USING IMPORTANCE SAMPLING IN ESTIMATING
WEAK DERIVATIVE

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Abstract
In this paper we study simulation-based methods for estimating gradients in stochastic networks. We derive a new method of calculating weak derivative estimator using importance sampling transform, and our method has less computational cost than the classical method. In the context of M/M/1 queueing network and stochastic activity network, we analytically show that our new method won’t result in a great increase of sample variance of the estimators. Our numerical experiments show that under same simulation time, the new method can yield a narrower confidence interval of the true gradient than the classical one, suggesting that the new method is more competitive.

1 Introduction
Stochastic gradient estimation plays an important role in many fields, such as simulation optimization[1] and the study of option price sensitivities ([2]). Suppose we are interested in
\[ \frac{dJ(\theta)}{d\theta}, \]
where \( J(\theta) \) is not directly available but instead the simulation model returns a randomized output \( Y(X, \theta) \) such that
\[ J(\theta) = E(Y(X, \theta)), \]
where, \( Y(X, \theta) \) can represent, for instance, the total cost time of stochastic activity network or the average waiting time in G/G/1 queue. Estimating the gradient in (1) can itself be a challenging task, which constitutes the subject of this paper.

A remarkable amount of stochastic gradient estimation methods have been developed in past few decades, and they can be essentially classified into two main categories—indirect or direct estimations. The most popular indirect gradient estimators method include finite difference and simultaneous perturbation. Direct estimators include score function(SF) method, infinite small perturbation analysis(IPA) and measure valued differentiation(weak derivative). We will write them respectively as SF, IPA and WD for the sake of simplicity in the rest of paper.

Unlike SF and IPA, which are single-run estimators, weak derivatives often requires more computational time to simulate random variable \( X^+ \) and \( X^- \) and calculate the difference of the values \( Y(X^+) \) and \( Y(X^-) \) [see section 2]. Such a disadvantage make WD estimator less widely used though it usually has less variance than single-run estimators.

The importance sampling method was originally developed for the purpose of variance reduction. However, it can been used in many cases other than variance reduction. For example, one can use
it to study one distribution while simulating another([3, 4, 5, 6]). Inspired by the idea of importance sampling, we develop a new way to estimate weak derivative, called importance sampling weak derivative (ISWD) estimator, which can be get in a single-run.

However, since the importance sampling transform may yield an estimator with variance dramatically larger than the original one, one has to be very cautious of using that [7, 8]. The remainder of this paper is devoted on discussing different cases where our new method is applicable and if so, whether it can outperform the classical way to estimate Weak Derivative.

Preview. This paper has the following structure. Section 2 introduces the direct gradient estimation problem and presents weak derivative estimators. Section 3 introduces importance sampling and present our new way of calculating the WD estimator.

2 WEAK DERIVATIVE ESTIMATOR

2.1 Introduction

We denote our objective function to be \( J(\Theta) \), the randomized output value to be \( Y(X) \), and the following equality holds:

\[
E\{Y(X)\} = J(\Theta)
\]

where \( X \) denote the vector of input random variables of the stochastic network, \( X = \{X_1,...X_N\} \), and \( \Theta = \{\theta_1,...\theta_n\} \) denote the parameter associated with \( \{X_1,...X_N\} \).

We are interested in the sensitivity of \( \theta_i \) in our objective function [9, 10], which can be expressed as

\[
\frac{dE(Y(X))}{d\theta_i} = \frac{dJ(\Theta)}{d\theta_i}.
\]

Writing equation (2) in the integration form, we have

\[
\frac{dE(Y(X))}{d\theta_i} = \int_{R} Y(x_1,...x_N) f_i(x_1,...x_N;\theta_i) dx_1...dx_N
\]

(3)

Suppose the r.v.s \( \{X_1,...X_N\} \) are independent to each other, i.e

\[
f(x_1,...x_N, \Theta) = \prod_{1}^{N} f(x_i;\theta_i)
\]

Where \( f(x_1,...x_N; \Theta) \) represents the joint density function of \( \{X_1,...X_N\} \).

