

A principled stopping rule for importance sampling

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Abstract: Importance sampling (IS) is a Monte Carlo technique that relies on weighted samples, simulated from a proposal distribution, to estimate intractable integrals. The quality of the estimators improves with the number of samples. However, for achieving a desired quality of estimation, the required number of samples is unknown and depends on the quantity of interest, the estimator, and the chosen proposal. We present a sequential stopping rule that terminates simulation when the overall variability in estimation is relatively small. The proposed methodology closely connects to the idea of an effective sample size in IS and overcomes crucial shortcomings of existing metrics, e.g., it acknowledges multivariate estimation problems. Our stopping rule retains asymptotic guarantees and provides users a clear guideline on when to stop the simulation in IS.

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1. Introduction

In a wide variety of applications, a key problem of interest is the estimation of intractable integrals through Monte Carlo techniques. Specifically, let $\pi(x)$ be a target distribution on $\mathcal{X} \subseteq \mathbb{R}^s$ with associated density function also denoted by π . Suppose $h : \mathcal{X} \rightarrow \mathbb{R}^p$ and interest is in estimating

$$\mu_h := \int_{\mathcal{X}} h(x) \pi(dx) < \infty. \quad (1.1)$$

Under independent and identically distributed (iid) sampling from π , the vanilla Monte Carlo estimator for μ_h is

$$\bar{\mu}_h := \frac{1}{n} \sum_{i=1}^n h(Y_i), \quad \text{where } Y_i \stackrel{\text{iid}}{\sim} \pi \text{ for } i = 1, \dots, n. \quad (1.2)$$

While iid sampling from the target density is often desirable, it may not always be feasible either due to the computational burden or the inefficiency of the resulting estimators (see [Denny, 2001](#)). In such cases, practitioners may resort to other Monte Carlo methods such as Markov chain Monte Carlo (MCMC) ([Robert and Casella, 2013](#); [Ekvall and Jones, 2014](#)) or importance sampling (IS) ([Kahn, 1950a,b](#); [Elvira and Martino, 2021](#)).

Importance sampling is a popular Monte Carlo technique often used for variance reduction. In IS, samples from a proxy *proposal* distribution are simulated and weighted averages of desired functions are calculated. Specifically, let $q(x)$ denote the density of a chosen proposal distribution. For a known or unknown normalizing constant Z , let $\tilde{\pi}(x) = Z\pi(x)$ be such that it can be evaluated (often called *unnormalized target*) for every $x \in \mathcal{X}$. Random samples, X_1, \dots, X_n drawn from the distribution with density q are assigned importance weights

$$w_i = \frac{\tilde{\pi}(X_i)}{q(X_i)}. \quad (1.3)$$

Based on Z being known or unknown, weighted averages of $h(X_i)$ yield estimators of μ_h , which we generically denote as μ_h^* . Often, μ_h^* is the unnormalized IS (UIS) estimator or the self-normalized IS (SNIS) estimator. Other IS estimators have also been proposed (see [Elvira et al., 2019](#); [Kuntz et al., 2022](#); [Martino et al., 2018](#); [Vehtari et al., 2015](#)).

In addition to the target and proposal distributions, variability in μ_h^* is critically dependent on: (i) the function of interest h and (ii) the choice of the estimator. Almost all methods assessing the quality of an IS algorithm only utilize the importance weights and do not factor h or the estimator employed to estimate μ_h . A key question that thus remains unanswered is, how should n be chosen so that μ_h^* is a *good* estimate of μ_h ?

Common diagnostics for IS algorithms measure the discrepancy between the target and proposal distributions. [Chatterjee et al. \(2018\)](#) obtain sample size requirements by utilizing the Kullback-Leibler divergence between π and q . [Sanz-Alonso \(2018\)](#) and [Sanz-Alonso and Wang \(2021\)](#) leverage the χ^2 divergence between π and q to quantify the variance of the weights and obtain an estimate of the necessary sample size. These methods are useful in understanding the quality of the weights, but since they are invariant to the choice of h and μ_h^* , they are not equipped to directly explain the quality of estimation of μ_h by μ_h^* . Another popular diagnostic is the effective sample size (ESS) which is meant to provide the number of iid samples from π that would yield the same variability in $\bar{\mu}_h$ as the variability in μ_h^* . Using a series of simplifying assumptions, [Kong \(1992\)](#) provides a popularly employed estimator of ESS. As described by [Elvira et al. \(2022\)](#), the simplifying assumptions make it so that the resulting estimator does not satisfy key desirable properties. As a consequence, although a reasonable diagnostic for assessing the suitability of the proposal distribution, the estimator fails to truly assess the quality of estimation of μ_h . Nevertheless,

it continues to be used in IS as a practical diagnostic owing to reasonable statistical properties, ease of implementation, and lack of better alternatives (see [Elvira et al., 2022](#), for more details).

Due to interest in several expectations, often μ_h and its estimator are multivariate. Naturally, the correlation among components of μ_h^* impacts the quality of estimation. Since most IS diagnostics do not depend on the choice of the function h , this correlation is left ignored.

The contributions of this paper are twofold. First, we present a multivariate analogue of the original definition of ESS, avoiding most of the simplifying assumptions of [Kong \(1992\)](#). The proposed metric, that we call M-ESS, acknowledges that changing q , h , and the estimator employed μ_h^* should yield different quality of estimation. Second, we adapt and integrate multivariate sequential stopping rule techniques of [Glynn and Whitt \(1992\)](#) to determine when enough weighted samples have been obtained in IS. Our proposed method stops simulation when the volume of the confidence region for μ_h^* is small, relative to the variability of h under π . We show that the confidence region constructed at the random time of termination is asymptotically valid, i.e., the probability that μ_h is contained in the $100(1 - \alpha)\%$ confidence region at termination is asymptotically $1 - \alpha$. Moreover, adapting ideas from the MCMC literature ([Vats et al., 2019](#)), we show that this stopping rule is asymptotically equivalent to stopping the IS simulation when the estimated M-ESS is larger than an *a priori* obtained lower bound. The proposed methodology provides users clear guidelines on when to stop their simulations while redeeming many shortcomings of the current practices.

We implement our proposed ESS and stopping rules in three examples. First, we set both π and q to be multivariate Gaussian densities and analytically obtain the true variance of two different IS estimators. Using these variances, we analyze the quality of estimation of M-ESS and the performance of our termination rule as a function of the problem dimension and the degree of correlation in the resulting estimators. Our second example is of a Bayesian Weibull multi-step stress model. Here, we employ our ESS for two different multivariate h of interest to demonstrate the difference in the quality of estimation for different choices of h . Our third example is a relatively large-dimensional approximate Bayesian inference problem using IS and integrated nested Laplace approximation, where the quality of estimation of our proposed M-ESS is upheld, despite the problem complexity.

2. Importance Sampling and Effective Sample Size

We recall that interest is in estimating $\mu_h = E_\pi[h(X)] \in \mathbb{R}^p$ where π may be such that

$$\tilde{\pi}(x) = Z\pi(x). \quad (2.1)$$

We assume that $\tilde{\pi}$ is known (can be evaluated at any $x \in \mathcal{X}$) while Z may be known or unknown; without loss of generality, we assume $Z = 1$ when π can be completely evaluated. For instance, in Bayesian inference, Z is the intractable marginal likelihood. Based on the availability of Z , one of the two popular IS

estimators may be employed. There certainly are situations where $\tilde{\pi}$ may also be unavailable (see [Park and Haran, 2018](#)); we exclude these from consideration in this work.

