

# Multiple Importance Sampling for Stochastic Gradient Estimation

Corentin Salaün<sup>1</sup><sup>a</sup>, Xingchang Huang<sup>1</sup><sup>b</sup>, Iliyan Georgiev<sup>2</sup><sup>c</sup>, Niloy Mitra<sup>2,3</sup><sup>d</sup> and Gurprit Singh<sup>1</sup><sup>e</sup>

<sup>1</sup>Max Planck Institute for Informatics, Saarland University, Saarbrücken, Germany

<sup>2</sup>Adobe Research, London, U.K.

<sup>3</sup>Department of Computer Science, University College London, London, U.K.

{csalaun, xhuang, gsingh}@mpi-inf.mpg.de, igeorgiev@adobe.com, n.mitra@cs.ucl.ac.uk

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Abstract: We introduce a theoretical and practical framework for efficient importance sampling of mini-batch samples for gradient estimation from single and multiple probability distributions. To handle noisy gradients, our framework dynamically evolves the importance distribution during training by utilizing a self-adaptive metric. Our framework combines multiple, diverse sampling distributions, each tailored to specific parameter gradients. This approach facilitates the importance sampling of *vector-valued* gradient estimation. Rather than naively combining multiple distributions, our framework involves optimally weighting data contribution across multiple distributions. This adapted combination of multiple importance yields superior gradient estimates, leading to faster training convergence. We demonstrate the effectiveness of our approach through empirical evaluations across a range of optimization tasks like classification and regression on both image and point cloud datasets.

## 1 INTRODUCTION


Stochastic gradient descent (SGD) is fundamental in optimizing complex neural networks. This iterative optimization process relies on the efficient estimation of gradients to update model parameters and minimize the optimization objective. A significant challenge in methods based on SGD lies in the influence of stochasticity on gradient estimation, impacting both the quality of the estimates and convergence speed. This stochasticity introduces errors in the form of noise, and addressing and minimizing such noise in gradient estimation continues to be an active area of research.


Various approaches have been introduced to reduce gradient estimation noise, including data diversification Zhang et al. (2019); Faghri et al. (2020); Ren et al. (2019), adaptive mini-batch sizes Balles et al. (2017); Alfarra et al. (2021), momentum-based estimation Rumelhart et al. (1986); Kingma and Ba


(2014), and adaptive sampling strategies Santiago et al. (2021). These methods collectively expedite the optimization by improving the gradient-estimation accuracy.


Another well-established technique for noise reduction in estimation is importance sampling (IS) Loshchilov and Hutter (2015); Katharopoulos and Fleuret (2017, 2018), which involves the non-uniform selection of data samples for mini-batch construction. Data samples that contribute more significantly to gradient estimation are selected more often. This allows computational resources to focus on the most critical data for the optimization task. However, these algorithms are quite inefficient and add significant overhead to the training process. Another limitation of importance sampling, in general, lies in determining the best sampling distribution to achieve maximal improvement, often necessitating a quality trade-off due to the simultaneous estimation of numerous parameters.


We propose an efficient importance sampling algorithm that does *not* require resampling, in contrast to Katharopoulos and Fleuret (2018). Our importance function dynamically evolves during training, utilizing a self-adaptive metric to effectively manage initial noisy gradients. Further, unlike existing IS meth-

<sup>a</sup> <https://orcid.org/0000-0002-5112-7488>

<sup>b</sup> <https://orcid.org/0000-0002-2769-8408>

<sup>c</sup> <https://orcid.org/0000-0002-9655-2138>

<sup>d</sup> <https://orcid.org/0000-0002-2597-0914>

<sup>e</sup> <https://orcid.org/0000-0003-0970-5835>

ods in machine learning where importance distributions assume scalar-valued gradients, we propose a multiple importance sampling (MIS) strategy to manage *vector-valued* gradient estimation (i.e., multiple parameters). We propose the simultaneous use of multiple sampling strategies combined with a weighting approach following the principles of MIS theory, well studied in the rendering literature in computer graphics Veach (1997). Rather than naively combining multiple distributions, our proposal involves estimating importance weights w.r.t. data samples across multiple distributions by leveraging the theory of optimal MIS (OMIS) Kondapaneni et al. (2019). This optimization process yields superior gradient estimates, leading to faster training convergence. In summary, we make the following contributions:

- An efficient IS algorithm with a self-adaptive metric for importance sampling is developed.
- An MIS estimator for gradient estimation is introduced to improve gradients estimation.
- A practical approach to computing the OMIS weights is presented to maximize the quality of vector-valued gradient estimation.
- The effectiveness of the approach is demonstrated on various machine learning tasks.

## 2 RELATED WORK

**Importance Sampling for Gradient Estimation.** Importance sampling (IS) Kahn (1950); Kahn and Marshall (1953); Owen and Zhou (2000) has emerged as a powerful technique in high energy physics, Bayesian inference, rare event simulation for finance and insurance, and rendering in computer graphics. In the past few years, IS has also been applied in machine learning to improve the accuracy of gradient estimation and enhance the overall performance of learning algorithms Zhao and Zhang (2015).

