = j | x_{<i}) \nabla_N^{(m)} \nabla(0) f(j)
\]

Using the recursion in Proposition 2 we see that \(\nabla_N^{(m)} \nabla(0) f(j) = \nabla_N^{(m)} f(j)\), since \(\nabla_N l_i = \nabla N 0 = 0\). So,

\[
\sum_{j=1}^{C_i} \sum_{m=0}^{n} \nabla_N^{(n-m)} p(x_i = j | x_{<i}) \nabla_N^{(m)} f(j) = \sum_{j=1}^{C_i} \nabla_N^{(n)} p(x_i = j | x_{<i}) f(j) = \nabla_N^{(n)} \mathbb{E}_x_i [f(x_i)].
\]

Condition 2 follows simply from \(a_i(x_i) = 0\), and condition 3 follows from the fact that \(\sum_{j=1}^{C_i} p(x_i = j | x_{<i}) = 1\), that is, constant. Condition 4 follows from the SCG being identical under evaluation, i.e. \(p(x_i = j | x_{<i}) = p(x_i = j | x_{<i})\).

It should be noted that this proof is not completely trivial, as it shows how to implement the expectation so that it can be combined with other gradient estimators while making sure the pathwise derivative through \(f\) also gets the correct gradient.

### D.2 Score Function

The score function is the best known general gradient estimator and is easy to fit in Stochastic.

#### D.2.1 Score Function with Replacement

We consider the case where we take \(m\) samples with replacement from the distribution \(p(x_i | x_{<i})\), and we use a baseline \(b_i(x_{<i}, \mathcal{X}_i \setminus \{x_i\})\) for the first-order gradient estimate.

1. \(w_i(x_i) = \frac{1}{m}\)
2. \(q_i = \prod_{j=1}^{m} p(x_{i,j} | x_{<i})\). That is, \(x_{i,1}, \ldots, x_{i,m} \sim p(x_i | x_{<i})\).
3. \(l_i(x_i) = \log p(x_i | x_{<i})\)
4. \(a_i(x_{<i}, \mathcal{X}_i) = (1 - \nabla_N l_i) b_i(x_{<i}, \mathcal{X}_i \setminus \{x_i\})\), where \(b_i(x_{<i}, \mathcal{X}_i \setminus \{x_i\})\) is not differentiable,

that is, \(\nabla_N^{(n)} b_i(x_{<i}, \mathcal{X}_i \setminus \{x_i\}) = 0\) for \(n > 0\).

We start by showing that condition 1 holds. We assume \(p(x_i | x_{<i})\) is a continuous distribution and note that the proof for discrete distributions is analogous.

We will show how to prove that sampling a set of \(m\) samples with replacement can be reduced in expectation to sampling a single sample. Here, we use that \(x_{i,1}, \ldots, x_{i,m}\) are all independently (line 1 to 2) and identically (line 2 to 3) distributed.

\[
\mathbb{E}_q \left[ \sum_{j=1}^{m} \nabla_N^{(n)} \frac{1}{m} \nabla(l_i) f(x_{<i}, x_{i,j}) \right] = \frac{1}{m} \sum_{j=1}^{m} \mathbb{E}_{x_{i,j} \sim p(x_i)} \left[ \nabla_N^{(n)} \nabla(l_i) f(x_{<i}, x_{i,j}) \right] \\
= \frac{1}{m} \sum_{j=1}^{m} \mathbb{E}_{x_i \sim p(x_i)} \left[ \nabla_N^{(n)} \nabla(l_i) f(x_{<i}) \right] = \mathbb{E}_x \left[ \nabla_N^{(n)} \nabla(l_i) f(x_{<i}) \right]
\]

A proof that \(\mathbb{E}_x \left[ \nabla_N^{(n)} \nabla(l_i) f(x_{<i}) \right] = \nabla_N^{(n)} \mathbb{E}_x [f(x_{<i})]\) was first given in [13]. For completeness, we give a similar proof here, using induction.
First, assume \( n = 0 \). Then, \( \mathbb{E}_{x_i}[\mathbb{E}_{l_i}(f(x_{\leq i}))] = \mathbb{E}_{x_i}[f(x_{\leq i})] = \mathbb{E}_{x_i}[f(x_{\leq i})] \).