Let q be an appropriately chosen proposal density and X_1, \dots, X_n be iid samples from q . If Z is known, μ_h may be estimated using the UIS estimator

$$\hat{\mu}_h := \frac{1}{n} \sum_{i=1}^n h(X_i) w_i. \quad (2.2)$$

When Z is unknown, the UIS estimator cannot be calculated, in which case μ_h can be estimated by the SNIS estimator

$$\tilde{\mu}_h := \frac{\sum_{i=1}^n h(X_i) w_i}{\sum_{i=1}^n w_i}. \quad (2.3)$$

If $q(x) > 0$ for all x such that $\pi(x) > 0$, both $\hat{\mu}_h$ and $\tilde{\mu}_h$ converge to μ_h with probability 1, as $n \rightarrow \infty$; see [Owen \(2013\)](#); [Robert and Casella \(2013\)](#) for more details. Recall, we denote any IS estimator of μ_h as μ_h^* , and will use the specific notations when referring to either UIS or SNIS. Further, often μ_h^* exhibits asymptotic normality, so that as $n \rightarrow \infty$,

$$\sqrt{n}(\mu_h^* - \mu_h) \xrightarrow{d} \mathcal{N}(0, \Omega^*), \quad (2.4)$$

where $\Omega^* := \lim_{n \rightarrow \infty} n \text{Var}_q(\mu_h^*)$. By a central limit theorem (CLT), asymptotic normality for $\hat{\mu}_h$ is straightforward, and Ω^* is denoted by Ω_U . For the SNIS estimator, when Ω^* is finite, asymptotic normality holds with

$$\Omega^* = \Omega := \frac{\mathbb{E}_q [w(X)^2 (h(X) - \mu_h)(h(X) - \mu_h)^T]}{\mathbb{E}_q [w(X)]^2}. \quad (2.5)$$

The form of Ω has been presented before in [Nilakanta \(2020\)](#); [Owen \(2013\)](#), but for the sake of completion, we provide the details in [Appendix A.1](#). Assuming finite variance, denoted by $\Sigma := \text{Var}_\pi(h(X))$, the vanilla Monte Carlo estimator, $\bar{\mu}_h$, also satisfies a CLT with a limiting covariance matrix

$$\lim_{n \rightarrow \infty} n \text{Var}_\pi(\bar{\mu}_h) = \Sigma. \quad (2.6)$$

For a univariate h , in order to quantify the relative quality of μ_h^* as compared to $\bar{\mu}_h$, [Kong \(1992\)](#) attempts to define the ESS as the ratio of the respective mean-squared errors. Since the bias of the SNIS estimator is difficult to ascertain, ESS is first described as $n \cdot \text{Var}(\bar{\mu}_h) / \text{Var}(\mu_h^*)$ (in the univariate case, both variances are scalars). Through a series of approximations, [Kong \(1992\)](#) obtains the following estimator of the above ESS:

$$K_n := \frac{1}{\sum_{i=1}^n \bar{w}_i^2}, \quad (2.7)$$

where $\bar{w}_i = w_i / \sum_{i=1}^n w_i$ are the normalized weights. [Elvira et al. \(2022\)](#) provide a full derivation of (2.7), including the assumptions and approximations,

and discuss various shortcomings of K_n . A critical undesirable quality of K_n is that it does not depend on the function of interest h and thus claims the same estimation quality irrespective of h . Consequently, K_n is also unable to acknowledge multivariate estimation in h . This may be an advantage in some scenarios, e.g., when there is not a particular targeted integral μ_h and IS is used to build a weighted particle approximation of the target. However, IS is mostly used as a variance reduction technique for the approximation of integrals, and thus, K_n not depending on h is a limitation in most applications of interest. For instance, in machine learning IS is used to estimate a gradient, and thus h is multivariate (see [Mohamed et al., 2020](#)). Moreover, in rare events events estimation, h can be a multivariate function composed of indicator functions ([Owen et al., 2019](#); [Miller et al., 2021](#)). Finally, since $1 \leq K_n \leq n$, the estimator is unable to detect improvements in statistical efficiency, a key feature of IS.

We propose a multivariate extension of the definition of ESS based on the original intention of [Kong \(1992\)](#), but replace the finite-time variances with the estimable limiting variances. That is, we define the multivariate ESS as

$$\text{M-ESS} := n \frac{|\Sigma|^{1/p}}{|\Omega^*|^{1/p}}. \quad (2.8)$$

The p th root of the determinant of covariance matrices is a dimension-free measure of variability ([SenGupta, 1987](#)) and is natural since the generalized variability of a random vector is quantified by the determinant of the corresponding covariance matrix ([Wilks, 1932](#)). [Vats et al. \(2019\)](#) employ a similar metric in the context of MCMC where Ω^* is the asymptotic variance in the Markov chain CLT of MCMC ergodic averages. This unified formulation of ESS allows us to compare the efficiency of different sampling methods whenever a meaningful estimator of Ω^* can be constructed. This is discussed in detail in Section 4.3.

We present estimators of Σ and $\Omega^* = \Omega$ for SNIS. Since

$$\Sigma = \mathbb{E}_\pi \left[(h(X) - \mu_h)(h(X) - \mu_h)^T \right] = \mathbb{E}_q \left[w(X)(h(X) - \mu_h)(h(X) - \mu_h)^T \right],$$

a plug-in estimator of Σ is

$$\hat{\Sigma} := \sum_{i=1}^n \bar{w}_i (h(X_i) - \tilde{\mu}_h)(h(X_i) - \tilde{\mu}_h)^T. \quad (2.9)$$

Similarly, for Ω from (2.5), a multivariate extension of the plug-in estimator of [Owen \(2013\)](#) is

$$\hat{\Omega} = \frac{n^{-1} \sum_{i=1}^n w_i^2 (h(X_i) - \tilde{\mu}_h)(h(X_i) - \tilde{\mu}_h)^T}{\left(n^{-1} \sum_{i=1}^n w_i \right)^2} = n \sum_{i=1}^n \bar{w}_i^2 (h(X_i) - \tilde{\mu}_h)(h(X_i) - \tilde{\mu}_h)^T. \quad (2.10)$$

Remark 1. For UIS, estimators for Σ and Ω_U , denoted by $\hat{\Sigma}_U$ and $\hat{\Omega}_U$, respectively, are:

$$\hat{\Sigma}_U := \frac{1}{n} \sum_{i=1}^n w_i (h(X_i) - \hat{\mu}_h)(h(X_i) - \hat{\mu}_h)^T \quad \text{and} \quad \hat{\Omega}_U := \sum_{i=1}^n (w_i h(X_i) - \hat{\mu}_h)(w_i h(X_i) - \hat{\mu}_h)^T.$$

Using the estimators described above, a plug-in estimator of the M-ESS is

$$\widehat{\text{M-ESS}} = n \frac{|\hat{\Sigma}|^{1/p}}{|\hat{\Omega}_*|^{1/p}}. \quad (2.11)$$

Remark 2. *The quality of estimation for both K_n and $\widehat{\text{M-ESS}}$ depends critically on the weights. Since $\widehat{\text{M-ESS}}$ requires second moment estimates, we recommend that users choose their ideal proposal before implementing our stopping rules to determine when to stop their simulation.*

Remark 3. *Throughout the manuscript we assume that IS and SNIS estimators exhibit asymptotic normality. This may not always be true, in which case Ω^* will be infinite. In such a case, for finite Σ , M-ESS is zero since the determinant of Ω^* will be infinite.*

The proposed $\widehat{\text{M-ESS}}$ indicates the quality of estimation of μ_h^* relative to the vanilla Monte Carlo estimator. As we discuss in next section, it also serves as basis for a principled stopping criterion and can greatly alleviate ambiguity in terminating simulation.

