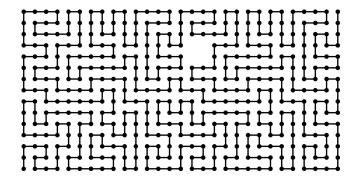
# Winsorized Importance Sampling

Paulo Orenstein February 8, 2019

Stanford University



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#### Introduction

Let f(x) be an arbitrary function, p(x), q(x) probability densities. Suppose we are interested in

$$\theta = \mathbb{E}_p[f(X)] = \int_{\mathbb{R}} f(x)p(x)dx.$$

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- Assume we can only sample from q, which is called the sampling distribution; p is the target distribution.
- $\triangleright$  The importance sampling estimator for  $\theta$  is

$$\hat{\theta}_n = \frac{1}{n} \sum_{i=1}^n f(X_i) \frac{p(X_i)}{q(X_i)}, \qquad X_i \sim q.$$

▶ The importance sampling (IS) estimator is unbiased:

$$\hat{\theta}_n \stackrel{n \to \infty}{\longrightarrow} \mathbb{E}\left[f(x)\frac{p(X)}{q(X)}\right] = \int f(x)\frac{p(x)}{q(x)}q(x)dx = \int f(x)p(x)dx = \theta,$$

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- ▶ But it can have huge or even infinite variance, leading to terrible estimates.
- Can we control the variance of the terms

$$Y_i = f(X_i) \frac{p(X_i)}{q(X_i)}$$

by sacrificing some small amount of bias?

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▶ Define the *winsorized importance sampling estimator* at level *M* as

$$\hat{\theta}_n^M = \frac{1}{n} \sum_{i=1}^n Y_i^M.$$

- ▶ Picking the right threshold level *M* is crucial.
- ▶ Bias-variance trade-off: smaller *M* implies less variance but more bias.

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## How to pick M?

▶ Let  $\{Y_i\}_{i=1}^n$  be random variables distributed iid with mean  $\theta$ .

Winsorized IS Theoretical Guarantees

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- Consider winsorizing  $Y_i$  at different threshold levels in a pre-chosen set  $\Lambda = \{M_1, \dots, M_k\}$  to obtain winsorized samples  $\{Y_i^{M_j}\}_{i=1}^n$ ,  $j = 1, \dots, k$ .

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- Pick the threshold level according to the rule

$$M_* = \min \left\{ M \in \Lambda : \forall M', M'' \ge M, |\overline{Y^{M'}} - \overline{Y^{M''}}| \le \alpha \cdot \left( \frac{\hat{\sigma}^{M'} + \hat{\sigma}^{M''}}{2} \right) \right\},$$

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where:

- $\alpha = c \cdot \frac{t}{\sqrt{n-t}}$

- $\frac{c}{Y^M} = \frac{1}{n} \sum_{i=1}^n Y_i^M$   $\hat{\sigma}^M = \sqrt{\frac{1}{n} \sum_{i=1}^n (Y_i^M \overline{Y^M})^2}$ .

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- Intuitively, if we have truncation levels M' > M'', we are willing to truncate further to M'' if the increase in bias  $|\frac{1}{n}\sum_{i=1}^n Y_i^{M'} \frac{1}{n}\sum_{i=1}^n Y_i^{M''}|$  is small relative to the standard deviation.

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- ▶ The actual rule can be thought of as a concrete version of the Balancing Principle (or Lepski's Method), which is reminiscent of oracle inequalities.
- ▶ With high probability, the mean-squared error using  $M_*$  is less than 5 times the error roughly incurred by choosing the best threshold level in the set.

#### Theorem

Let  $Y_i$  be iid with mean  $\theta$ . Consider winsorizing  $Y_i$  at different levels in  $\Lambda = \{M_1, \dots, M_k\}$  to obtain samples  $Y_i^{M_j}$ . Pick the threshold level

$$\mathit{M}_* = min \left\{ \mathit{M} \in \Lambda \ : \ \forall \mathit{M}', \mathit{M}'' \geq \mathit{M}, \quad |\overline{Y^{\mathit{M}'}} - \overline{Y^{\mathit{M}''}}| \leq \alpha \cdot \left( \frac{\hat{\sigma}^{\mathit{M}'} + \hat{\sigma}^{\mathit{M}''}}{2} \right) \right\},$$

