Towards a turnkey approach to unbiased Monte Carlo estimation of smooth functions of expectations

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Introduction

Joint work with Francesca R. Crucinio & Sumeetpal S. Singh

The math problem

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generate unbiased estimates of $f(m)$.

Taylor expansion

Taylor expansion of f around some x_0:

$$f(m) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!}(m - x_0)^k$$

$$= \sum_{k=0}^{\infty} \gamma_k \left(\frac{m}{x_0} - 1\right)^k$$

where $\gamma_k := f^{(k)}(x_0)x_0^k/k!$.

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where $\gamma_k := f^{(k)}(x_0)x_0^k/k!$.

Unbiased estimate for $(m/x_0 - 1)^k$: $\prod_{i=1}^{k}(X_i/x_0 - 1)$.

A Taylor-based sum estimator

This suggests using a **sum estimator** (McLeish, 2011; Glynn and Rhee, 2014; Rhee and Glynn, 2015):

$$\hat{f} = \sum_{k=0}^{R} \frac{\gamma_k U_{R,k}}{\mathbb{P}(R \geq k)} = \sum_{k=0}^{\infty} \gamma_k U_{R,k} \frac{\mathbf{1}\{R \geq k\}}{\mathbb{P}(R \geq k)}$$

where R takes values in $\mathbb{N} = \{0, 1, ...\}$, and

$$U_{r,k} = U_k = \prod_{i=1}^{k} (X_i / x_0 - 1).$$

Motivation I: Log and MLE

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For $f(x) = \log(x)$, $\gamma_k = (-1)^{k-1}/k$ (sub-geometric).

Motivation II: Reciprocal and un-normalised models

A model whose likelihood is of the form:

$$p(y|\theta) = g(y, \theta)/Z(\theta)$$

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For $f(x) = 1/x$, $\gamma_k = (-1)^{k-1}$, which is also sub-geometric.

Not a motivation: Exponential

Obviously

$$\exp(x) = \exp(x_0) \times \sum_{k=0}^{\infty} \frac{(x - x_0)^k}{k!}$$

has also many practical applications; however the decay of the coefficients is **super-geometric**, which leads to different considerations.

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See Papaspiliopoulos (2011).

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Robust/automatic guidelines on how to choose:

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- **sum** of random variables (when estimates are computed sequentially)
- **max** of random variables (when estimates are computed in parallel)

Theoretical properties

Variance decomposition

$$\mathrm{var}[\hat{f}] = \mathrm{var}\left[\mathbb{E}[\hat{f}|R]\right] + \mathbb{E}\left[\mathrm{var}[\hat{f}|R]\right]$$

where:

- the first term measures the variability induced by the random truncation.

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where:

- the first term measures the variability induced by the random truncation.
- the second term measures the variability due to the $U_{r,k}$'s (the unbiased estimates of $(m/x_0 - 1)^k$).

Analysing the first term

$$\mathbb{E}\left[\hat{f}\middle|R=r\right]=\sum_{k=0}^{\infty}\gamma_k\frac{\mathbf{1}\{r\geq k\}}{\mathbb{P}(R\geq k)}\left(\frac{m}{x_0}-1\right)^k.$$

Hence

$$\begin{aligned}\operatorname{var}\left[\mathbb{E}[\hat{f}|R]\right]=&\sum_{k=0}^{\infty}\gamma_k^2\left(\frac{m}{x_0}-1\right)^{2k}\left(\frac{1}{\mathbb{P}(R\geq k)}-1\right)\\&+2\sum_{k=0}^{\infty}\sum_{l=k+1}^{\infty}\gamma_k\gamma_l\left(\frac{m}{x_0}-1\right)^{k+l}\left(\frac{1}{\mathbb{P}(R\geq k)}-1\right).\end{aligned}$$

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These expressions suggest to take:

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- x_0 such that $\beta_0 := |m/x_0 - 1| < 1$;
- $R \sim \text{Geometric}(p)$, with $p < 1 - \beta_0$, so that $\mathbb{P}(R \geq k) > \beta_0^{2k}$.

Improving the $U_{r,k}$

Currently, we use the following unbiased estimate of $(m/x_0 - 1)^k$:

$$U_{r,k} = U_k = \prod_{i=1}^{k} (X_i/x_0 - 1).$$

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Currently, we use the following unbiased estimate of $(m/x_0 - 1)^k$:

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Computing $\hat{f}$ requires generating $X_1, \dots, X_R$ in order to compute the last term $U_{R,R}$, but we use only the k first inputs to estimate $(m/x_0 - 1)^k$. Seems inefficient.