3. Using ESS to Stop Simulation

A key practical question in any simulation paradigm is, when should sampling stop? Sequential stopping rules that check whether a desired criterion has been satisfied, have been useful in answering this question in steady-state simulations (Dong and Glynn, 2019; Glynn and Whitt, 1992), stochastic programming (Bayraksan and Pierre-Louis, 2012), general Monte Carlo (Frey, 2010; Vats et al., 2021), and MCMC (Flegal and Gong, 2015; Vats et al., 2019). Such stopping rules terminate simulation when the size of the confidence region of the estimator is small. For the rest of the paper, we focus our attention on the SNIS estimator (unless stated otherwise).

Ellipsoidal large-sample confidence regions for μ_h are available due to (2.4) and (2.10). Let $\chi_{1-\alpha,p}^2$ denote the $(1-\alpha)$ -quantile of a chi-squared distribution with p degrees of freedom. Then a large-sample $100(1-\alpha)\%$ confidence region around $\tilde{\mu}_h$ is,

$$C_\alpha(n) = \left\{ \mu_h \in \mathbb{R}^p : n(\tilde{\mu}_h - \mu_h)^T \hat{\Omega}^{-1}(\tilde{\mu}_h - \mu_h) < \chi_{1-\alpha,p}^2 \right\}. \quad (3.1)$$

The volume of the confidence region is,

$$\text{Vol}(C_\alpha(n)) = \frac{2\pi^{p/2}}{p\Gamma(p/2)} \left(\frac{\chi_{1-\alpha,p}^2}{n} \right)^{p/2} |\hat{\Omega}|^{1/2}. \quad (3.2)$$

For a user-chosen ϵ -tolerance, we derive a stopping rule that terminates the simulation when the estimated ESS is larger than a pre-determined lower-bound. In other words, consider stopping the simulation when the p th root of the volume

of $C_\alpha(n)$ is an ϵ th fraction of $|\widehat{\Sigma}|^{1/2p}$. Specifically, suppose $s(n)$ is a function on the integers such that $s(n) \rightarrow 0$ as $n \rightarrow \infty$. The process terminates the first time when

$$\text{Vol}(C_\alpha(n))^{1/p} + s(n) \leq \epsilon |\widehat{\Sigma}|^{1/2p}. \quad (3.3)$$

Often, $s(n)$ is chosen to ensure some minimum simulation effort. Equation (3.3) is the relative standard deviation sequential stopping rule of Vats et al. (2019). Ignoring $s(n)$ for large n , (3.2) implies that the stopping rule in (3.3) is equivalent to stopping the simulation when:

$$\widehat{\text{M-ESS}} \geq \frac{2^{2/p} \pi}{(p\Gamma(p/2))^{2/p}} \frac{1}{\epsilon^2} \chi_{1-\alpha, p}^2 =: L_{\alpha, \epsilon, p}. \quad (3.4)$$

This reformulation furnishes a rule that terminates the IS process when $\widehat{\text{M-ESS}}$ is larger than $L_{\alpha, \epsilon, p}$. A lower level of relative tolerance, ϵ , yields a higher $L_{\alpha, \epsilon, p}$. Notice that the lower bound $L_{\alpha, \epsilon, p}$ can be calculated even before the simulation begins. Implementations that yield large variability in the SNIS estimator will require more sample size to reach the desired lower bound. Such sequential stopping rules terminate simulation at a random time, and thus additional care must be taken to ensure asymptotic validity of the resulting confidence regions is retained. The following theorem is built on the works of Glynn and Whitt (1992); Vats et al. (2019) to establish this asymptotic validity in the context of IS. The theorem and proof (see Appendix A.2) is presented for the SNIS estimator; an analogous statement and proof is available for the UIS estimator.

Theorem 3.1. *Let $R_n(X)$ be a strongly consistent estimator of an attribute of the system, $R(X)$. That is, let $R_n(X) \rightarrow R(X)$ with probability 1 as $n \rightarrow \infty$. Define $s(n) = \epsilon R_n(X) I(n < n^*) + n^{-1}$ for some finite $n^* > 0$. Additionally, note that $\widehat{\Omega} \rightarrow \Omega$ as $n \rightarrow \infty$ with probability 1. For $\epsilon > 0$, consider the stopping rule*

$$T^*(\epsilon) = \inf \left\{ n \geq 0 : \text{Vol}(C_\alpha(n))^{1/p} + s(n) \leq \epsilon R_n(X) \right\}. \quad (3.5)$$

As $\epsilon \rightarrow 0$, $T^*(\epsilon) \rightarrow \infty$ and $\Pr\{\mu_h \in C_\alpha(T^*(\epsilon))\} \rightarrow 1 - \alpha$.

Due to the random-time termination, Glynn and Whitt (1992) show that strong consistency of $\widehat{\Omega}$ and $R_n(X)$ is necessary for asymptotic validity of the resulting confidence regions.

Remark 4. *The constant n^* is user-chosen and safeguards against premature termination occurring due to early bad estimates. When $n < n^*$, $s(n) = \epsilon R_n(X) + n^{-1}$, making it so that simulation cannot stop. Thus, this choice of $s(n)$ ensures termination occurs after a minimum simulation effort of n^* .*

Remark 5. *The attribute $R(X)$ denotes the quantity relative to which termination occurs. A common choice is setting $R(X) = \|\mu_h\|$, for some appropriate norm. This yields the relative magnitude sequential stopping rule (Glynn and Whitt, 1992). We will focus only on the relative standard-deviation sequential stopping rule, for which $R(X) = |\Sigma|^{1/2p}$.*

Setting $R(X) = |\Sigma|^{1/2p}$ and $R_n(X) = |\widehat{\Sigma}|^{1/2p}$, $T^*(\epsilon)$ the smallest n that satisfies (3.3). Thus, stopping the simulation by checking whether $\widehat{\text{M-ESS}} > L_{\alpha, \epsilon, p}$ will produce adequate confidence regions. The relative precision, ϵ , may be chosen depending on the desired quality of estimation. As $\epsilon \rightarrow 0$, $L_{\alpha, \epsilon, p} \rightarrow \infty$, implying the required sample size would also increase to infinity.

4. Examples

We implement our proposed multivariate ESS in three different examples.¹ First, we present a controlled scenario where the groundtruth is available, and therefore validation of the proposed methodology is possible. We estimate the mean vector of a multivariate normal distribution with a multivariate normal proposal using both UIS and SNIS. We arrive at an expression for the true Ω^* and use this to assess the proposed termination criterion. Next, we present a Bayesian multi-step step-stress model where interest is in estimating two different functions h . We demonstrate the utility of our $\widehat{\text{M-ESS}}$ in acknowledging these different estimation goals. Our last example is that of approximate Bayesian inference using IS and integrated nested Laplace approximation (INLA). We highlight that in this relatively large-dimensional problem, our proposed M-ESS is well-behaved and particularly well-suited for comparisons of IS with MCMC.