Next, assume it holds for \( n \) and consider \( n + 1 \). Using Proposition 2, we find that \( g^{(n+1)}(x_{\leq i}) = \nabla_N g^{(n)}(x_{\leq i}) + g^{(n)}(x_{\leq i}) \nabla_N \log p(x_{\leq i} | x_{<i}) \). Writing the expectation out, we find

\[
\mathbb{E}_{x_i}[\nabla_N g^{(n)}(x_{\leq i}) + g^{(n)}(x_{\leq i}) \nabla_N \log p(x_{\leq i} | x_{<i})]
\]

\[
= \int p(x_{\leq i} | x_{<i}) (\nabla_N g^{(n)}(x_{\leq i}) + g^{(n)}(x_{\leq i}) \frac{\nabla_N p(x_{\leq i} | x_{<i})}{p(x_{\leq i} | x_{<i})}) dx_i
\]

\[
= \int \nabla_N p(x_{\leq i} | x_{<i}) g^{(n)}(x_{\leq i}) dx_i = \nabla_N \mathbb{E}_{x_i}[g^{(n)}(x_{\leq i})]
\]

By Proposition 3, \( g^{(n)}(x_i) \) is identical under evaluation, since by the assumption of Theorem 1 both \( p(x_{\leq i} | x_{<i}) \) and \( f(x_{\leq i}) \) are identical under evaluation. As a result, \( \nabla_N \mathbb{E}_{x_i}[g^{(n)}(x_{\leq i})] = \nabla_N \mathbb{E}_{x_i}[g^{(n)}(x_{\leq i})] \). Therefore, by the induction hypothesis,

\[
\mathbb{E}_{\tilde{x}_i}[g^{(n+1)}(x_{\leq i})] = \nabla_N \mathbb{E}_{x_i}[g^{(n)}(x_{\leq i})] = \nabla_N^{(n+1)} \mathbb{E}_{x_i}[f(x_{\leq i})]
\]

Since the weights \( \frac{1}{m} \) are constant, condition 3 is satisfied.

### D.2.2 Importance Sampling

A common use case for weighting samples is importance sampling [44]. In the context of gradient estimation, it is often used in off-policy reinforcement-learning [32] to allow unbiased gradient estimates using samples from another policy. For simplicity, we consider importance sampling within the context of score function estimators, single-sample estimates, and use no baselines. The last two can be introduced using the techniques in Section D.2.1 and C.

1. \( w_i = \perp \frac{p(x_{\leq i} | x_{<i})}{q(x_{\leq i} | x_{<i})} \),
2. \( q(x_{\leq i} | x_{<i}) \) is the sampling distribution,
3. \( l_i(x_i) = \log p(x_{\leq i} | x_{<i}) \),
4. \( a_i(x_{\leq i}) = 0 \).

Condition 3 follows from the fact that \( \nabla_N^{(n)} w_i = 0 \) for \( n > 0 \), since the importance weights are detached from the computation graph. Condition 1:

\[
\mathbb{E}_{\tilde{x}_i}[\nabla_N^{(n)} \perp \frac{p(x_{\leq i} | x_{<i})}{q(x_{\leq i} | x_{<i})} \nabla(l_i) f(x_{\leq i})] = \int_{\Omega_i} q(x_{\leq i} | x_{<i}) \frac{p(x_{\leq i} | x_{<i})}{q(x_{\leq i} | x_{<i})} \nabla_N^{(n)} \nabla(l_i) f(x_{\leq i}) dx_i
\]

\[
= \mathbb{E}_{\tilde{x}_i}[\nabla_N^{(n)} \nabla(l_i) f(x_{\leq i})] = \mathbb{E}_{\tilde{x}_i}[f(x_{\leq i})]
\]

where in the last step we use the proven condition 1 of D.2.1 Note that this holds both for \( n = 0 \) and \( n > 0 \).

### D.2.3 Discrete Sequence Estimators

Recent literature introduced several estimators for sequences of discrete random variables. These are quite similar in how they are implemented in Stochastic, which is why we group them together.

The sum-and-sample estimator chooses a set of sequences \( \hat{\chi}_i \subset \Omega_i \) and chooses \( k = |\hat{\chi}_i| > 0 \) samples from \( \Omega_i \setminus \hat{\chi}_i \). This set can be the most probable sequences [30] or can be chosen randomly [25]. This is guaranteed not to increase variance through Rao-Blackwellization [6, 30]. It is often used together with deterministic cost functions \( f \), which allows memorizing the cost-function evaluations of the sequences in \( \hat{\chi}_i \). In this context, the estimator is known as Memory-Augmented Policy Optimization [28].