By strategically sampling data points from a non-uniform distribution, IS effectively focuses training resources on the most informative and impactful data, leading to more accurate gradient estimates. Bordes et al. (2005) developed an online algorithm (LASVM) that uses importance sampling to train kernelized support vector machines. Loshchilov and Hutter (2015) suggested employing data rankings based on their respective loss values. This ranking is then employed to create an importance sampling strategy that assigns greater importance to data with higher loss values. Katharopoulos and Fleuret (2017) proposed importance sampling the loss function. Subsequently,

Katharopoulos and Fleuret (2018) introduced an upper bound to the gradient norm that can be employed as an importance function. Their algorithm involves resampling and computing gradients with respect to the final layer. Despite the importance function demonstrating improvement over uniform sampling, their algorithm exhibits significant inefficiency.

**Multiple Importance Sampling.** The concept of Multiple Importance Sampling (MIS) emerged as a robust and efficient technique for integrating multiple sampling strategies Owen and Zhou (2000). Its core principle lies in assigning weights to multiple importance sampling estimator, each using a different sampling distribution, allowing each data sample to utilize the most appropriate strategy. Veach (1997) introduced this concept of MIS to rendering in computer graphics and proposed the widely adopted *balance heuristic* for importance (weight) allocation. The balance heuristic determines weights based on a data sample's relative importance across all sampling approaches, effectively mitigating the influence of outliers with low probability densities. While MIS is straightforward to implement and independent of the specific function, Variance-Aware MIS Grittmann et al. (2019) advanced the concept by using variance estimates from each sampling technique for further error reduction. Moreover, Optimal MIS Kondapaneni et al. (2019) derived optimal sampling weights that minimize MIS estimator variance. Notably, these weights depend not only on probability density but also on the function values of the samples. Supplemental document summarizes the theory behind (multiple) importance sampling. It also states the optimal MIS estimator and how to compute it.

## 3 PROBLEM STATEMENT

The primary goal of machine-learning optimization is to find the optimal parameters  $\theta$  for a given model function  $m(x, \theta)$  by minimizing a loss function  $\mathcal{L}$  over a dataset  $\Omega$ :

$$\theta^* = \underset{\theta}{\operatorname{argmin}} \underbrace{\int_{\Omega} \mathcal{L}(m(x_i, \theta), y) dx}_{\mathcal{L}_{\theta}}. \quad (1)$$

The loss function  $\mathcal{L}$  quantifies the dissimilarity between the model predictions  $m(x, \theta)$  and observed data  $y$ . In the common case of a discrete dataset, the integral becomes a sum.

In practice, the total loss is minimized via iterative gradient descent. In each iteration  $t$ , the gradient  $\nabla \mathcal{L}_{\theta_t}$ ,

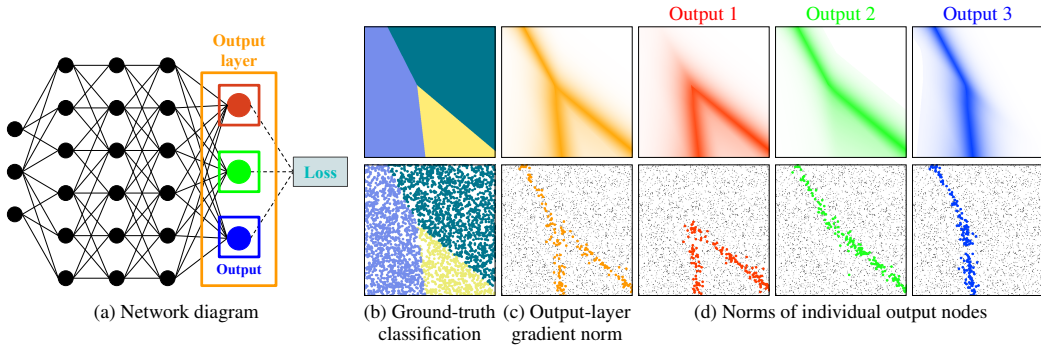


Figure 1: We visualize different importance sampling distributions for a simple classification task. We propose to use the output layer gradients for importance sampling, as shown in the network diagram (a). For a given ground-truth classification (top) and training dataset (bottom) shown in (b), it is possible to importance sample from the  $L_2$  norm of the output-layer gradients (c) or from three different sampling distributions derived from the gradient norms of individual output nodes (d). The bottom row shows sample weights from each distribution.

of the loss with respect to the current model parameters  $\theta_t$  is computed, and the parameters are updated as

$$\theta_{t+1} = \theta_t - \lambda \underbrace{\int_{\Omega} \nabla \mathcal{L}(m(x, \theta_t), y) dx}_{\nabla L_{\theta_t}}, \quad (2)$$

where  $\lambda > 0$  is the learning rate. It is also possible to use an adaptive learning rate instead of a constant.