where  $\alpha = c \cdot \frac{t}{\sqrt{n-t}}$  with c, t chosen constants. Let K > 0 be such that  $\mathbb{E}[|Y_i^{M_j} - \mathbb{E}[Y_i^{M_j}]|^3] \le K(\mathbb{V}[Y_i^{M_j}])^{3/2}$  for all j. Then, with probability

$$1-2|\Lambda|\left(1+rac{50K}{\sqrt{n}}-\Phi\left(t\sqrt{rac{n}{(\sqrt{n}-t)^2+t^2}}
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it holds

$$|\overline{Y^{M_*}} - \theta| \le C \min_{M \in \Lambda} \left\{ |\mathbb{E}[Y_i^M] - \theta| + \frac{t\sqrt{n}}{\sqrt{n} - t} \frac{\hat{\sigma}^M}{\sqrt{n}} \right\},\,$$

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Proof



Apply the Balancing Theorem:

### Balancing Theorem

Suppose  $\theta \in \mathbb{R}$  is an unknown parameter,  $\{\hat{E}^M\}_{M \in \Theta}$  is a sequence of estimators of  $\theta$  indexed by  $M \in \Theta \subset \mathbb{R}$ , with  $\Theta$  a finite set. Additionally, suppose that for each M we know  $|\hat{E}^M - \theta| \leq \text{bias}(M) + \hat{s}(M)$ , where we assume bias(M) is unknown but non-increasing in M, and  $\hat{s}(M) > 0$  is observed and non-decreasing in M. Fix c > 2, and take

$$M_* = \min \left\{ M \in \Theta : \forall M', M'' \ge M, |\hat{E}^{M'} - \hat{E}^{M''}| \le c \left( \frac{\hat{s}(M') + \hat{s}(M'')}{2} \right) \right\}.$$

Then we have that

$$|\hat{\mathcal{E}}^{M_*} - \theta| \le C \min_{M \in \Theta} \left\{ \hat{s}(M) + \text{bias}(M) \right\}$$
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► Then, use Berry-Esseen to get probabilistic bounds.

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# Proof (of Balancing Theorem)

▶ We must thus show that for all  $M \in \Theta$ , there exists  $C \ge 0$  such that  $|\hat{E}^{M_*} - \theta| \le C(\hat{s}(M) + \text{bias}(M))$ . For this we shall consider two cases.

## Proof (of Balancing Theorem)

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- $\triangleright$  (i) First, consider any fixed M such that  $M > M_*$ . Then, by our definition of  $M_*$ , and since  $\hat{s}(M)$  is non-decreasing in M,

$$|\hat{E}^{M_*} - \hat{E}^M| \le c \cdot \hat{s}(M).$$

Also, as  $|\hat{E}^M - \theta| < \text{bias}(M) + \hat{s}(M)$ , we get

$$|\hat{E}^{M_*} - \theta| \le |\hat{E}^{M_*} - \hat{E}^{M}| + |\hat{E}^{M} - \theta| \le c\hat{s}(M) + bias(M) + \hat{s}(M)$$
  
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(ii) The other side is harder.

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- Compare three estimators:
  - usual IS: no winsorization;
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- ► CV IS takes 10-20× longer than Balanced IS and is usually worse.

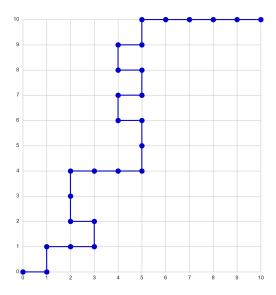
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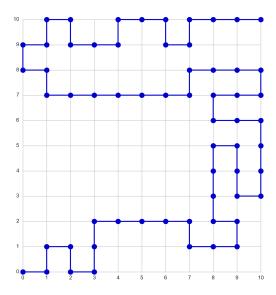
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- ► CV IS takes 10-20× longer than Balanced IS and is usually worse.
- ▶ For small variances Balanced IS matches usual IS; as the proposal distribution gets worse, Balanced IS performs much better.

