Adaptive Pareto Smoothed Importance Sampling

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Introduction

- Importance Sampling
- Measuring performance
- Improving performance
  - Modifications
  - Optimization

Importance Sampling

- Need to compute an expected value
  - $\mathbb{E}_F \varphi(X)$
- Can't do the integral

- Monte Carlo approximation
  - Simulating from F might be hard

Importance Sampling

- Introduce "proposal distribution", G:

$$\mathbb{E}_F \varphi(X) = \mathbb{E}_G \left[\varphi(X) \cdot \frac{f(X)}{g(X)} \right]$$
$$= \mathbb{E}_G \left[\varphi(X) \cdot w(X) \right]$$

- G can be nearly anything*
    - *Some choices will be better than others

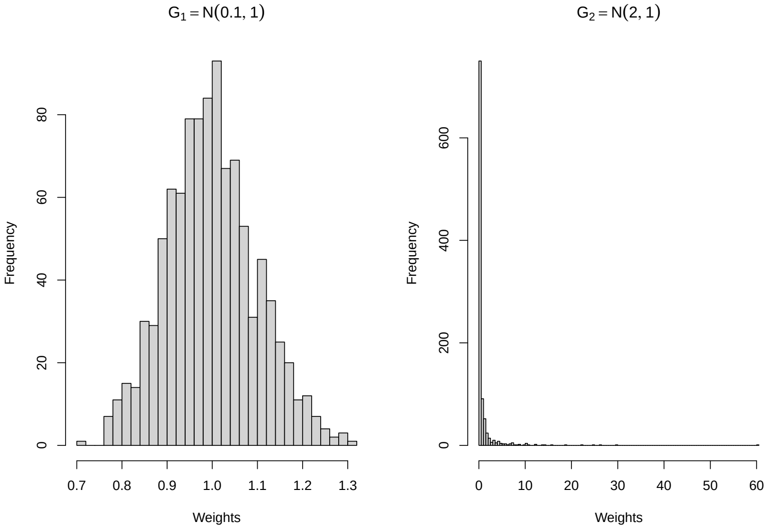
Example: Mystery Target

- f unknown, but can be evaluated
- $\varphi(X) = X^2$

- Try some proposals:
  - $G_1 \sim N(0.1, 1)$
  - $G_2 \sim N(2, 1)$

- Use $M = 1000$ samples from proposal
  - $\hat{\mathbb{E}}_1 = 0.974$
  - $\hat{\mathbb{E}}_2 = 0.603$

Example: Mystery Target



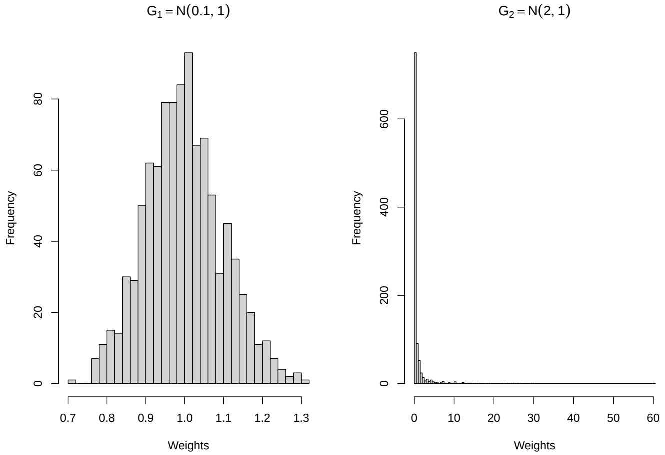
Importance Sampling

- We can make this difference precise
- "Effective Sample Size":

$$ESS = \frac{\left[\sum_i w(X_i)\right]^2}{\sum_i w(X_i)^2}$$

$$1 \leq ESS \leq M$$

Example: Mystery Target



$ESS_1 \approx 990$ $\quad$ $ESS_2 \approx 73$

Importance Sampling

- Problem: Low ESS $\rightarrow$ hard to estimate means
- But ESS is based on means
  - (Chatterjee and Diaconis, 2018)