4.1. Multivariate Normal

Let $\pi = \mathcal{N}(\mu, \Lambda)$ where $\mu \in \mathbb{R}^p$ and Λ is a $p \times p$ positive-definite matrix. Suppose h is the identity function so that the goal is to estimate $\mu_h = \mu$. Set the proposal to be $q = \mathcal{N}(\mu, \Upsilon)$. The limiting variance of the SNIS estimator $\tilde{\mu}_h$ is available (see Appendix A.3):

$$\Omega = \frac{|\Upsilon|^{1/2}}{|\Lambda||2\Lambda^{-1} - \Upsilon^{-1}|^{1/2}} (2\Lambda^{-1} - \Upsilon^{-1})^{-1}. \quad (4.1)$$

Additionally, for the UIS estimator

$$\Omega_U = \frac{|\Upsilon|^{1/2}}{|\Lambda||2\Lambda^{-1} - \Upsilon^{-1}|^{1/2}} \left[(2\Lambda^{-1} - \Upsilon^{-1})^{-1} + \mu\mu^T \right] - \mu\mu^T. \quad (4.2)$$

We first fix $p = 2$ and for $\sigma_1, \sigma_2, \sigma > 0$ and $0 < \lambda, \rho < 1$, consider Λ and Υ of the following form:

$$\Lambda = \begin{pmatrix} \sigma_1 & \lambda\sqrt{\sigma_1\sigma_2} \\ \lambda\sqrt{\sigma_1\sigma_2} & \sigma_2 \end{pmatrix} \quad \text{and} \quad \Upsilon = \begin{pmatrix} \sigma & \rho\sigma \\ \rho\sigma & \sigma \end{pmatrix}.$$

We compare the various ESSs for SNIS and UIS under three different settings:

¹Code is available at <https://github.com/medhaaga/Importance-Sampling-Stopping-Rule>

1. *Setting 1*: low target and proposal correlation, with $\lambda = \rho = 0.1$:

$$\Lambda = \begin{pmatrix} 2 & 0.1\sqrt{2} \\ 0.1\sqrt{2} & 1 \end{pmatrix} \quad \Upsilon = \begin{pmatrix} 2 & 0.2 \\ 0.2 & 2 \end{pmatrix}. \quad (4.3)$$

2. *Setting 2*: medium correlation in target and proposal, with $\lambda = \rho = 0.5$:

$$\Lambda = \begin{pmatrix} 2 & 0.5\sqrt{2} \\ 0.5\sqrt{2} & 1 \end{pmatrix} \quad \Upsilon = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}. \quad (4.4)$$

3. *Setting 3*: high and differing correlation, with $\lambda = 0.8$ and $\rho = 0.7$:

$$\Lambda = \begin{pmatrix} 2 & 0.8\sqrt{2} \\ 0.8\sqrt{2} & 1 \end{pmatrix} \quad \Upsilon = \begin{pmatrix} 2 & 1.4 \\ 1.4 & 2 \end{pmatrix}. \quad (4.5)$$

Throughout, we set $\mu = \mathbf{1}_p$. For $p = 2$, the covariance ellipse of Λ and Υ in the three settings, along with ellipses for Ω and Ω_U are shown in Figure 1 (top). It is evident that in all three settings the variance of UIS estimator is larger than that of the SNIS estimator. Figure 1 (bottom) shows the univariate and multivariate true ESS for UIS and SNIS vs the correlation between the two components in the proposal distribution; the chosen ρ for each setting is indicated through a vertical dashed line. First, the SNIS estimator is clearly preferred here over the UIS estimator; this is unsurprising given the ellipses in the top row. Second, the differing quality of univariate and multivariate ESS estimation is apparent. Not accounting for the complex dependence structures (as presented in the top row), leads to inadequate understanding of the overall estimation quality. Next we demonstrate the performance of the proposed stopping rule in (3.4). Controlling the desired quality of estimation through ϵ , we study the impact of i) the problem dimension, p , ii) the target/proposal setting, and iii) the choice of estimator (UIS and SNIS). Since dimensions will increase from $p = 2$, we present a general form of Λ and Υ , similar to the three previous settings:

$$\Lambda = \begin{pmatrix} A & B \\ B & C \end{pmatrix} \quad \Upsilon = \begin{pmatrix} A' & B' \\ B' & C' \end{pmatrix}, \quad (4.6)$$

where

$$A = \begin{pmatrix} \sigma_1 & \dots & \lambda\sigma_1 \\ \vdots & \ddots & \vdots \\ \lambda\sigma_1 & \dots & \sigma_1 \end{pmatrix}, B = \begin{pmatrix} \lambda\sqrt{\sigma_1\sigma_2} & \dots & \lambda\sqrt{\sigma_1\sigma_2} \\ \vdots & \ddots & \vdots \\ \lambda\sqrt{\sigma_1\sigma_2} & \dots & \lambda\sqrt{\sigma_1\sigma_2} \end{pmatrix}, \text{ and } C = \begin{pmatrix} \sigma_2 & \dots & \lambda\sigma_2 \\ \vdots & \ddots & \vdots \\ \lambda\sigma_2 & \dots & \sigma_2 \end{pmatrix}$$

$$A' = \begin{pmatrix} v_1 & \dots & \rho v_1 \\ \vdots & \ddots & \vdots \\ \rho v_1 & \dots & v_1 \end{pmatrix}, B' = \begin{pmatrix} \rho\sqrt{v_1v_2} & \dots & \rho\sqrt{v_1v_2} \\ \vdots & \ddots & \vdots \\ \rho\sqrt{v_1v_2} & \dots & \rho\sqrt{v_1v_2} \end{pmatrix}, \text{ and } C' = \begin{pmatrix} v_2 & \dots & \rho v_2 \\ \vdots & \ddots & \vdots \\ \rho v_2 & \dots & v_2 \end{pmatrix}.$$

We set $\sigma_1 = 2, \sigma_2 = 1$ and $v_1 = v_2 = 2$. Similar to before, for the three settings, we let 1) $\lambda = \rho = 0.1$ and 2) $\lambda = \rho = 0.5$, and 3) $\lambda = 0.8, \rho = 0.7$. These three

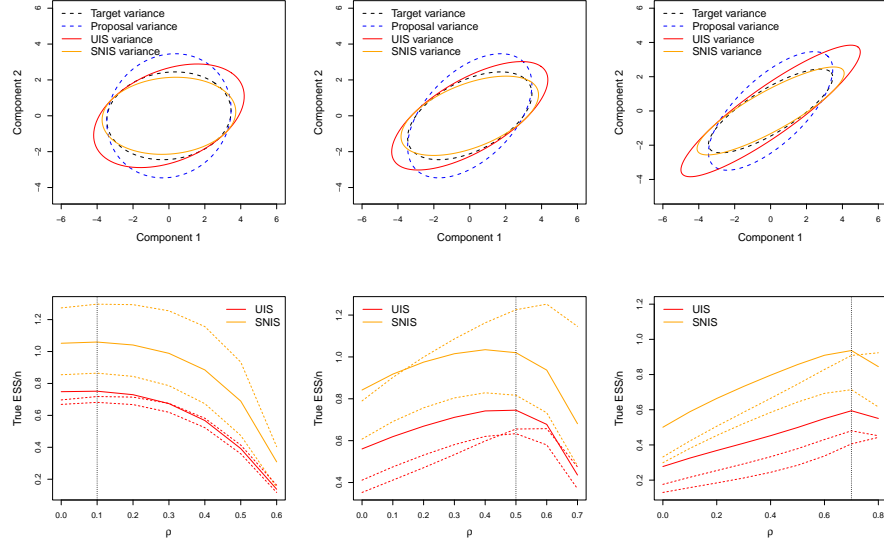


FIG 1. (Top row) The target, proposal, UIS, and SNIS covariance ellipses for Settings 1, 2, and 3 (left to right). (Bottom row) True ESS/n for SNIS and UIS from (4.1) and (4.2) for each setting. The vertical dotted line marks the value of ρ chosen in the three settings.

settings represent low, medium, and high correlation between components for all dimensions.