1. \( w_i(x_i) = I[x_i \in \hat{\chi}_i] p(x_i | x_{<i}) + I[x_i \notin \hat{\chi}_i] \frac{p(x_i \notin \hat{\chi}_i)}{k - |\hat{\chi}_i|} \)
2. \( q(x_i) = \delta \Delta_i (x_{i,1}, \ldots, x_{i,|\hat{X}|}) : \prod_{j=|\hat{X}|+1}^k p(x_{i,j} \mid x_{i,j} \notin \hat{X}, x_{<i}) \)

were \( p(x_i \notin \hat{X}) = 1 - \sum_{x_i' \in \hat{X}} p(x_i' \mid x_{<i}) \). This essentially always 'samples' the set \( \hat{X} \) using the Dirac delta distribution, and then samples \( k \) more samples out of the remaining sequences, with replacement. The estimator resulting from this implementation is

\[
\mathbb{E}_{q_i} \left[ \sum_{j=1}^{|\hat{X}|} p(x_{i,j} \mid x_{<i}) f(x_{<i}, x_{i,j}) + \sum_{j=|\hat{X}|+1}^k \frac{p(x_i \notin \hat{X})}{k - |\hat{X}|} \mathbb{E}^n(l_i f(x_{<i}, x_{i,j})) \right]
\]

Using the result from Section D.1, we see that

\[
\nabla_{N}^{(n)} \mathbb{E}_{q_i} \left[ \sum_{j=1}^{|\hat{X}|} p(x_{i,j} \mid x_{<i}) f(x_{<i}, x_{i,j}) \right] = \nabla_{N}^{(n)} \mathbb{E}_{p(x_i \in \hat{X})} \left[ \sum_{j=1}^{|\hat{X}|} p(x_{i,j} \mid x_{i,j} \in \hat{X}, x_{<i}, x_{i,j}) f(x_{<i}, x_{i,j}) \right]
\]

\[
= \nabla_{N}^{(n)} \mathbb{E}_{p(x_i \in \hat{X})} \left[ p(x_i \in \hat{X}) \mathbb{E}_{p(x_i \mid x_{<i}, x_{i,j})} [f(x_{<i})] \right].
\]

Similarly, from the result for sampling with replacement of score functions in Section D.2.1

\[
\nabla_{N}^{(n)} \mathbb{E}_{q_i} \left[ \sum_{j=|\hat{X}|+1}^k \frac{p(x_i \notin \hat{X})}{k - |\hat{X}|} \mathbb{E}^n(l_i f(x_{<i}, x_{i,j})) \right] = \nabla_{N}^{(n)} \mathbb{E}_{p(x_i \notin \hat{X})} \left[ p(x_i \notin \hat{X}) \mathbb{E}_{p(x_i \mid x_{<i} \notin \hat{X}, x_{i,j})} [f(x_{<i})] \right]
\]

Added together, these form \( \nabla_{N}^{(n)} \mathbb{E}_{q_i} [f(x_{<i})] \), which shows that the sum-and-sample estimator with the score function is unbiased for any-order gradient estimation. The variance of this estimator can be further reduced using a baseline from Section C, such as the leave-one-out baseline.

The unordered set estimator is a low-variance gradient estimation method for a sequence of discrete random variables \( S_i [25] \). It makes use of samples without replacement to ensure that each sequence in the sampled batch will be different. We show here how to implement this estimator within Stochastic, leaving the proof for validity of the estimator for [25].

1. \( q(x_i \mid x_{<i}) \) is an ordered sample without replacement from \( p(S_i \mid x_{<i}) \). For sequences, samples can efficiently be taken in parallel using ancestral gumbel-top-k sampling [24, 23]. An ordered sample without replacement means that we take a sequence of samples, where the \( i \)th sample cannot equal the \( i-1 \) samples before it.

2. \( u_i(x_i) = \mathbb{P}(x_{<i} \mid U = X_i \mid x_{<i}) \mathbb{P}(U = X_i \mid x_{<i}) \), where \( p(U = X_i \mid x_{<i}) \) is the probability of the unordered sample without replacement, and \( p(U = X_i | o_1 = x_i, x_{<i}) \) is the probability of the unordered sample without replacement, given that, if we were to order the sample, the first of those ordered samples is \( x_i \).