Cycling estimator

In order to use the **whole sample**, consider the following cycling estimator:

$$U^{\mathrm{C}}_{r,k} := \frac{1}{r}\Big[\prod_{i=1}^{k}\left(\frac{X_i}{x_0}-1\right)+\prod_{i=2}^{k+1}\left(\frac{X_i}{x_0}-1\right) + \dots + \left(\frac{X_r}{x_0}-1\right)\prod_{i=1}^{k-1}\left(\frac{X_i}{x_0}-1\right)\Big].$$

Second term of the decomposition

For the cycling estimator, one has (under weak assumptions)

$$\mathbb{E}\left[\mathrm{var}(\hat{f}^{\mathrm{C}}|R)\right] = \mathcal{O}(p\log(1/p))$$

as $p \to 0$.

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- We can have $\mathrm{var}[\hat{f}] \to 0$ by taking $\mathbb{E}[R] \to +\infty$. (This is not the case for the simple estimator.)
- Up to log factor, standard Monte Carlo rate, i.e. $\mathrm{var}[\hat{f}] = \mathcal{O}(\log \mathbb{E}[R]/\mathbb{E}[R])$.

Without cycling

The simple estimator does not converge as $\mathbb{E}[R] \to +\infty$.

Calibration of tuning parameters

Tuning x_0

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$\Rightarrow$ pilot run, bootstrap to ensure this condition with high probability.

Tuning p

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See paper.

Numerical experiments: log

log-likelihood (and gradient) of a latent variable model

Model with data y, latent z, parameter θ;

$$p(y|\theta) = \int p(y|z,\theta)p(z|\theta)dz$$

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To compute the MLE, use our approach to derive unbiased estimate of the **log-likelihood** and its **gradient** (stochastic gradient descent).

Alternative approach: SUMO (Luo et al, 2021)

Consider biased (but consistent) IS estimate:

$$\ell_k(\theta) = \log\left(\frac{1}{k}\sum_{i=1}^{k} w_i\right)$$

The SUMO estimator is a sum estimator based on the series:

$$\log p(y|\theta) = \mathbb{E}[\ell_1(\theta)] + \sum_{k=1}^{\infty} \mathbb{E}[\Delta_k], \quad \Delta_k = \ell_{k+1}(\theta) - \ell_k(\theta)$$

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Main issue: infinite variance.

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Variance is infinite, but the random CPU time may have infinite variance (and has always heavy tails).

Comparison on a toy model from Rob & Cornish (2021)

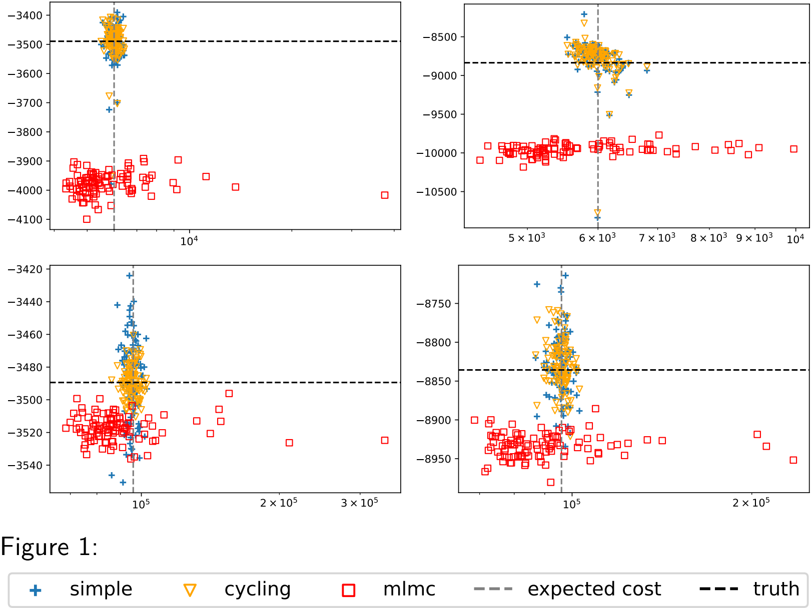

Figure 1:

Caption

Estimate vs CPU for an expected cost C of 6 (top) and 96 (bottom) samples per data point. Dimension is $d = 2$ (left) and $d = 5$ (right). The vertical dashed line denotes the expected cost while the horizontal one denotes the true value of $\sum_{i=1}^{n} \log p(y_i|\theta)$.