The derivative can then be written as

\[
\frac{dE(Y(X))}{d\theta_i} = \int_{R} Y(x_1,...x_N) \frac{\partial f_i(x_1,...x_N;\theta)}{\partial \theta_i} f_{-1}(x_1,...x_N) dx_1...dx_N
\]

(4)

Where \( f_{-1}(x_1,...x_N) \) denote the joint density function of all the r.v.s except \( X_i \).

Observe the fact that when the derivative \( \frac{\partial f_i(x_i;\theta_i)}{\partial \theta_i} \) can be decomposed weakly to the subtraction of two nonnegative functions, that is

\[
\frac{\partial f_i(x_i;\theta_i)}{\partial \theta_i} = c_i(\theta_i) (f_i^+(x_i;\theta_i) - f_i^-(x_i;\theta_i))
\]

(5)

Such weak decomposition of derivative can be seen by the property that

\[
\int_{-\infty}^{x} \frac{\partial f_i(x_i;\theta_i)}{\partial \theta_i} = \frac{\partial F_i(x_i;\theta_i)}{\partial \theta_i} = c_i(\theta_i) \int_{-\infty}^{x} f^+(t;\theta_i) - f^-(t;\theta_i) dt
\]

which is justified by the absolute continuity property of the derivative \( \frac{\partial F(x_i;\theta)}{\partial \theta} \).

According to The weak decomposition of derivative[11] of density function leads to the following relationship:
\[ \frac{dE(Y(X))}{d\theta_i} = \int_R Y(x_1, \ldots, x_N) c_i(\theta_i) f_i^+(x_i; \theta_i) - f_i^-(x_i; \theta_i)) f_{-1}(x_1, \ldots, x_N) dx_1 \ldots dx_N \]  

(6)

For simplicity, we denote (5) as

\[ \frac{dE(Y(X))}{d\theta_i} = \sum_{i=1}^{n} c_i(\theta_i) E(Y(X_1, \ldots, X_i^+, \ldots, X_n) - Y(X_1, \ldots, X_i^-, \ldots, X_n)) \]  

(7)

with \( X_i^+ \sim f_i^+(x_i; \theta_i) \), \( X_i^- \sim f_i^-(x_i; \theta_i) \) and \( X_i^+, X_i^- \) are all independent of r.vs \( X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n \). And a typical weak derivative estimator for the gradient can be written as

\[ \{ \sum_{i=1}^{N} c_i(\theta_i) (Y(X_1, \ldots, X_i^+, \ldots, X_N) - Y(X_1, \ldots, X_i^-, \ldots, X_N)) \} \]  

(8)

In the special case where \( X_i \)'s are i.i.d, \( c_i(\theta_i) \)'s and \( \theta_i \)'s are identical, denoted by \( \theta \) and \( c(\theta) \), and we let \( J(\theta) \) represents our objective function, and we are interested in estimating

\[ \frac{dE(Y(X))}{d\theta} = \frac{dJ(\theta)}{d\theta}. \]  

(9)

The WD estimator becomes

\[ c(\theta) \{ \sum_{i=1}^{N} (Y(X_1, \ldots, X_i^+, \ldots, X_N) - Y(X_1, \ldots, X_i^-, \ldots, X_N)) \} \]  

(10)

### 2.2 Motivational Examples

- **Gaussian distribution** [12]

  Suppose \( X \sim N(\theta, \sigma^2) \), with density function

  \[ \phi_{\theta, \sigma}(x) = \frac{1}{\sqrt{2\pi}\sigma^2} e^{-(x-\theta)^2/2\sigma^2} \]

  According to Fu(06), we can decompose the derivative weakly to the following:
  \( X^+ \sim \theta + Wei(2, \frac{1}{2\sigma^2}) \), and \( X^- \sim \theta - Wei(2, \frac{1}{2\sigma^2}) \).

- **Gamma Distribution** [13]

  Denote \( X \sim Gamma(\alpha, \theta) \) with density equal to

  \[ f_{\theta, \alpha}(x) = \frac{\theta^{-\alpha} x^{\alpha-1} e^{-x/\theta}}{\Gamma(\alpha)} \]

  one choice of weak derivative decomposition can be:
  \( X^+ \sim gamma(\alpha + 1, \theta) \), \( X^- \sim gamma(\alpha, \theta) \).