3. \( l_i(x_i) = \log p(x_i \mid x_{<i}) \)

4. \( a_i(x_{<i}, \lambda_i) = (1 - \mathbb{E}^n(l_i)) b_i(x_{<i}, \lambda_i) \), where \( b_i(x_{<i}, \lambda_i) = \sum_{x_i' \in X_i} \mathbb{P}(x_i' \mid x_{<i}) \mathbb{P}(U = X_i | o_1 = x_i, o_2 = x_i', x_{<i}) f(x_i') \)

This estimator essentially reweights each sample without replacement to ensure it remains unbiased under this sampling strategy. This estimator can be used for any-order differentiation, since \( \mathbb{E}_{q_i} \left[ \sum_{x_i \in X_i} w_i f(x_i) \right] = \mathbb{E}_{S_i} [f(x_i)] \) (see [25] for the proof) and \( \nabla_{N}^{(n)} w_i = 0 \) for \( n > 0 \). The baseline is 0 in expectation for the zeroth and first order evaluation [25]. We leave for future work whether it is also a mean-zero baseline for \( n > 1 \).

D.2.4 LAX, RELAX and REBAR

REBAR [47] and LAX and RELAX [16] are single-sample score-function based methods that learn a control variate to minimize variance. The control variate is implemented using reparameterization. We start with LAX as it is simplest, and then extend the argument to RELAX, since REBAR is a special case of RELAX. We use \( b_{i,\phi} \) to denote the learnable control variate. We have to assume there is
The control variate has expectation 0 for zeroth and first order differentiation. This is because it relies on the original Bernoulli formulation. This equality follows because the CDF of the logistic distribution has no pathwise dependency. As both are unbiased expectations of the \( N(0,1) \) parameter, their difference has to be 0 in expectation, proving condition 2. Furthermore, the 0th order evaluation is exactly 0. The parameters \( \phi \) are trained to minimize the gradient estimate variance.

The control variate for RELAX \([16]\), an extension of LAX to discrete random variables, is similar. It first samples a continuously relaxed input \( q(\tilde{z}|x_{<i}) \), which is then transformed to a discrete sample \( x_i \sim p(x_i|x_{<i}) \). See \([16, 47]\) for details on how this relaxed sampling works. It also samples a relaxed input conditional on the discrete sample, \( q(\tilde{z}|x_{<i}) \). The corresponding control variate is

\[
\tilde{a}_l(x_{<i}, x_i) = \tilde{b}_{i,\phi}(\tilde{z}_i) - \tilde{b}_{i,\phi}(\zeta_i) + (2 - \tilde{\Theta}(l_i)) \tilde{b}_{i,\phi}(\zeta_i)
\]

Here, we subtract \( \tilde{\Theta}(l_i) \) to ensure the first two terms together sum to 0 during 0th order evaluation, and add 2 \( \tilde{\Theta}(l_i) \) to ensure the last two terms sum to 0. Note that for \( n > 0 \),

\[
\nabla_N^m \tilde{a}_l(x_{<i}, x_i) = \nabla_N^m \tilde{b}_{i,\phi}(\tilde{z}_i) - \tilde{b}_{i,\phi}(\zeta_i) + (2 - \tilde{\Theta}(l_i)) \tilde{b}_{i,\phi}(\zeta_i)
\]

We refer the reader to \([16, 47]\) for details on why this control variate component has 0 expectation for all orders of differentiation.

\[E_S \left[ \nabla_N^m \tilde{b}_{i,\phi} \right] \] is the reparameterization estimate of \( \nabla_N^m E_S [b_{i,\phi}] \) and \( E_S [\nabla_N^m \tilde{\Theta}(l_i) \tilde{b}_{i,\phi}] \) is the score-function estimate under the assumption that \( b_{i,\phi} \) has no pathwise dependency. As both are unbiased expectations of the \( m \)-th order derivative, their difference has to be 0 in expectation, proving condition 2. Furthermore, the 0th order evaluation is exactly 0. The parameters \( \phi \) are trained to minimize the gradient estimate variance.

D.2.5 ARM

ARM is a score-function based estimator for multivariate Bernoulli random variables. For our implementation, we use the baseline formulation mentioned in \([8]\), and we follow the derivation in terms of the Logistic random variables from \([9]\). ARM assumes a real-valued parameter vector \( \alpha \), which can be the output of a neural network. The probabilities of the Bernoulli random variable are then assumed to be \( \sigma(\alpha) \) where \( \sigma \) is the sigmoid function.