We implement our multivariate stopping rule in (3.4) in 100 repeated simulations for varying choices of ϵ for both the UIS and SNIS estimators. Figure 2 presents the L_2 norm of the error in estimation of μ versus the sample size at ϵ -termination. That is, we calculate $\|\mu^* - \mu\|_2$ and plot it versus n at termination for each ϵ . The top row has results for $p = 2$ and the bottom row for $p = 10$. Here the circles represent the IS runs where μ^* is the UIS estimator and the triangles represent the SNIS estimator. First, we note that since UIS produces more inefficient estimators; for any given ϵ , UIS terminates later than SNIS. Additionally, as ϵ decreases, the variability in the squared error also decreases; this is a direct consequence of an increase in the required sample sizes. Finally, we note that the quality of estimation of the ESS over all three settings is sound. Setting 3, which has the most correlation in the target, exhibits the most variability in the termination time.

4.2. Weibull Multi-Step Step-Stress Model

Consider the fish dataset of Pal et al. (2021), described in Table 1, where the swimming performance of $n = 14$ fish was investigated with an initial swimming rate of 15 cm/sec. The time at which a fish could not maintain its natural position was recorded as the failure time. The flow rate was increased by 5

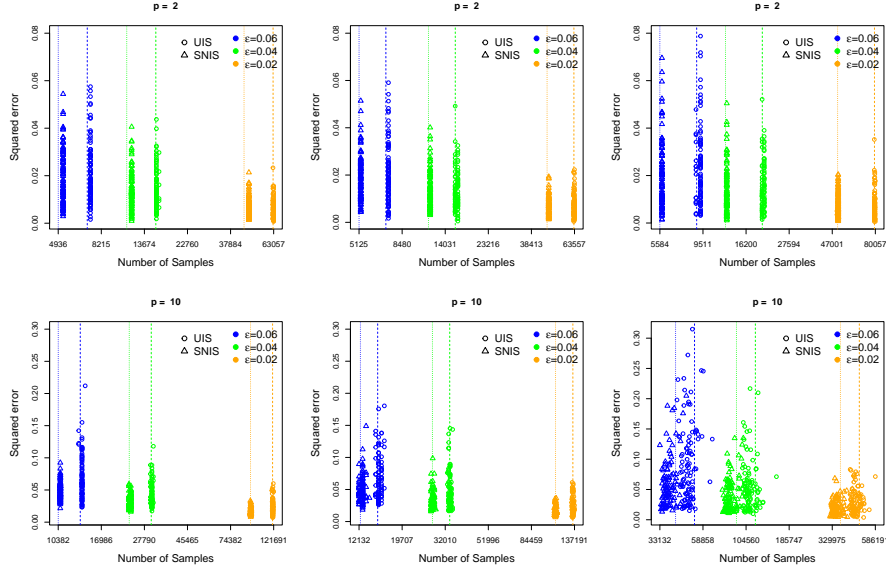


FIG 2. L_2 error of SNIS and UIS estimator vs termination time for varying ϵ for $p = 2$ and 10 (top and bottom row). The truth is marked with vertical lines for both estimators.

cm/sec every time after 110, 130, and 150 minutes. Here, the increased flow rate can be thought of as a stress factor. Thus, there are four stress levels and the observed number of failures at each level, n_k , $k = 1, 2, 3, 4$, is 6, 3, 3, and 2, respectively. The failure times are centered by 80 and scaled by 100 as recommended by Pal et al. (2021), so that time-points corresponding to stress change are $\tau_1 = 0.3, \tau_2 = 0.5, \tau_3 = 0.7$.

Stress level	Failure times
s_1	83.50, 91.00, 91.00, 97.00, 107.00, 109.50
s_2	114.00, 115.41, 128.61
s_3	133.53, 138.58, 140.00
s_4	152.08, 155.10

TABLE 1
Fish Dataset

Let $\bar{n}'_j = \sum_{i=1}^j n_i$ be the total number of failures observed during and before the j th stress-level and let t_r denote the time-to-failure of the r th fish. Let the collected data of ordered observed failure times be denoted by \mathcal{D} . Pal et al. (2021) assume that the lifetime distribution of the experimental units under a given stress level k , follows Weibull(α, λ_k) for $\alpha, \lambda_k > 0$ with probability density function

$$f_k(t) = \lambda_k \alpha t^{\alpha-1} e^{-\lambda_k t^\alpha}. \quad (4.7)$$

To allow for ordering in the time-to-failure with subsequent stress levels, the λ 's are assumed to be ordered so that, $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \lambda_4$. Let $\theta = (\alpha, \lambda_1, \lambda_2, \lambda_3, \lambda_4)$.

For $a > 0$, $b > 0$, $a_i > 0$; $i = 0, \dots, 4$ and $\mathbf{a} = (a_1, a_2, a_3, a_4)$, the following are the independent priors assumed by Pal et al. (2021):

$$\alpha \sim \text{Gamma}(a, b) \text{ and } \lambda \sim \text{ODG}(a_o, b_o, \mathbf{a}), \quad (4.8)$$

where ODG stands for the ordered Dirichlet Gamma distribution. Given the Bayesian paradigm, the resulting posterior distribution is the primary object of interest and can be written down as

$$\pi(\theta|\mathcal{D}) \propto \pi_1^*(\lambda|\mathcal{D}, \alpha) \pi_2^*(\alpha|\mathcal{D}) g(\alpha, \lambda|\mathcal{D}), \quad (4.9)$$

where π_1^* and π_2^* are densities of an ODG and Gamma distribution respectively; the exact parameters and details on g are given in Appendix A.4. We set $a = b = a_o = b_o = 0.5$ and $\mathbf{a} = (1, 1, 1, 1)$.