**Monte Carlo Gradient Estimator.** In practice, the parameter gradient is estimated from a small batch  $\{x_i\}_{i=1}^B$  of randomly selected data points:

$$\langle \nabla L_{\theta} \rangle = \sum_{i=1}^B \frac{\nabla \mathcal{L}(m(x_i, \theta), y_i)}{Bp(x_i)} \approx \nabla L_{\theta}, \quad x_i \sim p. \quad (3)$$

The data points are sampled from a probability density function (pdf)  $p$  or probability mass function in discrete cases. The mini-batch gradient descent substitutes the true gradient  $\nabla L_{\theta_t}$  with an estimate  $\langle \nabla L_{\theta_t} \rangle$  in Eq. (2) to update the model parameters in each iteration.

We want to estimate  $\nabla L_{\theta_t}$  accurately and also efficiently, since the gradient-descent iteration (2) may require many thousands of iterations until the parameters converge. These goals can be achieved by performing the optimization in small batches whose samples are chosen according to a carefully designed distribution  $p$ . For a simple classification problem, Fig. 1c shows an example importance sampling distribution derived from the output layer of the model. In Fig. 1d we derive multiple distributions from the individual output nodes. Below we develop theory and practical algorithms for importance sampling using a single distribution (Section 4) and for combining multiple distributions to further improve gradient estimation (Section 5).

## 4 MINI-BATCH IMPORTANCE SAMPLING

Mini-batch gradient estimation (3) notoriously suffers from Monte Carlo noise, which can make the parameter-optimization trajectory erratic and convergence slow. That noise comes from the often vastly different contributions of different samples  $x_i$  to that estimate.

Typically, the selection of the multiple samples constructing a mini-batch is done with uniform probability  $p(x_i) = 1/|\Omega|$ . Each data of the mini-batch is sampled with replacement following this distribution. Importance sampling is a technique for using a non-uniform pdf to strategically pick samples proportionally on their contribution to the gradient, to reduce estimation variance.

**Practical Algorithm.** We propose an importance sampling algorithm for mini-batch gradient descent, outlined in Algorithm 1. Similarly to Schaul et al. (2015), we use an importance function that relies on readily available quantities for each data point, introducing only negligible memory and computational overhead over classical uniform mini-batching. We store a set of persistent *un-normalized importance* scalars  $q = \{q_i\}_{i=1}^{|\Omega|}$  that are updated continuously during the optimization.

The first epoch is a standard SGD one, during which we additionally compute the initial importance of each data point (line 3). In each subsequent epoch, at each mini-batch optimization step  $t$  we normalize the importance values to a valid distribution  $p$  (line 6). We then choose  $B$  data samples (with replacement) according to  $p$  (line 7). The loss  $\mathcal{L}$  is evaluated

Algorithm 1: Mini-batch importance sampling for SGD.

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1:  $\theta \leftarrow$  random parameter initialization
2:  $B \leftarrow$  mini-batch size,  $N = |\Omega|$   $\leftarrow$  Dataset size
3:  $q, \theta \leftarrow$  Initialize( $x, y, \Omega, \theta, B$ )  $\leftarrow$  See Supplemental
4: until convergence do  $\leftarrow$  Loop over epochs
5:   for  $t \leftarrow 1$  to  $N/B$   $\leftarrow$  Loop over mini-batches
6:      $p \leftarrow q/\text{sum}(q)$   $\leftarrow$  Normalize importance to pdf
7:      $x, y \leftarrow B$  data samples  $\{x_i, y_i\}_{i=1}^B \propto p$ 
8:      $\mathcal{L}(x) \leftarrow \mathcal{L}(m(x, \theta), y)$ 
9:      $\nabla \mathcal{L}(x) \leftarrow$  Backpropagate( $\mathcal{L}(x)$ )
10:     $\langle \nabla L_{\theta} \rangle \leftarrow (\nabla \mathcal{L}(x) \cdot (1/p(x) \cdot B)^T) / B$   $\leftarrow$  Eq. (3)
11:     $\theta \leftarrow \theta - \lambda \langle \nabla L_{\theta} \rangle$   $\leftarrow$  SGD step
12:     $q(x) \leftarrow \alpha \cdot q(x) + (1 - \alpha) \cdot \left\| \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)} \right\|$ 
13:
14:    $q \leftarrow q + \epsilon$   $\leftarrow$  Accumulate importance
15: return  $\theta$ 

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for each selected data sample (line 8), and backpropagated to compute the loss gradient (line 9). The per-sample importance is used in the gradient estimation (line 10) to normalize the contribution. In practice lines 9-10 can be done simultaneously by backpropagating a weighted loss  $\mathcal{L}(x) \cdot (1/p(x) \cdot B)^T$ . Finally, the network parameters are updated using the estimated gradient (line 11). On line 12, we update the importance of the samples in the mini-batch; we describe our choice of importance function below. The blending parameter  $\alpha$  ensures stability of the persistent importance as discussed in Supplemental document. At the end of each epoch (line 14), we add a small value to the un-normalized weights of all data to ensure that every data point will be eventually evaluated, even if its importance is deemed low by the importance metric.