- **Exponential Distribution**

  Consider \( X \sim exp(\theta) \), a special case of Gamma distribution with density:

  \[ f_{\theta}(x) = \frac{1}{\theta} e^{-\frac{x}{\theta}} \]

  it’s weak derivative decomposition can be: \( X^+ \sim erlang(2, \theta) \), \( X^- \sim exp(\theta) \)
3 IMPORTANCE SAMPLING WEAK DERIVATIVE ESTIMATOR

3.1 Review of importance sampling

Suppose that our problem here is to find
\[ \mu_p = E_p(Y(X)) = \int_D Y(x)p(x)dx \]

where \( p \) is a probability density function of \( X \) with support in \( D \). If \( q \) is a positive probability density function with support larger than \( D \), then
\[ \mu_p = \int_D Y(x)p(x)dx = \int_D \frac{Y(x)p(x)}{q(x)}q(x)dx = E_q(\frac{Y(X)p(X)}{q(X)}) \]  \hspace{1cm} (11)

We denote \( \mu_q \) for the value \( E_q(Y(X)p(X)/q(X)) \) in the rest of this section.

Given that we have \( n \) samples with density \( q \), denoted by \( \{X_1, X_n\} \), the importance sampling estimator of \( \mu_p = E_p(Y(X)) \) is
\[ \hat{\mu}_p = \frac{1}{n} \sum_{i=1}^{n} \frac{Y(X_i)p(X_i)}{q(X_i)}, X_i \sim q. \]  \hspace{1cm} (12)

The variance of importance sampling transform is given in the theorem below without proof:

**Theorem 1.** Let \( \hat{\mu}_p \) be given by (2) where \( \mu = \int_D Y(x)p(x)dx \) and \( q(x) > 0 \) whenever \( Y(x)p(x) \neq 0 \). Then \( E_q(\hat{\mu}_q) = \mu \), and \( \text{Var}_q(\hat{\mu}_q) = \sigma_q^2/n \) where
\[ \sigma_q^2 = \int_D \frac{(Y(x)p(x))^2}{q(x)}dx - \mu^2 \]
\[ = \int_D \frac{(Y(x)p(x) - \mu q(x))^2}{q(x)}dx \]  \hspace{1cm} (13)

According to the theorem above, one can naturally find the estimator for the variance \( \sigma_q^2 \)
\[ \hat{\sigma}_q^2 = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{Y(X_i)p(X_i)}{q(X_i)} - \hat{\mu}_q \right)^2 \]

Therefore an approximate 95% CI for \( \mu \) is \( \hat{\mu}_q \pm 1.96 \hat{\sigma}_q^2/\sqrt{n} \)

- **Remark:** At this time the adjustment factor \( p(x)/q(x) \) is called the likelihood ratio. The distribution \( q \) is the importance distribution and \( p \) is the nominal distribution. In the above case the importance distribution \( q(x) \) doesn’t have to be positive everywhere. It’s sufficient that we have \( q(x) > 0 \) whenever \( Y(x)p(x) \neq 0 \).

3.2 Application in estimating Weak Derivative

Consider estimating weak derivative described in section 2, under the assumption all the input r.v.s \( \{X_1, ...X_n\} \) are independent to each other, with associated \( \{\theta_1, ...\theta_n\} \).

Observe that
\[ \frac{dE(Y(X_1,...X_n))}{d\theta_i} = c_i(\theta_i)(E(Y(X_1,X_1^+...X_n) - Y(X_1,...X_i^-...X_n))) \]