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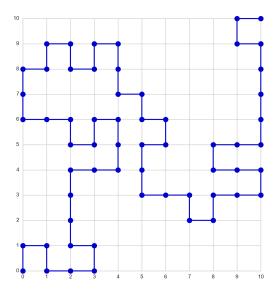
### Example: self-avoiding walk [Knuth, 1976]



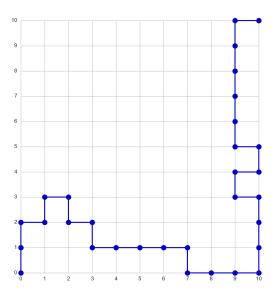
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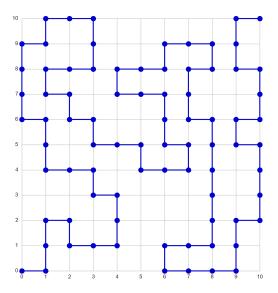
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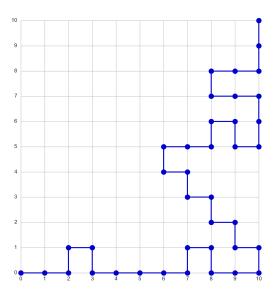
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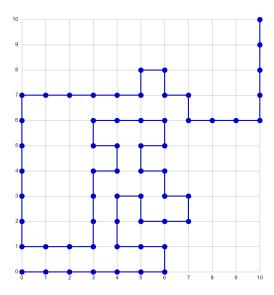
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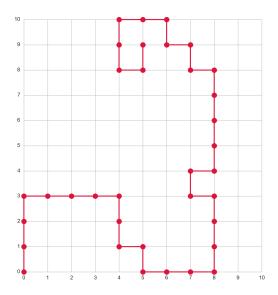
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Knuth suggested estimating the number of self-avoiding walks using importance sampling.

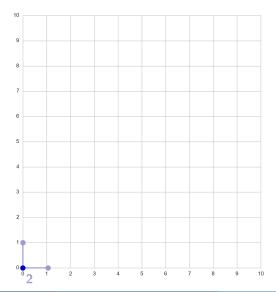
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- Knuth suggested estimating the number of self-avoiding walks using importance sampling.
- For this, we need to choose a sampling distribution, q(x), over the self-avoiding walks.

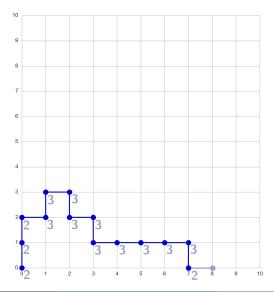
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- ▶ For this, we need to choose a sampling distribution, q(x), over the self-avoiding walks.
- Consider building one sequentially.

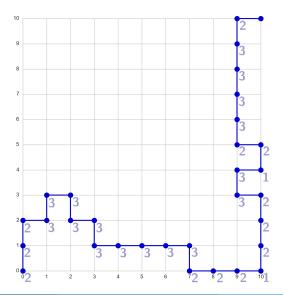
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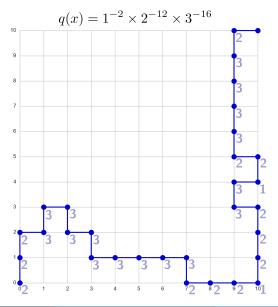
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- Define:
  - $p(x) = \frac{1}{Z_n} \mathbb{I}_{[SAW]}(x)$ ; note  $Z_n$  is the number of self-avoiding random walks;
  - $q(x) = \frac{1}{d_1 \cdot d_2 \cdot \cdot \cdot d_{m_X}}; d_i$  is the number of available neighbors to i (could be 0);
  - $f(x) = Z_n.$

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  - $f(x) = Z_n.$
- We would like to estimate

$$Z_n = \mathbb{E}_p[Z_n] = \mathbb{E}_p[f(X)] = \mathbb{E}_q\left[\frac{f(X)p(X)}{q(X)}\right] = \mathbb{E}_q\left[\frac{\mathbb{I}_{[SAW]}(X)}{q(X)}\right]$$
$$\approx \frac{1}{n}\sum_{i=1}^n d_1(X_i)d_2(X_i)\cdots d_{m_{X_i}}(X_i)\cdot \mathbb{I}_{[SAW]}(X).$$

► How does winsorization perform?

