Adaptive Pareto Smoothed Importance Sampling

William Ruth

Université de Montréal





Who am 1?

- PhD SFU (2023)
- Postdoc UdeM (present)
- Computational Statistics
 - Simulation and related methods
 - Latent variable models
- Infectious disease modelling

Topics

- Adaptive Pareto Smoothed Importance Sampling
- Multilevel Causal Mediation Analysis
- Modelling Tuberculosis in Foreign-Born Canadians

Topics

- Adaptive Pareto Smoothed Importance Sampling
- Multilevel Causal Mediation Analysis
- Modelling Tuberculosis in Foreign-Born Canadians

Outline

- 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 sum/integral
- Monte Carlo approximation
 - Simulating from F might be hard

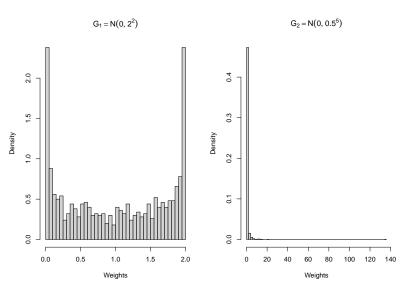
Importance Sampling

• Introduce "proposal distribution", G:

$$\mathbb{E}_{F}\varphi(X) = \mathbb{E}_{G}\left[\varphi(X)\cdot\frac{f(X)}{g(X)}
ight] = \mathbb{E}_{G}\left[\varphi(X)\cdot w(X)
ight]$$

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

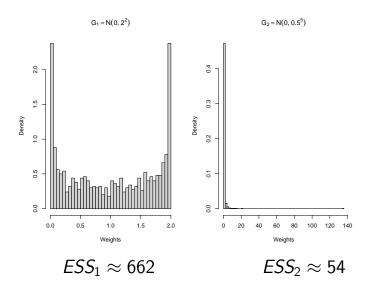
- f unknown, but can be evaluated
- $\varphi(X) = X^2$
- Try some proposals:
 - $G_1 \sim N(0, 2^2)$
 - $G_2 \sim N(0, 0.5^2)$
- Use M = 1000 samples from proposal
 - $\hat{\mathbb{E}}_1 = 0.99$, $\hat{SD} = 1.97$
 - $\hat{\mathbb{E}}_2 = 1.10$, $\hat{SD} = 2.32$



Importance Sampling

- *G*₁ weights look fine
- G₂ weights dominated by one large value
- We can make this difference precise
- "Effective Sample Size":

$$ESS = \frac{\left[\sum_{i} w(X_{i})\right]^{2}}{\sum_{i} w(X_{i})^{2}}$$



4□ > 4□ > 4□ > 4□ > 4□ > 4□ >

Importance Sampling

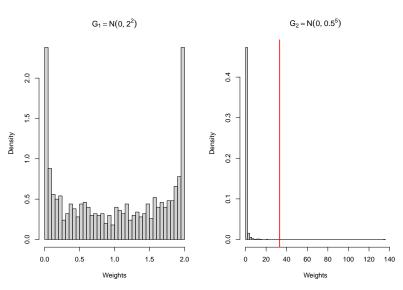
- ullet Problem: Low ESS o hard to estimate means
- But ESS is based on means
 - (Chatterjee and Diaconis, 2018)

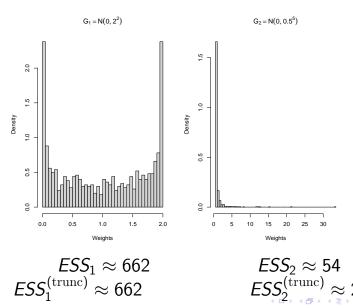
Improving IS

- Choose a good proposal
- Modify large weights
 - Truncated IS
 - Pareto Smoothed IS