1. \( q(x_i|x_{<i}) \) is a reparameterized sample from the multivariate Bernoulli distribution. First, it samples \( \epsilon \sim \text{Logistic}(0,1) \). Define \( z_i = \alpha + \epsilon \) and \( \tilde{z}_i = \alpha - \epsilon \). We find \( x_i \sim \text{Bernoulli}(\sigma(\alpha)) \).
   
   Then, with this procedure, \( x_i \sim \text{Bernoulli}(\sigma(\alpha)) \).

2. \( w_i(x_i) = 1 \)

3. \( l_i(x_i) = \log q_\alpha(z_i) \), where \( q_\alpha \) is the density function of \( \text{Logistic}(\alpha,1) \).

4. \( a_i(x_{<i}, x_i) = \Theta(1 - l_i(x_i)) \frac{1}{2} (f(x_{<i}, z_i > 0) + f(x_{<i}, \tilde{z}_i > 0)) \)

Since \( E_{x_i \sim \text{Bernoulli}(\sigma(\alpha))} [f(x_i)] = E_{\epsilon \sim \text{Logistic}(0,1)} [f(\alpha_\theta + \epsilon > 0)] = E_{z_i \sim \text{Logistic}(\alpha,1)} [f(z_i > 0)] \), any unbiased estimate of the logistic reparameterization must also be an unbiased estimate of the original Bernoulli formulation. This equality follows because the CDF of the logistic distribution is the logistic function (that is, the sigmoid function). \( l_i(x_i) \) is the (unbiased) score function of the logistic reparameterization, which we proved to be an unbiased estimator.

The control variate has expectation 0 for zeroth and first order differentiation. This is because it relies on the score function being an odd function \([5]\), that is, \( \nabla_N \log q_\alpha(z_i) = -\nabla_N \log q_\alpha(\tilde{z}_i) \). Therefore, \( E_F [\nabla(x_{<i}, z_i > 0) + f(x_{<i}, \tilde{z}_i > 0)] = E_F [f(x_{<i}, z_i > 0) - f(x_{<i}, \tilde{z}_i > 0)] \).

Note that, by symmetry of the logistic distribution, \( E_F [f(x_{<i}, z_i > 0)] = -E_F [f(x_{<i}, \tilde{z}_i > 0)] \), meaning the baseline is zero in expectation. However, this derivation only holds for odd functions! Unfortunately, the second-order score function \( \frac{\nabla_N^2}{\log q_\alpha(z_i)} \) is an even function since the derivative of an odd function is always an even function. Therefore, the ARM estimator will only be unbiased for first-order gradient estimation.
D.2.6 GO Gradient

The GO gradient estimator [7] is a method that uses the CDF of the distribution to derive the gradient. For continuous distributions, it reduces to implicit reparameterization gradients which can be implemented through transforming the computation graph, like other reparameterization methods. For \( m \) independent discrete distributions of \( d \) categories, the first-order gradient is given as:

\[
\mathbb{E}_p(x_i | x < i) \left[ \sum_{j=1}^{m} \left( f(x_{\leq i}) - f(x_{\leq i}, x_{i,j} + 1) \right) \frac{\nabla_N \sum_{k=1}^{x_{i,j}} p_j(k | x < i)}{p_j(x_{i,j} | x < i)} \right]
\]

Note that if \( x_{i,j} = d \), then the estimator evaluates to zero since \( \nabla_N \sum_{k=1}^{d} p_j(k | x < i) = 0 \).

We derive the Storchastic implementation by treating the GO estimator as a control variate of the single-sample score function. To find this control variate, we subtract the score function from this estimator, that is, we subtract \( f(x_{\leq i}) \nabla_N \log p(x_i | x < i) \).

\[
f(x_{\leq i}) \nabla_N \log p(x_i | x < i) = f(x_{\leq i}) \sum_{j=1}^{m} \frac{\nabla_N p(x_i | x < i)}{p(x_i | x < i)}
\]

where we use that each discrete distribution is independent. By unbiasedness of the GO gradient, the rest of the estimator is 0 in expectation, as we will show.