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- ▶ 1000 simulations of 1000 SAWs.
- $\theta = 1.56 \cdot 10^{24}$ :  $c = 1 + \sqrt{3}$ . t = 2.
- $M \in \{10^{21}, 5 \cdot 10^{23}, 10^{25}, 5 \cdot 10^{26}, 10^{28}\}.$

- ▶ How does winsorization perform?
- ▶ 1000 simulations of 1000 SAWs.
- $\theta = 1.56 \cdot 10^{24}$ ;  $c = 1 + \sqrt{3}$ , t = 2.
- $M \in \{10^{21}, 5 \cdot 10^{23}, 10^{25}, 5 \cdot 10^{26}, 10^{28}\}.$

	IS	CV IS	Balanced IS
MSE	$2.075 \cdot 10^{49}$	$2.457 \cdot 10^{48}$	$2.437 \cdot 10^{48}$
MAD	$1.817 \cdot 10^{24}$	$1.567 \cdot 10^{24}$	$1.561 \cdot 10^{24}$

- ▶ Procedure is run as follows:
  - Let  $M_1 = 10^{28}$ ;
    - ightharpoonup set  $M_* = M_1$

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    - $\triangleright$  set  $M_* = M_1$
  - Let  $M_2 = 5 \cdot 10^{26}$ ;
    - if  $|\overline{Y}^{M_1} \overline{Y}^{M_2}| \le \alpha \left(\frac{\hat{\sigma}^{M_1} + \hat{\sigma}^{M_2}}{2}\right)$ , set  $M_* = M_2$ , and consider further truncation;

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    - set M<sub>∗</sub> = M<sub>1</sub>
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    - else, stop
  - Let  $M_3 = 10^{25}$ 
    - $\qquad \text{if } |\overline{Y}^{M_1} \overline{Y}^{M_3}| \leq \alpha \left(\frac{\hat{\sigma}^{M_1} + \hat{\sigma}^{M_3}}{2}\right) \text{ and } |\overline{Y}^{M_2} \overline{Y}^{M_3}| \leq \alpha \left(\frac{\hat{\sigma}^{M_2} + \hat{\sigma}^{M_3}}{2}\right), \text{ set } M_* = \\$  $M_3$ , and consider further truncation:

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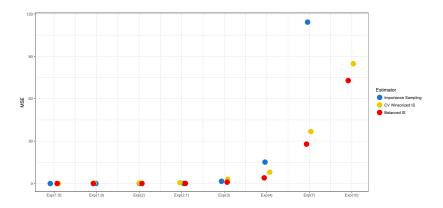
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    - else, stop
  - . . . .
- Computational complexity:  $O(|\Lambda| \cdot (|\Lambda| + n))$

## Simulation 1: Exponential

- $p = \frac{1}{\theta} Expo$ ,
- ightharpoonup q = Expo,
- ightharpoonup f(x) = x
- $\theta \in \{1.3, 1.5, 1.9, 2, 2.1, 3, 4, 10\}$
- $M \in \{550, 500, 400, 200, 100, 10\}$

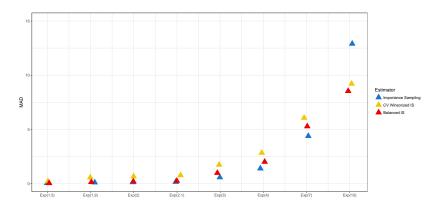
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# Simulation 1: Exponential



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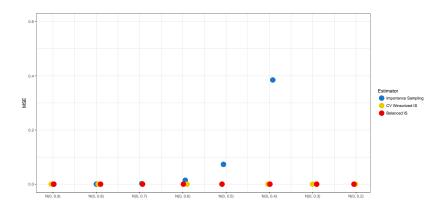


### Simulation 2: Normal

- P = N(0, 1),
- $ightharpoonup q = N(0, \theta),$
- ightharpoonup f(x) = x
- $\theta = \{0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.9\}$
- ► *M* ∈ {550, 500, 400, 200, 100, 10}

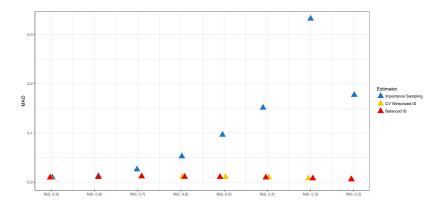
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### Simulation 2: Normal