Interest may be in the posterior mean or the average lifetime units for a stress level. For a Weibull(α, λ) distribution, the mean is $\lambda^{-1/\alpha} \Gamma(1 + 1/\alpha)$, so two functions of interest are

$$h_1(\theta) = \theta \quad h_2(\theta) = \left(\lambda_1^{-1/\alpha} \Gamma(1 + 1/\alpha), \dots, (\lambda_4^{-1/\alpha} \Gamma(1 + 1/\alpha)) \right). \quad (4.10)$$

Similar to Pal et al. (2021), we employ IS with proposal

$$q(\alpha, \lambda) \sim \pi_1^*(\lambda|\mathcal{D}, \alpha) \pi_2^*(\alpha|\mathcal{D}). \quad (4.11)$$

Using this proposal, the weight function is $g(\alpha, \lambda|\mathcal{D})$. Since the normalizing

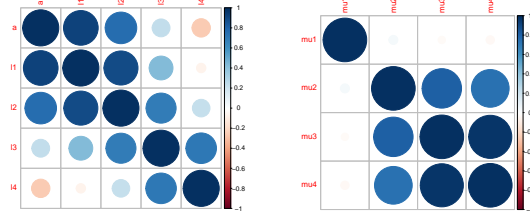


FIG 3. Estimated pairwise correlations for $\tilde{\mu}_{h_1}$ (left) and $\tilde{\mu}_{h_2}$ (right).

constants in the posterior distribution are unknown, only the SNIS estimator can be implemented. First, in order to visualize the complex correlation structures of $\tilde{\mu}_{h_1}$ and $\tilde{\mu}_{h_2}$, Figure 3 plots the estimated sample correlation matrices of the corresponding $\hat{\Omega}$. Since significant correlation between components for both $\tilde{\mu}_{h_1}$ and $\tilde{\mu}_{h_2}$ is evident, multivariate assessment of the quality of estimation is warranted.

The disparity between ESS estimation using multivariate ESS and univariate ESS with five different components of θ can be seen in left side plot of Figure 4. Here we present the estimated M-ESS for h_1 , univariate ESS for each component of h_1 , and K_n . Since interest is in estimating *all* components of h_1 , the individual univariate ESSs only provide partial information about the quality of estimation,

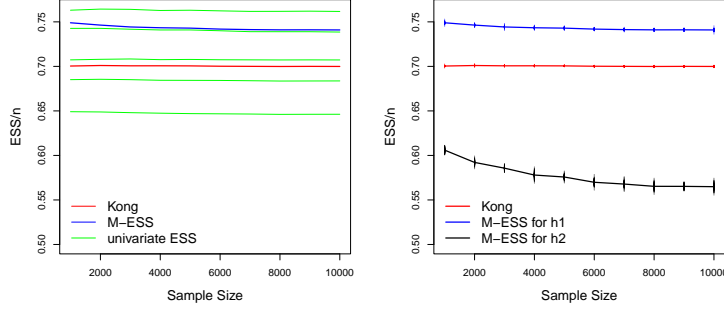


FIG 4. Left: ESS/n (Kong, univariate ESS, and M-ESS) vs sample size for $h(\theta) = h_1(\theta)$ where $\theta = (\alpha, \lambda_1, \dots, \lambda_4)$. Right: ESS/n (Kong and M-ESS) vs sample size for $h_1(\theta)$ and $h_2(\theta)$. For each sample size, simulations are run for 500 replications and the error bars for estimated ESS/n are drawn using two standard deviations.

whereas M-ESS provides a complete understanding of the relative quality of estimation.

In Figure 4 (right), K_n is limited to only quantifying the quality of the proposal distribution in relation to π , and does not account for the different h functions of interest. Further, it is evident that for any same sample size n , the M-ESS for estimating h_2 is significantly smaller than the M-ESS for h_1 . This indicates requirement of increased simulation effort for estimating μ_{h_2} and enables users to make informed decisions motivated by their primary objective. For instance, running the simulations with $\epsilon = 0.05$, we find that the necessary sample size (averaged over 10 replications) using (3.4) is 1.209×10^4 for estimating μ_{h_1} and 1.589×10^4 for estimating μ_{h_2} .

4.3. Bayesian Lasso using INLA

Berild et al. (2022) propose an importance sampling based extension of INLA. INLA is an approximate Bayesian inference tool for models with a latent Gaussian structure. INLA focuses on quick approximate marginal posterior inference, as opposed to exact joint inference often done by MCMC. Although INLA is applicable to a relatively small class of models, Berild et al. (2022) propose an importance sampling based method to expand this class to conditional latent Gaussian models.

Let $y \in \mathbb{R}^m$ be the vector of observed m responses and X be an $m \times p$ model matrix made of p regression covariates. For $\tau > 0$, consider the following Gaussian likelihood:

$$y \sim \mathcal{N}_m(X\beta, \tau^{-1}I_m).$$

For Bayesian lasso, a Laplace prior is put on β and Berild et al. (2022); Gómez-Rubio and Rue (2018) assume the default R-INLA prior for τ : $\tau \sim \text{Gamma}(1, .00005)$.

Since the Laplace prior is not available in R-INLA (Lindgren and Rue, 2015), Gómez-Rubio and Rue (2018) propose a method that combines MCMC and INLA to fit this model by conditioning on β . Using this key idea, Berild et al. (2022) combine IS and INLA to fit this model. Using notation in Berild et al. (2022), let $z = (\beta, \tau)$ with $z_c = \beta$ and $z_{-c} = \tau$; z_c denotes the parameters being conditioned on and z_{-c} denotes all other parameters. Given z_c , R-INLA provides numerical approximations to conditional posterior marginal $\pi(z_{-c}|y, z_c)$ and conditional marginal likelihood $\pi(y|z_c)$. In this situation, note that

$$\pi(z_c|y) \propto \pi(y|z_c)\pi(z_c),$$

where $\pi(y|z_c)$ can be approximated by R-INLA. Therefore, the posterior expectation of z_c , denoted by $\mu_{z_c} := \int z_c \pi(z_c|y) dz_c$, can be estimated using SNIS; $h(x)$ here is thus the identity function. The samples $\{z_c^i\}_{i=1}^n$ are generated from a proposal density g and the corresponding weights are

$$w_i := \frac{\pi(y|z_c^i)\pi(z_c^i)}{g(z_c^i)}.$$

Berild et al. (2022, Section 4.2) presents a detailed discussion on the need for an effective sample size that accounts for both the choice of $h(x)$ and does not require looking at many univariate ESSs. They acknowledge and indicate that one of the only possible quantities available is the modified ESS of Owen (2013). Let $h_j(x)$ denote the j th component of the function h , then Owen (2013) proposes the following:

$$\tilde{w}_i(h_j) := \frac{|h_j(X_i)|w_i}{\sum_{t=1}^n |h_j(X_t)|w_t} \quad \text{and} \quad \text{oESS}_j := \frac{1}{\sum_{t=1}^n \tilde{w}_t(h_j)^2}.$$

Berild et al. (2022) analyze the `Hitters` dataset available in `ISLR` library in R. Here the response is the salary variable and although they choose five numerical covariates, we analyze the complete dataset with all 19 covariates. Similar to Berild et al. (2022), we use a multivariate Student- t proposal, $t_\nu(\mu_k, \Sigma_k)$ with $\nu = 3$; the mean μ_k and covariance Σ_k are chosen via preliminary IS explorations.

Figure 5 presents ESS/ n versus Monte Carlo sample size n for $\widehat{\text{M-ESS}}$, K_n , and oESS_j (for each component), averaged over 10 replications. It is evident that the quality of estimation of the proposed $\widehat{\text{M-ESS}}$ remains reasonably steady as a function of n and there is significant difference between $\widehat{\text{M-ESS}}$ and K_n . Further, oESS_j , although accounting for the choice of h , ignores the multivariate nature of the estimation problem and returns vastly differing estimation quality over the components.