It is important to note that the first epoch is done without importance sampling to initialize each sample importance. This does not add overhead as it is equivalent to a classical epoch running over all data samples. While similar schemes have been proposed in the past Loshchilov and Hutter (2015), they often rely on a multitude of hyperparameters, making their practical implementation challenging. This has led to the development of alternative methods like re-sampling Katharopoulos and Fleuret (2018); Dong et al. (2021); Zhang et al. (2023). Tracking importance across batches and epochs minimizes the computational overhead, further enhancing the efficiency and practicality of the approach.

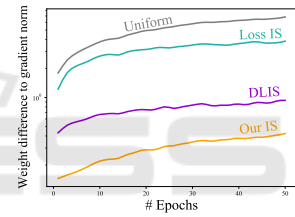
**Importance Function.** In combination with the presented algorithm, we propose an importance function that is efficient to evaluate. While the gradient  $L_2$  norm has been shown to be optimal Zhao and Zhang (2015); Needell et al. (2014); Wang et al. (2017); Alain et al. (2015), calculating it can be computation-

ally expensive as it requires full backpropagation for every data point. To this end, we compute the gradient norm only for a subset of the parameters, specifically the output nodes of the network:  $q(x) = \left\| \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)} \right\|$ . This choice is based on an upper bound of the gradient norm, using the chain rule and the Cauchy–Schwarz inequality Katharopoulos and Fleuret (2018):

$$\begin{aligned} \left\| \frac{\partial \mathcal{L}(x_i)}{\partial \theta} \right\| &= \left\| \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)} \cdot \frac{\partial m(x, \theta)}{\partial \theta} \right\| \leq & (4) \\ & \left\| \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)} \right\| \cdot \left\| \frac{\partial m(x, \theta)}{\partial \theta} \right\| \leq \underbrace{\left\| \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)} \right\|}_{q(x)} \cdot C, \end{aligned}$$

where  $C$  is the Lipschitz constant of the parameters gradient. That is, our importance function is a bound of the gradient magnitude based on the output-layer gradient norm.

We tested the relationship between four different importance distributions: uniform, our proposed importance function, the loss function as importance Katharopoulos and Fleuret (2017), and the work by Katharopoulos and Fleuret (2018)



using an other gradient norm bound. The inline figure plots the  $L_2$  difference between these importance distributions and the ground-truth gradient-norm distribution across epochs for an MNIST classification task. It shows that **Our IS** distribution has the smallest difference, i.e., it achieves high accuracy while requiring only a small part of the gradient.

For some specific task when the output layer has predictable shape, it is possible to derive a closed form definition of the proposed importance metric. Supplemental document derives the close form importance for classification task using cross entropy loss.

Note that any importance heuristic can be used on line 12 of Algorithm 1, such as the gradient norm Zhao and Zhang (2015); Needell et al. (2014); Wang et al. (2017); Alain et al. (2015), the loss Loshchilov and Hutter (2015); Katharopoulos and Fleuret (2017); Dong et al. (2021), or more advanced importance Katharopoulos and Fleuret (2018). For efficiency, our importance function reuses the forward-pass computations from line 8, updating  $q$  only for the current mini-batch samples.



## 5 MULTIPLE IMPORTANCE SAMPLING

The parameter gradient  $\nabla L_{\theta}$  is vector with dimension equal to the number of model parameters. The individual parameter derivatives vary uniquely across the data points, and estimation using a single distribution (Section 4) inevitably requires making a trade-off, e.g., only importance sampling the overall gradient magnitude. Truly minimizing the estimation error requires estimating each derivative using a separate importance sampling distribution tailored to its variation. However, there are two practical issues with this approach: First, it would necessitate sampling from all of these distributions, requiring “mini-batches” of size equal at least to the number of parameters. Second, it would lead to significant computation waste, since backpropagation computes all parameter derivatives but only one of them would be used per data sample. To address this issue, we propose using a small number of distributions, each tailored to the variation of a parameter subset, and combining *all* computed derivatives into a low-variance estimator, using multiple importance sampling theory. As an example, Fig. 1d shows three sampling distributions for a simple classification task, based on the derivatives of the network’s output nodes, following the boundary of each class.