Independent component analysis (Allassonnière and Younes, 2012)

$$y = \sum_{j=1}^{k} z_j a_j + \sigma\epsilon \quad \text{where}$$

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Aim is to estimate θ using SGD.

Stochastic gradient descent

Given data $(y_1, \ldots, y_n)$, do gradient descent, where at east step, the gradient is replaced by an unbiased estimate of the gradient of a **single** term (chosen uniformly).

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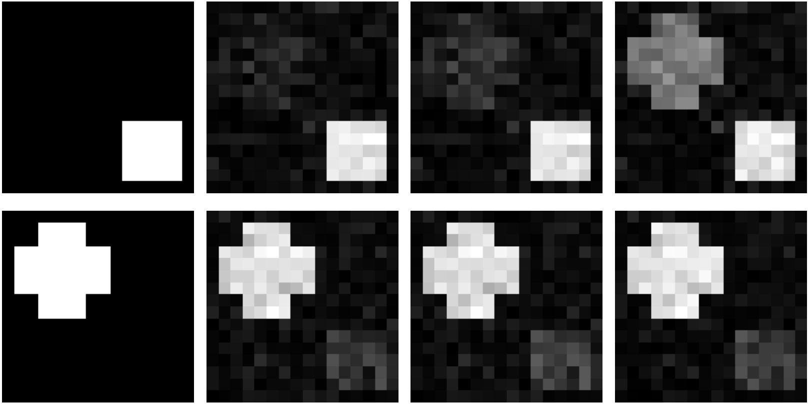
A good illustration on the need for automation, i.e. at each iteration, the actual value of m, σ^2, and thus x_0 and p must change.

Estimated images



(a) true (a) simple (a) cycle (a) SAEM

Numerical experiments: reciprocal

Exponential random graph model

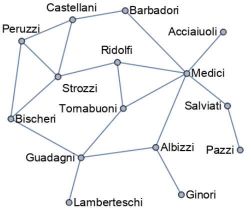


Figure 6: Florentine family business network

$$p(y|\theta) = \exp\{\theta^T s(y)\}/Z(\theta) \quad \text{where}$$

- $y = (y_{ij})$, with $y_{ij} = 1$ (resp. 0) if nodes i and j are connected

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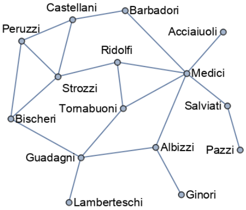

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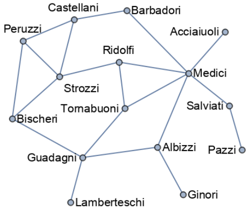

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- $s(y)$ is a collection of network statistics (number of edges, number of $k-$stars, etc.)
- $Z(\theta)$ is a sum over $2^{\binom{k}{2}}$ terms (intractable)

Bayesian inference (and model choice)

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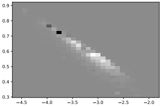
Pseudo-marginal approach: replace $1/Z(\theta)$ by an unbiased estimate.

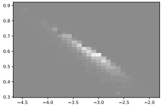
Details

For a fixed θ, run a tempering SMC algorithm to obtain an unbiased estimate of $Z(\theta)$.

Posterior approximation



(a) Simple



(a) Cycling

Figure 8: Bivariate weighted histograms approximating the posterior distributions obtained with the simple and the cycling estimator using $n = 1024$ samples from proposal q.

Cycling gives better performance II

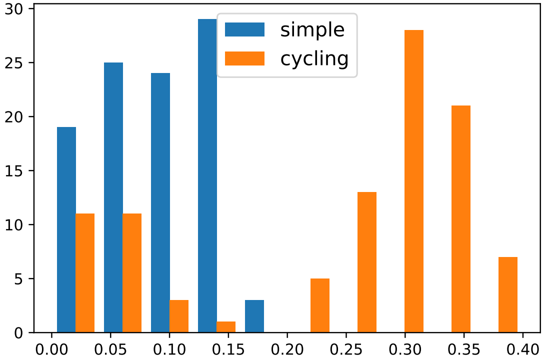


Figure 9: ESS accross simulated θ_j

Conclusion

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- No free lunch. Cannot work without pilot runs.
- Garbage in, garbage out: if the variance of the inputs is very large, the variance of our estimator will be large as well.

Paper

Chopin N., Crucinio F.R. and S. S. Singh (2024). Towards a turnkey approach to unbiased Monte Carlo estimation of smooth functions of expectations, arxiv 2403.20313.