It is important here to also add that Berild et al. (2022) compare their IS based method to the MCMC based method of Gómez-Rubio and Rue (2018), by comparing the effective sample sizes of the two algorithms; Berild et al. (2022) use the ESSs of both Kong (1992) and Owen (2013). However, although still

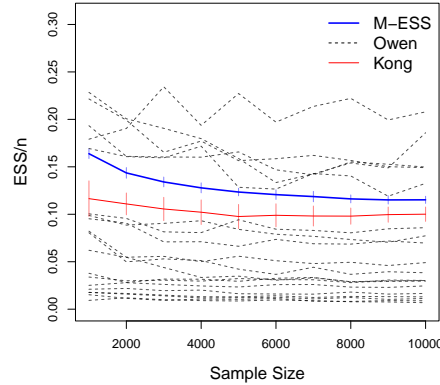


FIG 5. Estimated ESS/n vs n (sample size), averaged over 10 replications.

called “effective sample size”, both K_n and oESS diverge significantly from the effective sample size used in MCMC. M-ESS, on the other hand, can directly be used to compare quality of estimation between IS and MCMC. In other words, if the M-ESS of an IS estimator is more than the effective sample size of an MCMC estimator, it can be correctly concluded that IS yields a more efficient estimator. The same conclusion cannot be made for K_n and oESS.

5. Discussion

We present a practical sequential stopping rule for IS, based on self-assessing the quality of estimation in a multivariate setting. Choosing and adapting a proposal distribution is a rich and important area of work, known as adaptive importance sampling (AIS), and many existing algorithms are devoted to this task, e.g., PMC (Cappé et al., 2004), AMIS (Cornuet et al., 2012), M-PMC (Cappé et al., 2008), LAIS (Martino et al., 2015), DM-PMC (Elvira et al., 2017), or O-PMC (Elvira and Chouzenoux, 2022) (see Bugallo et al., 2017, for a detailed review). These existing methods do not consider an adaptive choice of the number of proposals nor the number of samples. We are confident that the proposed methodology can be useful to develop more efficient AIS algorithms. Traditionally, ESS is defined as the relative variance of the vanilla Monte Carlo estimator and the chosen estimator (see Kong (1992) and the discussion in Elvira et al. (2022)). One can argue against the choice of the vanilla Monte Carlo estimator as the baseline; this may be seen in applications to rare event simulation (Owen et al., 2019), and therefore, the ESS would not be as informative in such scenarios. Our proposed stopping rule in (3.4) and Theorem 3.1 can be adapted to such changes in the baseline.

As highlighted in the example in Section 4.2, the stopping rule and quality of

estimation critically depends on the function of interest h . It is then imperative that users first decide their h of interest, before commencing the IS procedure. In scenarios where a specific h may not be of interest, the K_n metric of Kong (1992) would be useful. While K_n does not translate into the number of effective samples from the target, it can still be useful in understanding the quality of the weights. Thus, K_n can be used as a qualifier to ascertain the quality of the proposal distribution for a particular target.

Other IS estimators have been proposed that promise improvement in estimation quality (see Martino et al., 2018; Elvira et al., 2019; Vehtari et al., 2015) by utilising weight modification techniques. These methods exhibit variance reduction in theory, but there are no known methods of estimating their variance other than bootstrap. Thus, variance estimation of other IS estimators is an interesting and critical line of future research.

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Appendix A: Appendix

A.1. Variance of the SNIS estimator

Versions of the proof of the asymptotic normality of $\tilde{\mu}_h$ is available in Rice (2006); Nilakanta (2020), however, we present the proof here for completeness. Define the mapping $k : \mathbb{R}^s \rightarrow \mathbb{R}^{p+1}$ such that $X \mapsto (h(X)w(X), w(X))$. If $\{X_i\}_{i=1}^n$ are i.i.d. samples from the proposal, this allows us to define iid random variables $Y_i := (h(X_i)w_i, w_i)$, for $i = 1, \dots, n$ so that $\theta := \mathbb{E}_q[Y_1] = (Z\mu_h, Z)^T$ and let $\Lambda := \text{Var}_q(Y_1)$ denote the $(p+1) \times (p+1)$ covariance matrix of Y_1 and we assume that $\Lambda < \infty$. Let \bar{Y}_n denote the sample average of $\{Y_i\}_{i=1}^n$. By a standard central limit theorem,

$$\sqrt{n}(\bar{Y}_n - \theta) \xrightarrow{d} \mathcal{N}(0, \Lambda) \quad \text{as } n \rightarrow \infty.$$

Define the function $g : \mathbb{R}^p \times \mathbb{R} \rightarrow \mathbb{R}^p$ as $g(a, b) = a/b$ for $a \in \mathbb{R}^p$ and $b \in \mathbb{R}$. Then using the multivariate delta method (see Lehmann, 2004) for variance of ratio of means and a second-order approximation,

$$\sqrt{n}(g(\bar{Y}_n) - g(\theta)) \xrightarrow{d} \mathcal{N}_p(0, \nabla g(\theta)^T \Lambda \nabla g(\theta)) \quad \text{as } n \rightarrow \infty,$$

where

$$\nabla g(\theta) = \begin{pmatrix} I_p & \\ \frac{\mu_h}{Z} & -\frac{\mu_h}{Z^2} \end{pmatrix}^T.$$

Note that g translates the sample average \bar{Y}_n to the SNIS estimator as

$$g(\bar{Y}_n) = g\left(\frac{\sum_{i=1}^n h(X_i)w_i}{n}, \frac{\sum_{i=1}^n w_i}{n}\right) = \frac{\sum_{i=1}^n h(X_i)w_i}{\sum_{i=1}^n w_i} = \tilde{\mu}_h.$$

Therefore, as $n \rightarrow \infty$, we have

$$\sqrt{n}(\tilde{\mu}_h - \mu_h) \xrightarrow{d} \mathcal{N}_p(0, \Omega), \quad (\text{A.1})$$

with

$$\Omega = \nabla g(\theta)^T \Lambda \nabla g(\theta) = \frac{\mathbb{E}_q[w(X)^2(h(X) - \mu)(h(X) - \mu)^T]}{\mathbb{E}_q[w(X)]^2}.$$

A.2. Proof of Theorem 3.1

Proof. For the purpose of this proof, we extend the notation of $\tilde{\mu}_h$ and $\hat{\Omega}$ to explicitly display the number of samples used in estimation. Let $\tilde{\mu}_h(m)$ and $\hat{\Omega}(m)$ denote the estimators $\tilde{\mu}_h$ and $\hat{\Omega}$ constructed using m importance samples. First, we show that as $\epsilon \rightarrow 0$, $T^*(\epsilon) \rightarrow \infty$. Consider $t^*(\epsilon) = \inf \{n \geq 0 : s(n) \leq \epsilon R_n(X)\}$. As $\epsilon \rightarrow 0$, $t^*(\epsilon) \rightarrow \infty$ and $T^*(\epsilon) > t^*(\epsilon)$, yielding $T^*(\epsilon) \rightarrow \infty$. Define $V(n) = \text{Vol}(C_\alpha(n))^{1/p} + s(n)$ and

$$d_{\alpha,p} := \frac{2\pi^{p/2}}{p\Gamma(p/2)} (\chi_{1-\alpha,p}^2)^{p/2}.$$

Recall from (3.1) and the statement of Theorem 3.1

$$\text{Vol}(C_\alpha(n)) = \frac{2\pi^{p/2}}{p\Gamma(p/2)} \left(\frac{\chi_{1-\alpha,p}^2}{n}\right)^{p/2} |\hat{\Omega}|^{1/2} \quad \text{and} \quad s(n) = \epsilon R_n(X) I(n < n^*) + n^{-1}.$$