Improving IS

- Choose a good proposal
- Modify large weights

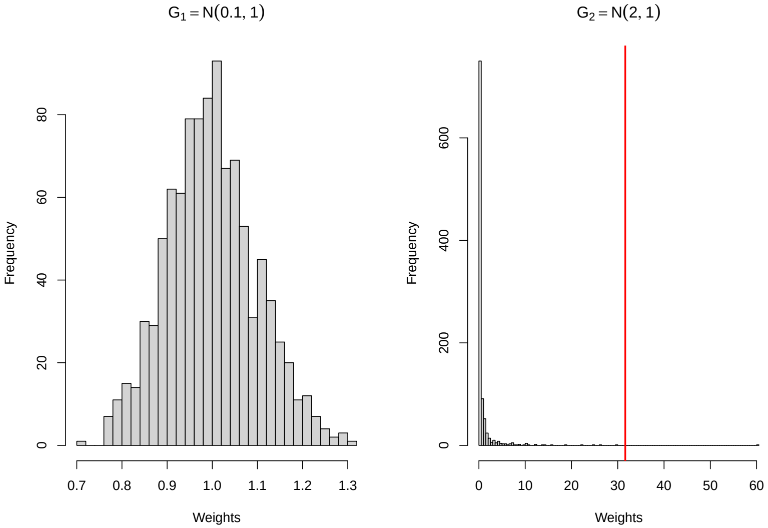
- Truncated IS
- Pareto Smoothed IS

Improving IS

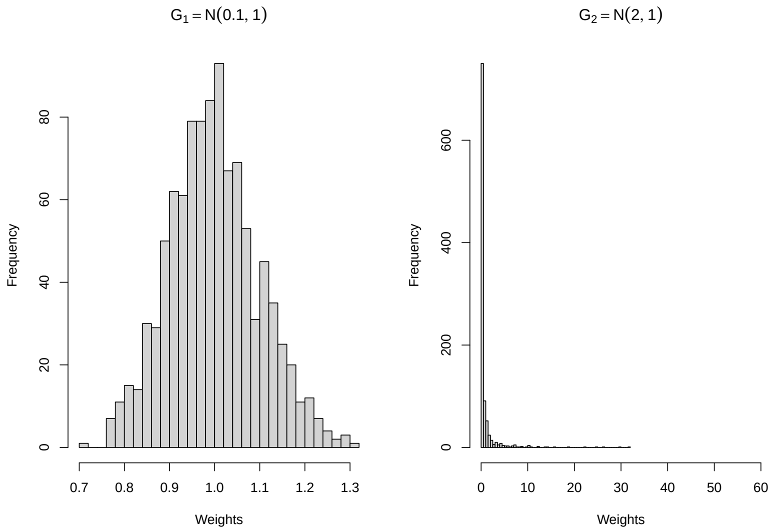
- Truncated Importance Sampling:
  - (Ionides, 2008)

1. Choose a threshold
2. Set any weights above threshold equal to threshold

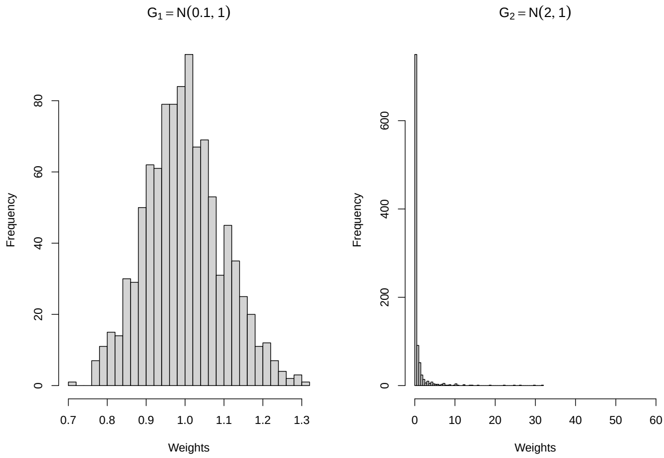
Example: Mystery Target



Example: Mystery Target



Example: Mystery Target



$$ESS_1 \approx 990$$
$$ESS_1^{(\text{trunc})} \approx 990$$

$$ESS_2 \approx 73$$
$$ESS_2^{(\text{trunc})} \approx 93$$

Improving IS

- Pareto Smoothed Importance Sampling:
  - (Vehtari et al., 2022)

1. Choose a threshold
   - Weights above threshold represent tail of their dist.
2. Approximate tail with Generalized Pareto Dist.
   - Fit GPD to weights above threshold
   - (Zhang and Stephens, 2009)
3. Replace large weights with quantiles of fitted GPD

Example: Mystery Target

Histograms of weights with threshold

Example: Mystery Target

Histograms of weights with threshold and fitted GPD density above threshold

Example: Mystery Target

Histograms of smoothed weights

Example: Mystery Target

Histograms of smoothed weights with ESS for raw, truncated and smoothed weights

Adaptive IS

- Modifications are nice, but require creativity
- Alternative: directly optimize ESS

- Adaptive Importance Sampling:
  - (Akyildiz and Míguez, 2021)

1. Choose a family of proposals
2. Iteratively update the proposal to maximize ESS

Adaptive IS

- Actually, we want to maximize a population-level analog: $\overline{ESS}$
- We only get ESS, not $\overline{ESS}$

Stochastic Approximation

- If we had $\overline{ESS}$, we would do gradient descent
- $\theta_{k+1} = \theta_k - \alpha \nabla \overline{ESS}(\theta_k)$

- Instead, do gradient descent on ESS
- $\hat{\theta}_{k+1} = \hat{\theta}_k - \alpha_k \nabla ESS(\hat{\theta}_k)$

- Stochastic Approximation
  - (Robbins and Monro, 1951)

Stochastic Approximation

- Have to choose $\{\alpha_k\}$ carefully
- May not have ∇ESS
  - Finite difference approximation
  - (Kiefer and Wolfowitz, 1952)

Example: Mystery Target

- Trajectory of $\hat{\theta}$
- Trajectory of ESS and $\overline{ESS}$

- Values of above at convergence

Our Method

- Recall: Be careful using IS means to diagnose IS
- Vehtari et al. give an alternative
  - Shape parameter of fitted tail distribution, $\hat{k}$
  - "Tail Index"
  - Smaller is better

Our Method

- Use diagnostic as objective function
- Apply stochastic approximation to minimize $\hat{k}$
  - More precisely, $k(\theta)$

Example: Mystery Target

- Trajectory of $\hat{\theta}$
- Trajectory of $\hat{k}$ and k

- Values of above at convergence

- Big reveal!

Recap

- Importance sampling and extensions
  - Truncation
  - Pareto Smoothing
- Diagnostics for importance sampling
  - Effective sample size
  - Pareto tail index
- Adaptive importance sampling
  - Stochastic approximation

Acknowledgements

Thank You

Some References

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