Define \( f_{j,k} = f(x_{\leq i}, x_{i,j} = k) \), \( p_{j,k} = p_j(k | x < i) \) and \( P_{j,k} = \sum_{k'=1}^{k} p_j(k' | x < i) \). Then the GO control variate is:

\[
a_i(x_{\leq i}) = \sum_{j=1}^{m} I[x_{i,j} < d] \left( \frac{f_{j,x_{i,j}} - f_{j,x_{i,j}+1}}{p_{j,x_{i,j}}} \right) \frac{P_j(x_{i,j}) - 1}{P_j(x_{i,j})} - \frac{f_{j,d}}{P_j(x_{i,j})}
\]

The first line will evaluate to the GO gradient estimator when differentiated, and the second to the single-sample score function gradient estimator.

Note that this gives a general formula for implementing any unbiased estimator into Storchastic. Use it as a control variate with the score function subtracted to ensure interoperability with other estimators in the stochastic computation graph.

D.3 SPSA

Simultaneous perturbation stochastic approximation (SPSA) [46] is a gradient estimation method based on finite difference estimation. It stochastically perturbs parameters and uses two functional evaluations to estimate the (possibly stochastic) gradient. Let \( \theta \) be the \( d \)-dimensional parameters of the distribution \( p_\theta(x_i | x < i) \). SPSA samples \( d \) times from the Rademacher distribution (a Bernoulli distribution with 0.5 probability for 1 and 0.5 probability for -1) to get a noise vector \( \epsilon \). We then get two new distributions: \( x_{i,1} \sim p_{\theta + \epsilon} \) and \( x_{i,2} \sim p_{\theta - \epsilon} \) where \( \epsilon > 0 \) is the perturbation size.

The difference \( f(x_{i,1}) - f(x_{i,2}) \) is then an estimate of the first-order gradient. Higher-order derivative estimation is also possible, but left for future work.

An easy way to implement SPSA in Storchastic is by using importance sampling (Appendix D.2.2). Assuming \( p_{\theta + \epsilon} \) and \( p_{\theta - \epsilon} \) have the same support as \( p \), we can set the weighting function to \( \frac{p(x_i | x < i)}{p_{\theta + \epsilon}(x_i | x < i)} \) for the first sample, and \( \frac{p(x_i | x < i)}{p_{\theta - \epsilon}(x_i | x < i)} \) for the second sample.

To ensure the gradients distribute over the parameters, we define the gradient function as \( \theta \nabla (p_{\theta + \epsilon}(x_i | x < i)) \) for the first sample and \( -\theta \nabla (p_{\theta - \epsilon}(x_i | x < i)) \) for the second sample. This cancels out the weighting function, resulting in the SPSA estimator.

D.4 Measure Valued Derivatives

Storchastic allows for implementing Measure Valued Derivatives (MVD) [18], however, it is only unbiased for first-order differentiation and cannot be easily extended to higher-order differentiation. The implementation is similar to SPSA, but with some nuances. We will give a simple overview for how to implement this method in Storchastic, and leave multivariate distributions and higher-order differentiation to future work.

First, define the weak derivative for parameter \( \theta \) of \( p \) as the triple \( (c_\theta, p^+, p^-) \) by decomposing \( p(x_i | x < i) \) into the positive and negative parts \( p^+(x_i^+) \) and \( p^-(x_i^-) \), and let \( c_\theta \) be a constant. For
We then set \( a_i(x_i, X_i) = 0 \) and use the following gradient function: 
\[
  l_i(x_i) = \theta \cdot \mathbb{1}(c_{\theta} \frac{p(x_i^+ | x_{<i})}{2p^+(x_i^+)})
\]
for positive samples and 
\[
  l_i(x_i) = -\theta \cdot \mathbb{1}(c_{\theta} \frac{p(x_i^- | x_{<i})}{2p^-(x_i^-)})
\]
for negative samples. This will compensate for the weighting function by ensuring the importance weights are not applied over the gradient estimates. For the first-order gradient, this results in the MVD \( \nabla_N \theta \mathbb{1}(c_{\theta})(f(x_i^+) - f(x_i^-)) \).

For other distributions for which \( p^+ \) and \( p^- \) do not cover an equal proportion of \( p \), more specific implementations have to be derived. For example, for the Poisson distribution one can implement its MVD by noting that \( p^+ \) has the same support as \( p \). Then, we can use one sample from \( p^+ \) using the importance sampling estimator using score function (Appendix \ref{sec:appendix_2.2}), and use a trick similar to the GO gradient by defining a control variate that subtracts the score function and adds the MVD, which is allowed since the MVD and score function are both unbiased estimators.