Improving IS

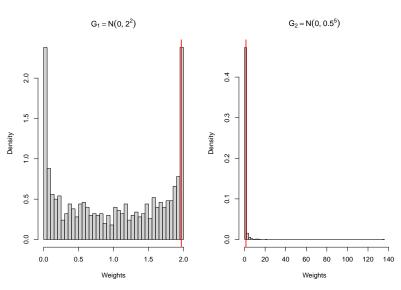
- Truncated Importance Sampling:
 - (Ionides, 2008)
- 1. Choose a threshold
- 2. Apply hard thresholding to any large weights
 - Still consistent for the target

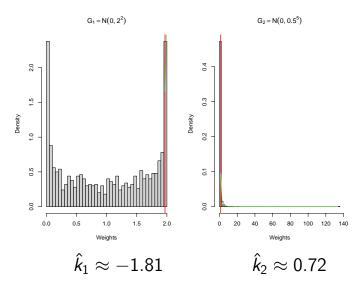




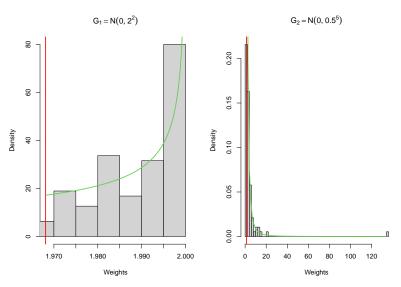
Improving IS

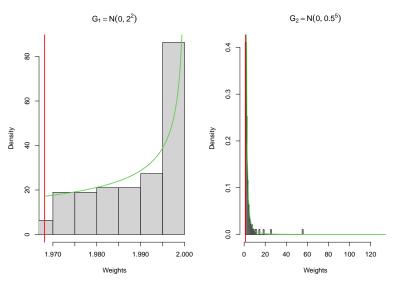
- Pareto Smoothed Importance Sampling:
 - (Vehtari et al., 2024)
- 1. Choose a threshold
 - Weights above threshold represent tail of their dist.
- 2. Approximate tail with Generalized Pareto Dist.
 - Fit GPD to weights above threshold
 - (Zhang and Stephens, 2009)
- 3. Replace large weights with quantiles of fitted GPD

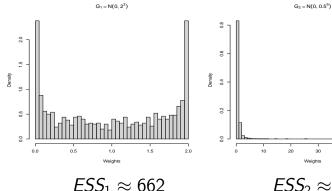




◆ロト→ (費) → (量) → (量) → (量) → (量) → (量) → (型) → (U) → (U)







$$ESS_1 \approx 662$$

 $ESS_1^{(\mathrm{trunc})} \approx 662$
 $ESS_1^{(\mathrm{PS})} \approx 662$

$$ESS_2 \approx 54$$

 $ESS_2^{(\mathrm{trunc})} \approx 245$
 $ESS_2^{(\mathrm{PS})} \approx 160$

Adaptive IS

- Alternative approach: directly optimize ESS
- Adaptive Importance Sampling:
 - (Akyildiz and Míguez, 2021)
- 1. Choose a (parametric) family of proposals
- 2. Iteratively update the proposal to maximize ESS

Stochastic Approximation

Actually, minimize a population-level analog:

•
$$\rho = \mathbb{E}_G w^2(X) \approx \frac{\dot{N}}{ESS}$$

• If we had ρ , we would do gradient descent

•
$$\theta_{k+1} = \theta_k - \alpha_k \nabla \rho(\theta_k)$$

• Instead, do gradient descent on $\hat{\rho}$

$$\bullet \ \hat{\theta}_{k+1} = \hat{\theta}_k - \alpha_k \nabla \hat{\rho}(\hat{\theta}_k)$$