Therefore, based on the equation above, we can develop a modified weak derivative estimator (will call it ISWD in the following paper) of \( \frac{dE(Y(\theta_i))}{d\theta_i} \) to be
\[ c_i(\theta_i)Y(X_1,...X_i,...X_n)(\frac{f^+_{i}(X_i)}{f_i(X_i)} - \frac{f^-_{i}(X_i)}{f_i(X_i)}) \]
Observe that if we assume all $X_i$s are i.i.d, the expression in (7) can also be written as

$$\sum_{i=1}^{n} c_i(\theta_i)E(Y(X_1, \ldots X_i^+, \ldots X_n) - Y(X_1, \ldots X_i^−, \ldots X_n)) = \sum_{i=1}^{n} c_i(\theta)E(Y(X_1, \ldots X_i, \ldots X_n)(\frac{f^+(X_i)}{f_i(X_i)} - \frac{f^-(X_i)}{f_i(X_i)}))$$

(14)

And based on (11), a sample of Modified weak derivative estimator for $\frac{dE(Y(X))}{d\theta}$ shall be

$$\sum_{i=1}^{n} c(\theta)(Y(X_1, \ldots X_i, \ldots X_n)(\frac{f^+(X_i)}{f_i(X_i)} - \frac{f^-(X_i)}{f_i(X_i)}))$$

(15)

3.3 ISWD estimator in M/M/1 FCFS queue

- **Notations:**
  Let $T_N(X_1, \ldots X_N, A_1, \ldots A_N)$ denote the system time of the $N$th customer, with $X_1, \ldots X_N$ represent the r.v.s of the service time [14] and $A_1, \ldots A_N$ represent the r.v.s of the inter arrival time. Denote $\theta$ the mean of service time, and we assume all $X_1, \ldots X_N$ are i.i.d exponentially distributed. Denote $f$ to be the density of $X_i$, and $f^+, f^−$ been respectively, the density from weak decomposition of $\partial f(\theta)/\partial \theta$.

  We are interested in estimating the sensitivity [15, 16, 17, 18] of expectation of $N$th customer’s system time w.r.t the mean service time, which is

$$\frac{dE(T_N(X_1, \ldots A_N))}{d\theta}$$

- **Typical weak derivative estimator** [19]:
  Notice that since all $X_i$s are i.i.d, $c_i(\theta)$ are identical to each other, we denote them as $c(\theta)$. The sensitivity of system time w.r.t the mean service time can be written as

$$\frac{dE(T_N(X_1, \ldots A_N))}{d\theta} = c(\theta) \sum_{i=1}^{N} E(T_N(X_1, \ldots X_i^+, \ldots X_N, A_1, \ldots A_N) - T_N(X_1, \ldots X_i^−, \ldots X_N, A_1, \ldots A_N)).$$

(16)

Where $X_i^+$ and $X_i^−$ are random variables whose densities come from weak derivative decomposition of density of $\partial f/\partial \theta$.

The sample estimator for the sensitivity becomes

$$c(\theta) \sum_{i=1}^{N} (T_N(X_1, \ldots X_i^+, \ldots X_N, A_1, \ldots A_N) - T_N(X_1, \ldots X_i^−, \ldots X_N, A_1, \ldots A_N))$$

- **ISWD estimator:**
  Inspired by the framework of importance sampling, one can instead estimate the expectations through ratio of the density function $f^+/f$ and $f^−/f$, i.e,

$$\frac{dE(T_N(X_1, \ldots A_N))}{d\theta} = \sum_{i=1}^{N} c(\theta)(E(T_N(X_1, \ldots A_N) \frac{f^+(X_i)}{f(X_i)}) - E(T_N(X_1, \ldots A_N) \frac{f^-(X_i)}{f(X_i)}))$$

(17)

This time, the estimator is been reduced to

$$c(\theta) \sum_{i=1}^{N} T(A_1, \ldots X_N) \frac{f^+(X_i)}{f(X_i)} - T(A_1, \ldots X_N) \frac{f^-(X_i)}{f(X_i)}$$

- **Computation time comparison:**
  The computational time for the typical estimator include the following three parts:
  1. simulate $X_i^+$ and $X_i^−$,
2. calculate $T_N(X_1, \ldots, X^+_i, \ldots, X_N, A_1, \ldots, A_N)$ and $T_N(X_1, \ldots, X^-_i, \ldots, X_N, A_1, \ldots, A_N)$ accordingly

3. subtracting the above two values.