**MIS Gradient Estimator.** Combining multiple sampling distributions into a single robust estimator has been well studied in the Monte Carlo rendering literature. The best known method is *multiple importance sampling* (MIS) Veach (1997). In our case of gradient estimation, the MIS estimator takes for form

$$\langle \nabla L_{\theta} \rangle_{\text{MIS}} = \sum_{j=1}^J \sum_{i=1}^{n_j} w_j(x_{ij}) \frac{\nabla \mathcal{L}(m(x_{ij}, \theta), y_{ij})}{n_j p_j(x_{ij})}, \quad (5)$$

where  $J$  is the number of sampling distributions,  $n_j$  the number of samples from distribution  $j$ , and  $x_{ij}$  the  $i^{\text{th}}$  sample from the  $j^{\text{th}}$  distribution. Each sample is modulated by a weight  $w_j(x_{ij})$ ; the estimator is unbiased as long as  $\sum_{j=1}^J w_j(x) = 1$  for every data point  $x$  in the dataset.

**Optimal Weighting.** Various MIS weighting functions  $w_j$  have been proposed in literature, the most universally used one being the balance heuristic Veach (1997). In this work we use the recently derived optimal weighting scheme Kondapaneni et al. (2019) which minimizes the estimation variance for a

given set of sampling distributions  $p_j$ :

$$w_j(x) = \alpha_j \frac{p_j(x)}{\nabla \mathcal{L}(m(x, \theta), y)} + \frac{n_j p_j(x)}{\sum_{k=1}^J n_k p_k(x)} \left( 1 - \frac{\sum_{k=1}^J \alpha_k p_k(x)}{\nabla \mathcal{L}(m(x, \theta), y)} \right). \quad (6)$$

Here,  $\boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_J]$  is the solution to the linear system

$$\mathbf{A}\boldsymbol{\alpha} = \mathbf{b}, \text{ with } \begin{cases} a_{j,k} = \int_{\Omega} \frac{p_j(x)p_k(x)}{\sum_i n_i p_i(x)} d(x,y), \\ b_j = \int_{\Omega} \frac{p_j(x)\nabla \mathcal{L}(m(x, \theta), y)}{\sum_i n_i p_i(x)} d(x,y), \end{cases} \quad (7)$$

where  $a_{j,k}$  and  $b_j$  are the elements of the matrix  $\mathbf{A} \in \mathbb{R}^{J \times J}$  and vector  $\mathbf{b} \in \mathbb{R}^J$  respectively.

Instead of explicitly computing the optimal weights in Eq. (6) using Eq. (7) and plugging them into the MIS estimator (5), we can use a shortcut evaluation that yields the same result Kondapaneni et al. (2019):

$$\langle \nabla L_{\theta} \rangle_{\text{OMIS}} = \sum_{j=1}^J \alpha_j. \quad (8)$$

In Supplemental document we provide an overview of MIS and the aforementioned weighting schemes. Importantly for our case, the widely adopted balance heuristic does not bring practical advantage over single-distribution importance sampling (Section 4) as it is equivalent to sampling from a mixture of the given distributions; we can easily sample from this mixture by explicitly averaging the distributions into a single one. In contrast, the optimal weights are different for each gradient dimension as they depend on the gradient value.

**Practical Algorithm.** Implementing the optimal-MIS estimator (8) amounts to drawing  $n_j$  samples from each distribution, computing  $\boldsymbol{\alpha}$  for each dimension of the gradient and summing its elements. The integrals in  $\mathbf{A}$  and  $\mathbf{b}$  (sums in the discrete-dataset case) can be estimated as  $\langle \mathbf{A} \rangle$  and  $\langle \mathbf{b} \rangle$  from the drawn samples, yielding the estimate  $\langle \boldsymbol{\alpha} \rangle = \langle \mathbf{A} \rangle^{-1} \langle \mathbf{b} \rangle$ .

Algorithm 2 shows a complete gradient-descent algorithm. The main differences with Algorithm 1 are the use of multiple importance distributions  $\mathbf{q} = \{q_j\}_{j=1}^J$  (line 5) and the linear system used to compute the OMIS estimator (line 6). This linear system is updated (lines 15-18) using the mini-batch samples and solved to obtain the gradient estimation (line 22). Since the matrix  $\langle \mathbf{A} \rangle$  is independent of the gradient estimation (see Eq. (7)), its inversion can be shared across all parameter estimates.