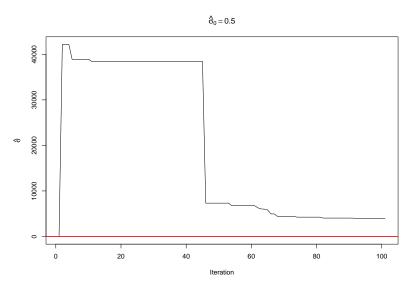
Stochastic approximation

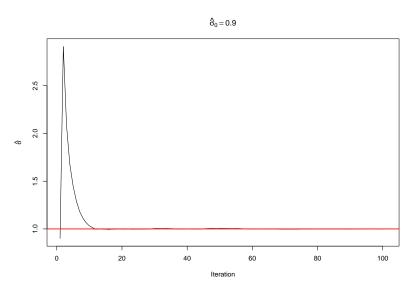
Stochastic Approximation

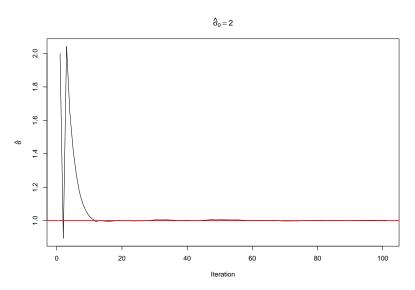
- Originally developed for root finding with noise
 - (Robbins and Monro, 1951)
- Quickly adapted for optimization
 - Use noisy evaluations for finite difference
 - (Kiefer and Wolfowitz, 1952)

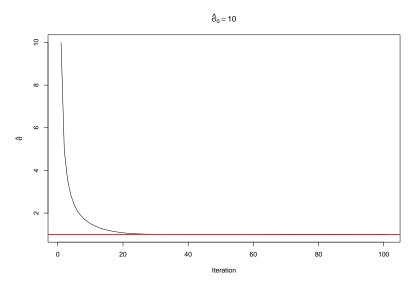
Stochastic Approximation

- Very well developed theory
- Step size $\rightarrow 0$
 - Called the "learning rate"
- Stochastic gradient descent
 - Popular in machine learning
 - Resample a (very) large dataset







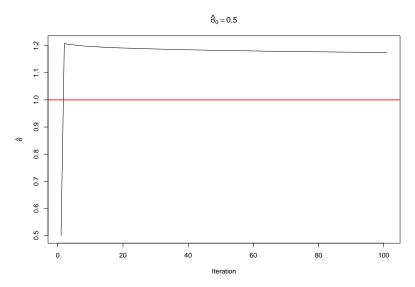


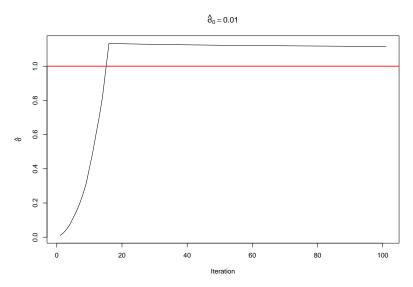
Our Method

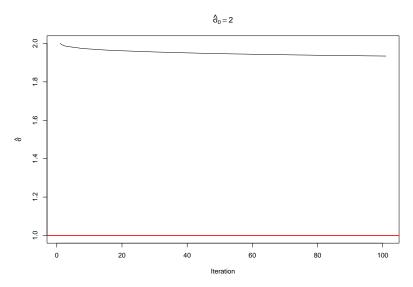
- Recall: Be careful using IS means to diagnose IS
- Vehtari et al. give an alternative
 - Shape parameter of fitted tail distribution, \hat{k}

Our Method

- Use diagnostic as objective function
- Apply stochastic approximation to minimize \hat{k}
 - More precisely, its population analog: $k(\theta)$
- Use finite difference approximation to $\hat{k}'(\theta)$
 - This is subtle







Our Method - Future Directions

- Refining the finite difference approximation
 - Generalize ESS version outside exponential families
- Analytical tail indices
- Convergence theory for stochastic approximation
- Applications
 - Latent variable models (e.g. GLMMs)
 - Bayesian inference in high-dimensions

Recap

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

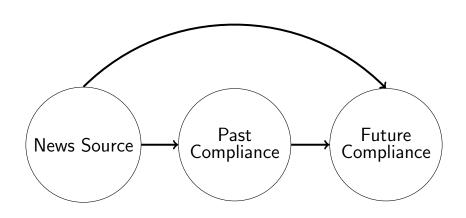
Topics

- Adaptive Pareto Smoothed Importance Sampling
- Multilevel Causal Mediation Analysis
- Modelling Tuberculosis in Foreign-Born Canadians