Among the three parts, calculating $T_N$ consumes the most and especially when $N$ is large, it often take a long time. However, the modified estimator will only consume as much as the 3rd part of typical estimator.

References

[1] W. K. Hastings. Monte carlo sampling methods using markov chains and their applications. *Biometrika*, 57:97–109, 1970.

[2] Michael C. Fu. Optimization for simulation: Theory vs. practice. 2002.

[3] Art B. Owen, Yury Maximov, and Michael Chertkov. Importance sampling the union of rare events with an application to power systems analysis. *ArXiv*, abs/1710.06965, 2019.

[4] Boning Zhang, Richard A. Regueiro, Andrew M. Druckrey, and Khalid Alshibli. Construction of poly-ellipsoidal grain shapes from smt imaging on sand, and the development of a new dem contact detection algorithm. *Engineering Computations*, 35(2):733–771, 2018.

[5] R.A. Regueiro, B. Zhang, and F. Shahhabi. Micromorphic continuum stress measures calculated from three-dimensional ellipsoidal discrete element simulations on granular media. *IS-Cambridge*, 2014:1–6, 2014.

[6] Boning Zhang and Richard A Regueiro. On large deformation granular strain measures for generating stress-strain relations based upon three-dimensional discrete element simulations. *International Journal of Solids and Structures*, 66:151–170, 2015.

[7] Cheng Jie, Zigeng Wang, Da Xu, and Wei Shen. Multi-objective cluster based bidding algorithm for e-commerce search engine marketing system. *Frontiers in Big Data*, 5, 2022.

[8] Cheng Jie. *Decision Making Under Uncertainty: New Models and Applications*. PhD thesis, 2018.

[9] Kun Lin, Cheng Jie, and Steven I. Marcus. Probabilistically distorted risk-sensitive infinite-horizon dynamic programming. *Automatica*, 97:1–6, 2018.

[10] Cheng Jie, Da Xu, Zigeng Wang, Lu Wang, and Wei-Yuan Shen. Bidding via clustering ads intentions: an efficient search engine marketing system for e-commerce. *ArXiv*, abs/2106.12700, 2021.

[11] Cheng Jie, A. PrashanthL., M. Fu, S. Marcus, and Csaba Szepesvari. Stochastic optimization in a cumulative prospect theory framework. *IEEE Transactions on Automatic Control*, 63:2867–2882, 2018.

[12] Andreas Winkelbauer. Moments and absolute moments of the normal distribution. *ArXiv*, abs/1209.4340, 2012.

[13] L.A. Prashanth, Cheng Jie, Michael Fu, Steve Marcus, and Csaba Szepesvári. Cumulative prospect theory meets reinforcement learning: Prediction and control. In *Proceedings of The 33rd International Conference on Machine Learning*, pages 1406–1415, 2016.

[14] Liao Zhu, Sumanta Basu, Robert A. Jarrow, and Martin T. Wells. High-dimensional estimation, basis assets, and the adaptive multi-factor model. *The Quarterly Journal of Finance*, 10(04):2050017, 2020.

[15] Liao Zhu, Ningning Sun, and Martin T. Wells. Clustering structure of microstructure measures. *Applied Economics and Finance*, 9(1):85–95, 2022.

[16] Xinyan Zhao, Mengqi Zhan, and Cheng Jie. Examining multiplicity and dynamics of publics’ crisis narratives with large-scale twitter data. *Public Relations Review*, 44(4):619–632, 2018.
[17] Christopher T Senseney, Zheng Duan, Boning Zhang, and Richard A Regueiro. Combined spheropolyhedral discrete element (de)-finite element (fe) computational modeling of vertical plate loading on cohesionless soil. *Acta Geotechnica*, 12:593–603, 2017.

[18] Boning Zhang, Eric B. Herbold, Michael A. Homel, and Richard A. Regueiro. DEM Particle Fracture Model. Technical report, Lawrence Livermore National Lab.(LLNL), Livermore, CA (United States), 12 2015.

[19] Thomas Flynn and Felisa V’azquez-Abad. A simultaneous perturbation weak derivative estimator for stochastic neural networks. *Comput. Manag. Sci.*, 16:715–738, 2019.
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