**Algorithm 2: Optimal multiple importance sampling SGD.**

```

1:  $\theta \leftarrow$  random parameter initialization
2:  $B \leftarrow$  mini-batch size,  $J \leftarrow$  number of pdf
3:  $N = |\Omega| \leftarrow$  dataset size
4:  $n_j \leftarrow$  sample count per technique, for  $j \in \{1, \dots, J\}$ 
5:  $\mathbf{q}, \theta \leftarrow$  InitializeMIS( $x, y, \Omega, \theta, B$ )  $\leftarrow$  see Supplemental
6:  $\langle \mathbf{A} \rangle \leftarrow 0^{J \times J}, \langle \mathbf{b} \rangle \leftarrow 0^J$   $\leftarrow$  OMIS linear system
7: until convergence do  $\leftarrow$  Loop over epochs
8:   for  $t \leftarrow 1$  to  $N/B$   $\leftarrow$  Loop over mini-batches
9:      $\langle \mathbf{A} \rangle \leftarrow \beta \langle \mathbf{A} \rangle, \langle \mathbf{b} \rangle \leftarrow \beta \langle \mathbf{b} \rangle$ 
10:    for  $j \leftarrow 1$  to  $J$   $\leftarrow$  Loop over distributions
11:       $p_j \leftarrow q_j / \text{sum}(q_j)$ 
12:       $x, y \leftarrow B$  data samples  $\{x_i, y_i\}_{i=1}^{n_j} \propto p_j$ 
13:       $\mathcal{L}(x) \leftarrow \mathcal{L}(m(x, \theta), y)$ 
14:       $\nabla \mathcal{L}(x) \leftarrow$  Backpropagate( $\mathcal{L}(x)$ )
15:       $S(x) \leftarrow \sum_{k=1}^J n_k p_k(x)$ 
16:       $\mathbf{W} \leftarrow n_i p_i(x) / \sum_{k=1}^J n_k p_k(x)$   $\leftarrow$  Momentum estim.
17:       $\langle \mathbf{A} \rangle \leftarrow \langle \mathbf{A} \rangle + (1 - \beta) \sum_{i=1}^{n_j} \mathbf{W}_i \mathbf{W}_i^T$ 
18:       $\langle \mathbf{b} \rangle \leftarrow \langle \mathbf{b} \rangle + (1 - \beta) \sum_{i=1}^{n_j} \nabla \mathcal{L}(x_i) \mathbf{W}_i / S(x_i)$ 
19:       $\mathbf{q}(x) \leftarrow \alpha \mathbf{q}(x) + (1 - \alpha) \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)}$ 
20:
21:     $\langle \alpha \rangle \leftarrow \langle \mathbf{A} \rangle^{-1} \langle \mathbf{b} \rangle$ 
22:     $\langle \nabla L_{\theta} \rangle_{\text{OMIS}} \leftarrow \sum_{j=1}^J \langle \alpha_j \rangle$ 
23:     $\theta \leftarrow \theta - \eta \langle \nabla L_{\theta} \rangle_{\text{OMIS}}$   $\leftarrow$  SGD step
24:
25: return  $\theta$ 
    
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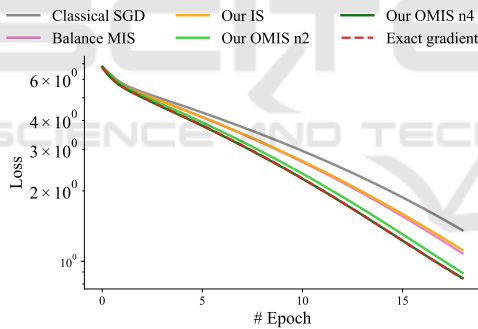


Figure 2: Convergence comparison of polynomial regression of order 6 using different method. Exact gradient show a gradient descent as baseline and classical SGD. For our method, we compare importance sampling and OMIS using  $n = 2$  or 4 importance distributions. Balance heuristic MIS is also visible. Our method using OMIS achieve same convergence as exact gradient.

**Momentum-Based Linear-System Estimation.** If the matrix estimate  $\langle \mathbf{A} \rangle$  is inaccurate, its inversion can be unstable and yield a poor gradient estimate. The simplest way to tackle this problem is to use a large number of samples per distribution, which produces accurate estimates of both  $\mathbf{A}$  and  $\mathbf{b}$  and thus a stable solution to the linear system. However, this approach is computationally expensive. Instead, we keep the sample counts low and reuse the estimates from previous mini-batches via momentum-based accumulation, shown in lines 17–18, where  $\beta$  is the parameter con-

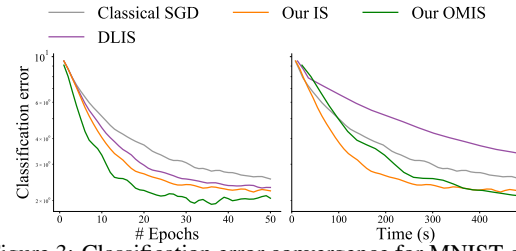


Figure 3: Classification error convergence for MNIST classification for various methods. Both Katharopoulos and Fleuret (2018) (DLIS) and resampling SGD approach. In comparison, our two method use the presented algorithm without resampling. It is visible that while DLIS perform similarly to our IS at equal epoch, the overhead of the method makes ours noticeably better at equal time for our IS and OMIS.

trolling the momentum; we use  $\beta = 0.7$ . This accumulation provides stability, yields an estimate of the momentum gradient Rumelhart et al. (1986), and allows us to use 1–4 samples per distribution in a mini-batch.