Example

- Goal: Understand adherence to restrictive measures
 - E.g. Lockdowns
 - Both past and future
- Influence of news source
 - How trustworthy?
- Disentangle influence on future from influence on past

Example



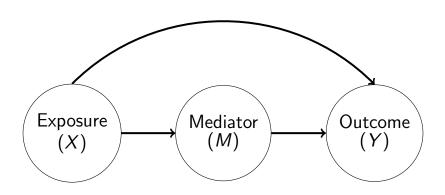
Example

Terminology

- Top path: Direct effect
- Center path: Indirect effect
- Combined: Total effect

- Exposure: X
- Outcome: Y
- Mediator: M

Mediation Analysis



Mediation Analysis

- Separate **Total Effect** of *X* on *Y* into
 - Direct Effect
 - Indirect Effect
- Define effects formally using counterfactuals

Mediation Analysis

- Under "identification assumptions", expected counterfactuals equal conditional expectations
- Use regression
 - Linear vs logistic
 - Single-level vs multi-level

Multi-Level Models

- Grouped data
 - E.g. By country
- Mediation effects differ by group
 - Mixed-effects regression

Multilevel Mediation Analysis

- Uncertainty quantification is messy
 - Bootstrap
 - Quasi-Bayesian Monte Carlo
 - δ -method
- Monte Carlo studies look promising

Topics

- Adaptive Pareto Smoothed Importance Sampling
- Multilevel Causal Mediation Analysis
- Modelling Tuberculosis in Foreign-Born Canadians

Tuberculosis

- Massive problem worldwide
 - Prevalence of 20-25%
 - (Cohen et al., 2019)
- Infection includes a latent period
 - Can last months or entire lifetime

Tuberculosis in Canada

- Relatively rare in Canada
- Mostly present in foreign-born and indigenous communities
 - We focus on foreign-born
- Immigration screens for active TB but not latent

Tuberculosis in Canada

- We model TB in foreign-born Canadians using a system of ODEs
 - Includes immigration and domestic transmission
- Some parameters from literature
- Others fit using data
- Not on track to meet our goal of 90% reduction by 2035

Acknowledgements

Collaborators:

- Payman Nickcki (UBC), Richard Lockhart (SFU)
- Bouchra Nasri (UdeM), Bruno Remillard (HEC), Rado Ramasy (UdeM), Rowin Alfaro (UdeM)
- Jeremy Chiu (SFU), Albert Wong (Langara)

Funding:

CANSSI

Thank You

Some References

- Akyildiz, Ö. D. and Míguez, J. (2021). Convergence rates for optimized adaptive importance samplers. *Statistics and Computing*, 31(12).
- Chatterjee, S. and Diaconis, P. (2018). The sample size required in importance sampling. *The Annals of Applied Probability*, 28(2).
- Cohen, A., Mathiasen, V. D., and Schön, T. (2019). The global prevalence of latent tuberculosis: a systematic review and meta-analysis. *European Respiratory Journal*, 53(3).
- Ionides, E. L. (2008). Truncated importance sampling. *Journal of Computational and Graphical Statistics*, 17(2).
- Kiefer, J. and Wolfowitz, J. (1952). Stochastic estimation of the maximum of a regression function. *The Annals of Mathematical Statistics*, 23(3).
- Robbins, H. and Monro, S. (1951). A stochastic approximation method. *The Annals of Mathematical Statistics*, 22(3).
- Vehtari, A., Simpson, D., Gelman, A., Yao, Y., and Gabry, J. (2022). Pareto smoothed importance sampling. *ArXiv*.
- Vehtari, A., Simpson, D., Gelman, A., Yao, Y., and Gabry, J. (2024). Pareto smoothed importance sampling. *Journal of Machine Learning Research*, 25(72).
- Zhang, J. and Stephens, M. A. (2009). A new and efficient estimation method for the generalized Pareto distribution. *Technometrics*, 51(3).

4□ > 4률 > 4률 > 4률 > 4률 > 4률 > 4률 > 9