Behaviour of informed ESS estimators

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Introduction

After reviewing the notion of an *informed ESS estimator* we show some numerical experiments to assess the behaviour of informed ESS estimators in a range of regimes including efficient as well as very inefficient MCMC algorithms.

Background

Consider a setup where we are benchmarking an MCMC method. To do so, we often pick a test function with known mean μ and variance σ^2 under the target distribution π. Here we review the construction of an *informed ESS estimator* based on these known parameters.

Markov chain CLT: Fix a Markov Kernel and a test function satisfying a central limit theorem for Markov chains, which motivates approximations of the form:

$$\sqrt{k}(\hat{I}_k - \mu) \approx \mathcal{N}(0, \sigma_a^2),$$

where $\hat{I}_k = \frac{1}{k}\sum_{i=1}^{k} g(X_i)$ and $\mu = \mathbb{E}[g(X)]$ for $X \sim \pi$, and σ_a^2 is the *asymptotic variance*, a constant that depends on g, π and the mixing of the Markov chain.

Now from the CLT for Markov chains it follows that if we have a Monte Carlo average I_k based on a MCMC chain of length k, then

$$k\mathrm{Var}(\hat{I}_k) \approx \sigma_a^2. \tag{1}$$

Independent MCMC chains: Suppose first we had a_n independent copies of MCMC (we will relax this shortly), each of length b_n. Let $\hat{I}^{(1)}, \dots, \hat{I}^{(a_n)}$ denote a_n independent estimators, the first one based on the first copy, second on second copy, etc. Since the $I^{(i)}$ are independent and identically distributed,

$$\mathrm{Var}(I^{(1)}) \approx \frac{1}{a_n}\sum_{i=1}^{a_n}(I^{(i)} - \mu)^2. \tag{2}$$

Combining Equation 1 and Equation 2, we obtain:

$$\frac{b_n}{a_n}\sum_{i=1}^{a_n}(I^{(i)}-\mu)^2 \approx \sigma_a^2.$$

Batch mean trick: view a trace of length n as a_n subsequent batches of length b_n. A popular choice is $a_n = b_n = \sqrt{n}$.

Effective sample size: recall the effective sample size (ESS) is defined as $\text{ESS} = \sigma_a^2/\sigma^2$. This is the quantity we seek to estimate.

Applying the batch mean trick with $a_n = b_n = \sqrt{n}$, we obtain:

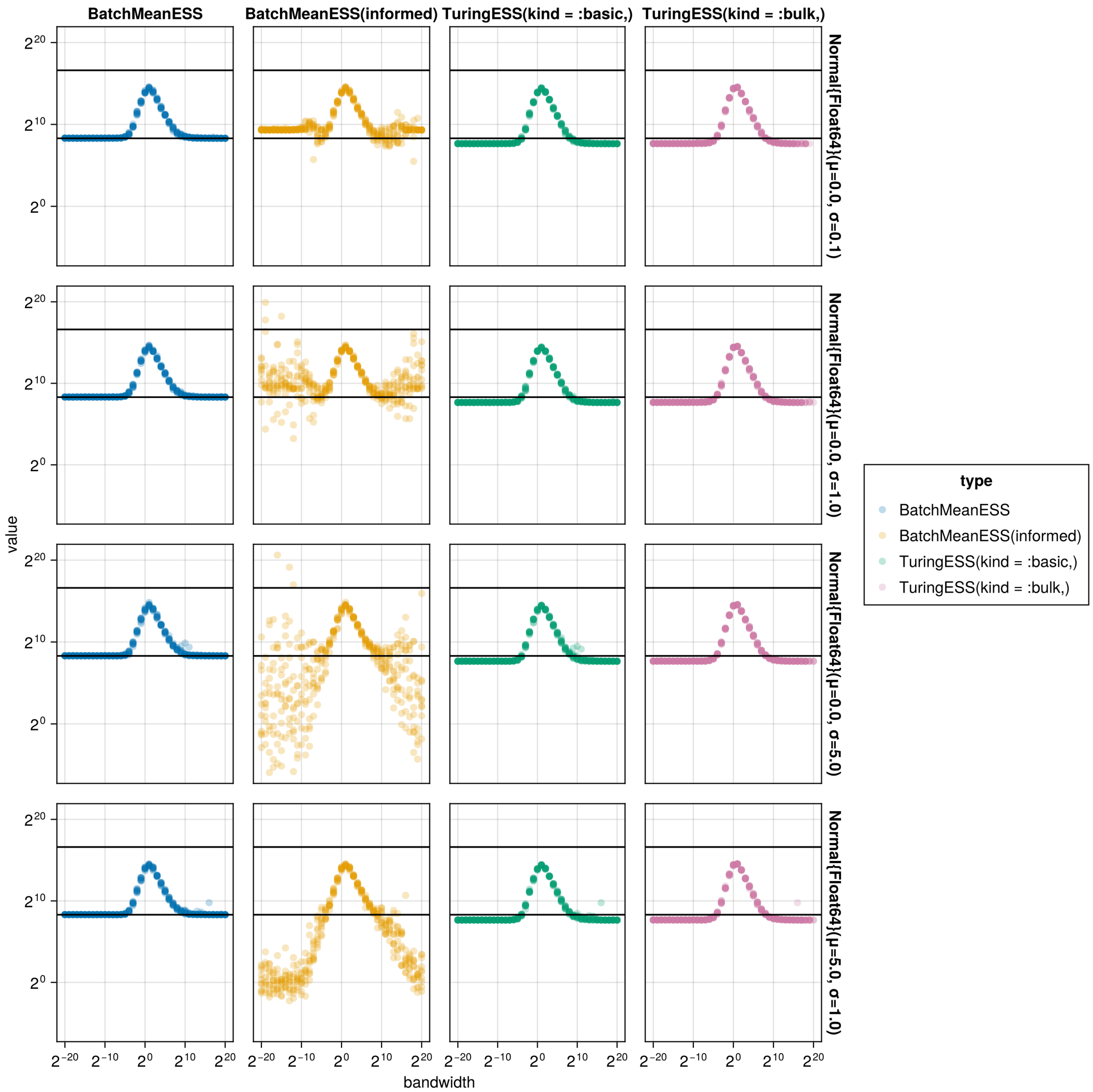
$$\text{ESS} = \frac{\sigma_a^2}{\sigma^2} \approx \frac{1}{\sigma^2}\frac{b_n}{a_n}\sum_{i=1}^{a_n}(I^{(i)}-\mu)^2 = \sum_{i=1}^{\sqrt{n}}\left(\frac{I^{(i)}-\mu}{\sigma}\right)^2. \tag{3}$$