**Importance functions.** To derive our importance distributions, we expand on the approach from Section 4. Instead of taking the norm of the entire output layer of the model, we take the different gradients separately as  $\mathbf{q}(x) = \frac{\partial \mathcal{L}(x)}{\partial m(x, \theta)}$  (see Fig. 1d). Similarly to Algorithm 1, we apply momentum-based accumulation of the per-data importance (line 19 in Algorithm 2). If the output layer has more nodes than the desired number  $J$  of distributions, we select a subset of the nodes. Many other ways exist to derive the distributions, e.g., clustering the nodes into  $J$  groups and taking the norm of each; we leave such exploration for future work.

## 6 EXPERIMENTS

**Implementation Details.** We evaluate our importance sampling (IS) and optimal multiple importance sampling (OMIS) methods on a set of classification and regression tasks with different data modalities (images, point clouds). We compare them to classical SGD (which draws mini-batch samples uniformly without replacement), DLIS Katharopoulos and Fleuret (2018), and LOW Santiago et al. (2021). DLIS uses a resampling scheme that samples an initial, larger mini-batch uniformly and then selects a fraction of them for backpropagation and a gradient step. This resampling is based on an importance sampling metric computed by running a forward pass for each initial sample. LOW applies adaptive weighting to uniformly selected mini-batch samples to give importance to data with high loss. All reported metrics

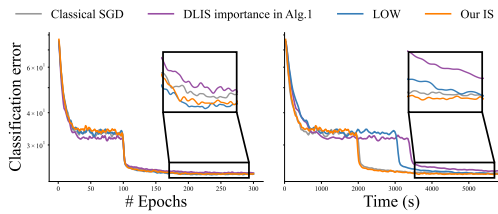


Figure 4: On CIFAR-100, we use the DLIS importance metric in our Algorithm 1 instead of the DLIS resampling algorithm. The zoom-in highlights show error drops when the learning rate decreases after epoch 100. Our method (Our IS) outperforms LOW Santiago et al. (2021) and DLIS weights at equal epochs (left). It also converges faster than LOW and DLIS weights at equal time (right).

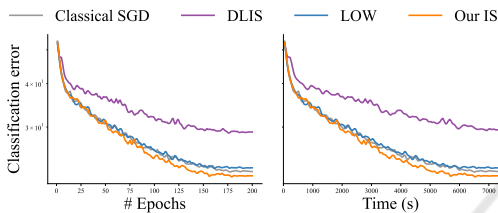


Figure 5: Comparisons on CIFAR-10 using Vision Transformer (ViT) Dosovitskiy et al. (2020). The results show our importance sampling scheme (Our IS) can improve over classical SGD, LOW Santiago et al. (2021) and DLIS Katharopoulos and Fleuret (2018) on modern transformer architecture.

are computed on data unseen during training, with the exception of the regression tasks.

All experiments are conducted on a single NVIDIA Tesla A40 graphics card. Details about the optimization setup of each experiment can be found in Supplemental document.

**Convex Problem.** We performed a basic convergence analysis of IS and OMIS on a convex polynomial-regression problem. Figure 2 compares classical SGD, our IS, and three MIS techniques: balance heuristic Veach (1997) and our OMIS using two and four importance distributions. The exact gradient serves as a reference point for optimal convergence. Balance-heuristic MIS exhibits similar convergence to IS. This can be attributed to the weights depending solely on the relative importance distributions, disregarding differences in individual parameter derivatives. This underscores the unsuitability of the balance heuristic as a weighting method for vector-valued estimation. Both our OMIS variants achieve convergence similar to that of the exact gradient. The four-distribution variant achieves the same quality as the exact gradient using only 32 data samples per mini-batch. This shows the potential of OMIS to achieve low error in gradient estimation even at low mini-batch sizes.

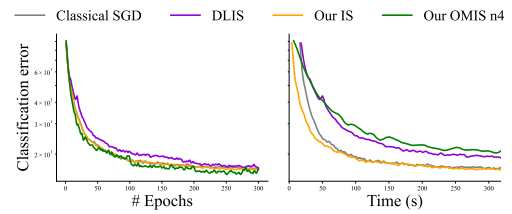


Figure 6: Comparison of our two methods (Our IS, Our OMIS) on point-cloud classification using PointNet Qi et al. (2017) architecture. Our OMIS achieves lower classification error at equal epochs, though it introduces computation overhead as shown at equal-time comparisons. At equal time, our method using importance sampling achieves the best performance.

**Classification.** In Fig. 3, we compare our algorithms to the DLIS resampling algorithm of Katharopoulos and Fleuret (2018) on MNIST classification. Our IS performs slightly better than DLIS, and our OMIS does best. The differences between our methods and the rest are more pronounced when comparing equal-time performance. DLIS has a higher computational cost as it involves running a forward pass on a large mini-batch to compute resampling probabilities. Our OMIS requires access to the gradient of each mini-batch sample; obtaining these gradients in our current implementation is inefficient due to technical limitations in the optimization framework we use (PyTorch). Nevertheless, the method manages to make up for this overhead with a higher-quality gradient estimate. In Fig. 3 we compare classification error; loss-convergence plots are shown in Supplemental document.

In Fig. 4, we compare our IS against using the DLIS importance function in Algorithm 1 and LOW Santiago et al. (2021) on CIFAR-100 classification. At equal number of epochs, the difference between the methods is small (see close-up view). Our IS achieves similar classification accuracy as LOW and outperforms the DLIS variant. At equal time the difference is more important as our method has lower computational cost. This experiment shows that our importance function achieves better performance than that of DLIS within the same optimization algorithm.