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### Simulation 2: Normal



$$p = t_{21}(0, 1),$$

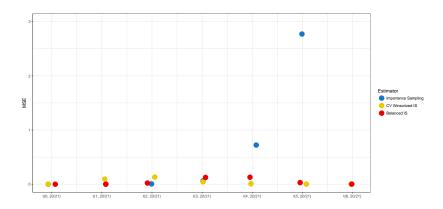
$$ightharpoonup q = t_{21}(\theta, 1 - 1/21),$$

$$ightharpoonup f(x) = x$$
,

$$\theta = \{0, 0.5, 1, 1.5, 2, 2.5, 3\}$$

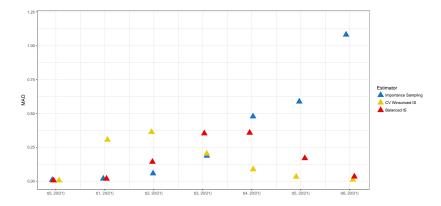
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### Simulation 3: t



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## Simulation 3: t

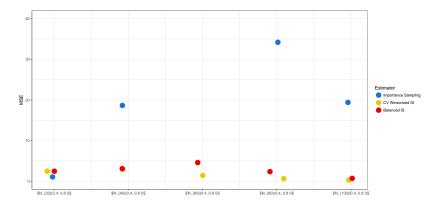


## Simulation 4: Multivariate Normal

- ▶  $p = N_{\theta}(0, 1),$
- $ightharpoonup q = t_{21,\theta}(0.4 \cdot 1, 0.8 \cdot 1),$
- $f(\mathbf{x}) = \sum_{i=1}^{\theta} x_i,$
- $\theta = \{20, 40, 60, 80, 100\}$
- $M \in \{550, 500, 400, 200, 100, 50, 10\}$

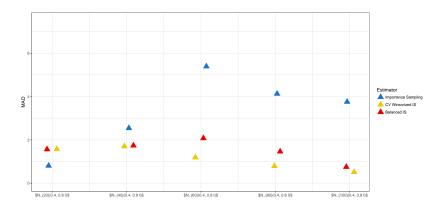
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## Simulation 4: Multivariate Normal



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## Simulation 4: Multivariate Normal

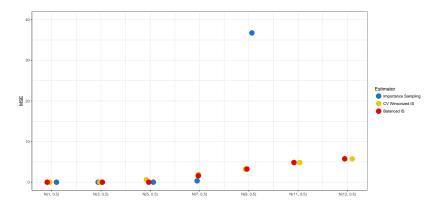


## Simulation 5: Normal Mixture

- $p = 0.8 \cdot N(0, 0.5) + 0.2 \cdot N(\theta, 0.5),$
- ightharpoonup q = N(0,4),
- ightharpoonup f(x) = x,
- $\theta = \{1, 3, 5, 7, 9, 11, 12\}$
- ► *M* ∈ {550, 500, 400, 200, 100, 10}

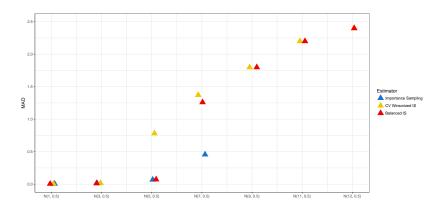
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## Simulation 5: Normal Mixture



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## Simulation 5: Normal Mixture



ction Winsorized IS Theoretical Guarantees Empirical Performance Conclusion

# Is it worth winsorizing?

- Negative aspects:
  - theory requires high n, at least  $10^8$  (but can be improved);
  - must be provided truncation values;
  - why winsorize symmetrically around 0?

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  - theory requires high n, at least  $10^8$  (but can be improved);
  - must be provided truncation values;
  - why winsorize symmetrically around 0?
- ► Positive aspects:
  - works well in practice;
  - adaptive to the sample;
  - comes with finite-sample optimality properties.

roduction Winsorized IS Theoretical Guarantees Empirical Performance Conclusion

## Conclusion

Importance sampling should not rely only on sample mean.

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Importance sampling should not rely only on sample mean.

▶ We need robust, adaptive alternatives.

Winsorized IS Theoretical Guarantees Empirical Performance Conclusion

### Conclusion

- Importance sampling should not rely only on sample mean.
- ▶ We need robust, adaptive alternatives.
- ▶ Balanced IS has theoretical guarantees and performs well in practice:
  - in high-variance settings, it outperforms usual IS
  - in low-variance settings, it matches it.

### Conclusion

- Importance sampling should not rely only on sample mean.
- ▶ We need robust, adaptive alternatives.
- ▶ Balanced IS has theoretical guarantees and performs well in practice:
  - in high-variance settings, it outperforms usual IS
  - in low-variance settings, it matches it.
- Many future extensions.

Winsorized IS Theoretical Guarantees Empirical Performance Conclusion

### References

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