The right hand side of this equation is the *informed ESS estimator.*

Numerical investigation

We replicate and expand a numerical experiment reported by Trevor Campbell (personal communication, January 2025). The setup is the following:

- Target distribution is $\mathcal{N}(0,1)$ in all experiment.
- We consider Metropolis-Hastings algorithms with normal proposals. We vary the proposal bandwidth (x-axis, log-scale).
- Facet rows: different initial distributions for the MCMC.
- Facet columns: different ESS estimators:
  - *Batch mean ESS (informed)*: the estimator reviewed above.
  - *Batch mean ESS*: the same as Equation 3 but where μ and σ are replaced by the sample mean and standard deviation (based on the full trace; this is equivalent to the classical batch mean ESS estimator).
  - *TuringESS basic and bulk*: ESS estimators based on truncated spectral estimation, default algorithms in the Turing.
- For each initial distribution and proposal bandwidth, we ran 10 independent chains and estimate 10 ESS from each chain separately.
- Each chain contains the samples from 100,000 iteration.
- The top solid black line denotes an idealized effective sample size of 100,000, the bottom solid black line denotes the square root of that.
- The test function used here is $g(x) = x^2$, so the reference distribution is a χ^2 with one degree of freedom. The values of μ and σ are computed from that distribution.



Observations:

- As bandwith goes to zero or infinity, we expect the effective sample size to go to zero.
- The only setup achieving this is the informed ESS with an initialization far from the target.
- However, for the other initial distributions considered, some of the informed ESS estimates are the worst observed, sometimes taking non-sense values higher than the number of MCMC samples, which is not possible in reversible chains.

Next steps

- Maybe time to move away from batch mean methods
  - Check this page benchmarking various ESS estimators.
    - They have a nice benchmark for detecting non-convergence due to multimodality. Covers both well mixing case and multi-chains detecting poor mixing. Batch means is not the winner. Geyer's method comes up better.
  - Pierre Jacob's handbook highlights the slow convergence of batch mean methods (slower than MC).
- Might still be interesting to look into the variance bias square decomposition
  - Optimal burn-in
  - Detecting when ESS estimation is meaningless.
  - Debunking some misinformation (use high dim normal initialized at zero). 1 2 3

Update: started working on informed spectral, then realized it would probably not be able either to detect ESS values much lower than $\sqrt{n}$ either. Added that lines to plot and indeed all methods seem to fail around there. So maybe a pragmatic solution here is to just have a threshold at $\sqrt{n}$ and give NA for these.

TODO: discuss and package-up a square-root check in our nextflow scripts.

- Still helpful to do jack-knife bias estimation
- Would be interesting to add a multimodal example?