Figure 5 shows a similar experiment on CIFAR-10 using a vision transformer Dosovitskiy et al. (2020). Our IS method achieves consistent improvement over the state of the art. The worse convergence of (original, resampling-based) DLIS can be attributed to its resampling tending to exclude some training data with very low importance, which can cause overfitting.

Figure 6 shows point-cloud classification, where our IS is comparable to classical SGD and our OMIS outperforms other methods in terms of classification error at equal epochs. In complex cases where impor-

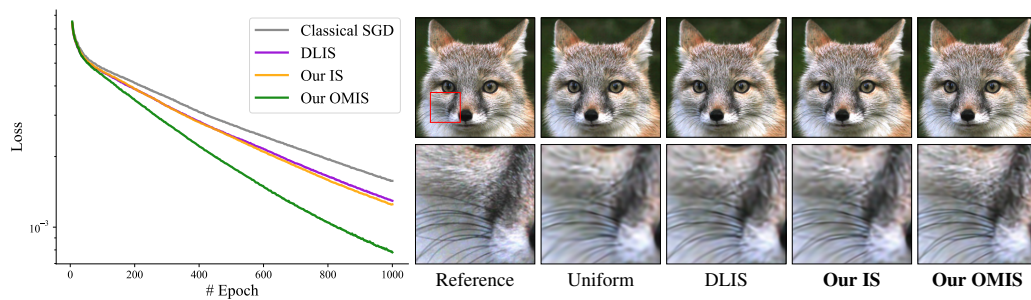


Figure 7: Comparison at equal step for image 2D regression. Left side show the convergence plot while the right display the result regression and a close-up view. Our method using MIS achieves the lower error on this problem while IS and DLIS perform similarly. On the images it is visible that our OMIS recover the finest details of the fur and whiskers.

tance sampling cannot enhance convergence by providing a more accurate gradient estimator, our method is still as efficient as SGD due to minimal overhead. This means that even though importance sampling does not offer additional benefits in these scenarios, our implementation remains competitive with classical methods. In his case DLIS and our OMIS both suffer from computational overhead.

**Regression.** Figure 7 shows results on image regression, comparing classical SGD, DLIS, and our IS and OMIS. Classical SGD yields a blurry image, as seen in the zoom-ins. DLIS and our IS methods achieves similar results, with increased whisker sharpness but still blurry fur, though ours has slightly lower loss and is computationally faster, as discussed above. Our OMIS employs three sampling distributions based on the network’s outputs which represent the red, green and blue image channels. This method achieves the lowest error and highest image fidelity, as seen in the zoom-in.

## 7 LIMITATIONS AND FUTURE WORK

We have showcased the effectiveness of importance sampling and optimal multiple importance sampling (OMIS) in machine-learning optimization, leading to a reduction in gradient-estimation error. Our current OMIS implementation incurs some overhead as it requires access to individual mini-batch sample gradients. Modern optimization frameworks can efficiently compute those gradients in parallel but only return their average. This is the main computational bottleneck in the method. The overhead of the linear system computation is negligible; we have tested using up to 10 distributions.

Our current OMIS implementation is limited to sequential models; hence its absence from our ViT

experiment in Fig. 5. However, there is no inherent limitation that would prevent its use with such more complex architectures. We anticipate that similar improvements could be achieved, but defer the exploration of this extension to future work.

In all our experiments we allocate the same sampling budget to each distribution. Non-uniform sample distribution could potentially further reduce estimation variance, especially if it can be dynamically adjusted during the optimization process.

Recent work from Santiago et al. (2021) has explored a variant of importance sampling that forgoes sample-contribution normalization, i.e., the division by the probability  $p(x)$  in Eq. (3) (and on line 10 of Algorithm 1). This heuristic approach lacks proof of convergence but can achieve practical improvement over importance sampling in some cases. We include a such variant of our IS method in Supplemental document.

## 8 CONCLUSION

This work proposes a novel approach to improve gradient-descent optimization through efficient data importance sampling. We present a method incorporates a gradient-based importance metric that evolves during training. It boasts minimal computational overhead while effectively exploiting the gradient of the network output. Furthermore, we introduce the use of (optimal) multiple importance sampling for vector-valued, gradient estimation. Empirical evaluation on typical machine learning tasks demonstrates the tangible benefits of combining several importance distributions in achieving faster convergence.



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