### E Discrete VAE Case Study Experiments

We report test runs on MNIST \cite{26} generative modeling using discrete VAEs in Table \ref{table:1}. We use Storchastic to run 100 epochs on both a latent space of 20 Bernoulli random variables and 20 Categorical random variables of 10 dimensions, and report training and test ELBOs. We run these on the gradient estimation methods currently implemented in the PyTorch library.

Although results reported are worse than similar previous experiments, we note that we only run 100 epochs (900 epochs in \cite{25}) and we do not tune the methods. However, the results reflect the order expected from \cite{25}, where score function with leave-one-out baseline also performed best, closely followed by the Unordered set estimator. Furthermore, the Gumbel softmax \cite{19, 31} still outperforms the other score-function based estimators, although the results in \cite{25} suggest that with more epochs and better tuning, better ELBO than reported here can be achieved.

These results are purely presented as a demonstration of the flexbility of the Storchastic library: Only a single line of code is changed to be able to compare the different estimators! A more thorough and fair comparison, also in different settings, is left for future work.

|                      | 20 Bernoulli VAE |                      | 10 Discrete VAE |
|----------------------|------------------|---------------------|-----------------|
|                      | Train ELBO       | Validation ELBO     | Train ELBO      | Validation ELBO |
| Score@1              | 191.3            | 191.9               | 206.3           | 206.7           |
| ScoreLOO@5 \cite{22} | 110.8            | 110.4               | 111.2           | 110.4           |
| REBAR@1 \cite{47}    | 220.0            | 1000                | 155.6           | 154.9           |
| RELAX@1 \cite{16}    | 210.6            | 205.9               | 202.5           | 201.7           |
| Unordered set@5 \cite{25} | 117.1         | 138.4               | 115.4           | 117.2           |
| Gumbel@1 \cite{19, 31} | 107.0           | 106.6               | 92.9            | 92.6            |
| GumbelIST@1 \cite{19} | 113.0           | 112.9               | 98.3            | 98.0            |
| ARM@1 \cite{51}      | 131.3            | 130.8               |                 |                 |
| DisARM@1 \cite{19}   | 125.1            | 124.3               |                 |                 |

Table 1: Test runs on MNIST VAE generative modeling. We report the lowest train and validation ELBO over 100 epochs. The number after the ‘@’ symbol denotes the amount of samples used to compute the estimator. We note that the ARM and DiSARM methods are specific for binary random variables, and do not evaluate it in the 100\textsuperscript{2} discrete VAE.

examples on how to perform this decomposition, see for example \cite{37}. To implement MVDs in Storchastic, we use the samples from \( p^+ \) and \( p^- \), and, similar to SPSA, treat them as importance samples (Appendix \ref{sec:appendix_2.2}) for the zeroth order evaluation.

That is, the proposal distribution is defined over tuples \( X_i = (x_i^+, x_i^-) \) such that \( q(X_i | x_{<i}) = p^+(x_i^+)p^-(x_i^-) \). The weighting function can be derived depending on the support of the positive and negative parts of the weak derivative. For weak derivatives for which the positive and negative part both cover an equal proportion of the distribution \( p(x_i | x_{<i}) \), the weighting function can be found using importance sampling by \( \mathbb{1}(\frac{p(x_i^+ | x_{<i})}{2p^+(x_i^+)}) \) for samples from the positive part, and \( \mathbb{1}(\frac{p(x_i^- | x_{<i})}{2p^-(x_i^-)}) \) for samples from the negative part. This gives unbiased zeroth order estimation by using importance sampling.

We then set \( a_i(x_i, X_i) = 0 \) and use the following gradient function: 
\[
  l_i(x_i) = \theta \cdot \mathbb{1}(c_{\theta} \frac{p(x_i^+ | x_{<i})}{2p^+(x_i^+)})
\]
for positive samples and 
\[
  l_i(x_i) = -\theta \cdot \mathbb{1}(c_{\theta} \frac{p(x_i^- | x_{<i})}{2p^-(x_i^-)})
\]
for negative samples. This will compensate for the weighting function by ensuring the importance weights are not applied over the gradient estimates. For the first-order gradient, this results in the MVD \( \nabla_N \theta \mathbb{1}(c_{\theta})(f(x_i^+) - f(x_i^-)) \).