Using the fact that $s(n) = o(n^{-1/2})$ and $\hat{\Omega}$ is consistent, we have $n^{1/2}V(n) \rightarrow (d_{\alpha,p}|\Omega|^{1/2})^{1/p}$ as $n \rightarrow \infty$. The following limit follows directly from Vats et al. (2019)

$$\lim_{\epsilon \rightarrow 0} \epsilon T^*(\epsilon)^{1/2} = d_{\alpha,p}^{1/p} \frac{|\Omega|^{1/2p}}{R(X)}.$$

Using the above, a functional delta method, and a standard random time change argument (Billingsley, 2013, p. 144) we have,

$$\sqrt{T^*(\epsilon)} \left[\hat{\Omega}(T^*(\epsilon)) \right]^{-1/2} (\tilde{\mu}_h(T^*(\epsilon)) - \mu_h) \xrightarrow{d} \mathcal{N}_p(0, I_p).$$

As a consequence, as $\epsilon \rightarrow 0$, with probability, $\Pr[\mu_h \in C_\alpha(T^*(\epsilon))] \rightarrow 1 - \alpha$. \square

A.3. True Variances for Multivariate Gaussian

Recall from Eq.(2.5), the limiting variance of $\tilde{\mu}_h$ is given by

$$\Omega = \int_{\mathbb{R}^p} \frac{(h(x) - \mu_h)(h(x) - \mu_h)^T \pi(x)^2}{q(x)} dx.$$

In Section 4.1, $h(x) = x$, $\pi = \mathcal{N}(\mu, \Lambda)$, and $q = \mathcal{N}(\mu, \Upsilon)$. Plugging this in (2.5), we get

$$\begin{aligned} \Omega &= \int_{\mathbb{R}^p} \frac{(x - \mu)(x - \mu)^T \pi(x)^2}{q(x)} dx \\ &= \frac{|\Upsilon|^{1/2}}{|\Lambda|} \int_{\mathbb{R}^p} \frac{(x - \mu)(x - \mu)^T}{(2\pi)^{p/2}} \exp \left\{ -(x - \mu)^T \Lambda^{-1} (x - \mu) + \frac{(x - \mu)^T \Upsilon^{-1} (x - \mu)}{2} \right\} dx \\ &= \frac{|\Upsilon|^{1/2}}{|\Lambda| |2\Lambda^{-1} - \Upsilon^{-1}|^{1/2}} (2\Lambda^{-1} - \Upsilon^{-1})^{-1}. \end{aligned}$$

Next,

$$\Omega_U = \int_{\mathbb{R}^p} \frac{(h(x)h(x)^T \pi(x)^2)}{q(x)} dx - \mu\mu^T \quad (\text{A.2})$$

$$\begin{aligned} &= \int_{\mathbb{R}^p} \frac{xx^T \pi(x)^2}{q(x)} dx - \mu\mu^T \\ &= \frac{|\Upsilon|^{1/2}}{|\Lambda|} \int_{\mathbb{R}^p} \frac{xx^T}{(2\pi)^{p/2}} \exp \left\{ -(x - \mu)^T \Lambda^{-1} (x - \mu) + \frac{(x - \mu)^T \Upsilon^{-1} (x - \mu)}{2} \right\} dx - \mu\mu^T \\ &= \frac{|\Upsilon|^{1/2}}{|\Lambda| |2\Lambda^{-1} - \Upsilon^{-1}|^{1/2}} \left[(2\Lambda^{-1} - \Upsilon^{-1})^{-1} + \mu\mu^T \right] - \mu\mu^T. \quad (\text{A.3}) \end{aligned}$$

A.4. Details of Bayesian Multi-Step Step-Stress Model

The combined likelihood for the fish dataset in Section 4.2 with $\theta = (\alpha, \lambda_1, \lambda_2, \lambda_3, \lambda_4)$ is,

$$L(\theta | \mathcal{D}) \propto \alpha^r \lambda_1^n \lambda_2^n \lambda_3^n \lambda_4^n \left(\prod_{i=1}^n t_i^{\alpha-1} \right) e^{-(\lambda_1 D_1(\alpha) + \lambda_3 + \lambda_4 D_4(\alpha))},$$

where with $\bar{n}_0 = \tau_0 = 0$, $\bar{n}_4 = n$,

$$D_j(\alpha) = \left(\sum_{i=\bar{n}_{j-1}-1}^{\bar{n}_j} t_i^\alpha + (n - \bar{n}_j) \tau_j^\alpha - (n - \bar{n}_{j-1}) \tau_{j-1}^\alpha \right).$$

Let $S(\alpha) = \min \{D_1(\alpha), D_2(\alpha), D_3(\alpha), D_4(\alpha)\}$ and $J = \min(n_1, n_2, n_3, n_4)$, then $\pi_1^*(\lambda|\alpha, \mathcal{D})$, $\pi_2^*(\alpha|\mathcal{D})$, and $g(\alpha, \lambda|\mathcal{D})$ from the full posterior distribution in (4.9) are

$$\pi_1^*(\lambda|\alpha, \mathcal{D}) = \text{density of ODG}(a_o + 4J, b_o + S(\alpha), a_1 + J, a_2 + J, a_3 + J, a_4 + J),$$

$$\pi_2^*(\alpha|\mathcal{D}) = \text{density of Gamma} \left(n + a, b - \sum_{i=1}^n \ln t_i \right),$$

$$g(\alpha, \lambda|\mathcal{D}) = \frac{\prod_{j=1}^4 \left[\lambda_j^{n_j - J} e^{-\lambda_j (D_j(\alpha) - S(\alpha))} \right]}{[b_o + S(\alpha)]^{a_o + 4J}}.$$

References

- Bayraksan, G. and Pierre-Louis, P. (2012). Fixed-width sequential stopping rules for a class of stochastic programs. *SIAM Journal on Optimization*, 22:1518–1548.
- Berild, M. O., Martino, S., Gómez-Rubio, V., and Rue, H. (2022). Importance sampling with the integrated nested Laplace approximation. *Journal of Computational and Graphical Statistics*, pages 1–13.
- Billingsley, P. (2013). *Convergence of Probability Measures*. John Wiley and Sons.
- Bugallo, M. F., Elvira, V., Martino, L., Luengo, D., Miguez, J., and Djuric, P. M. (2017). Adaptive importance sampling: the past, the present, and the future. *IEEE Signal Processing Magazine*, 34(4):60–79.
- Cappé, O., Douc, R., Guillin, A., Marin, J. M., and Robert, C. P. (2008). Adaptive importance sampling in general mixture classes. *Statistical Computing*, 18:447–459.
- Cappé, O., Guillin, A., Marin, J. M., and Robert, C. P. (2004). Population Monte Carlo. *Journal of Computational and Graphical Statistics*, 13(4):907–929.
- Chatterjee, S., Diaconis, P., et al. (2018). The sample size required in importance sampling. *The Annals of Applied Probability*, 28(2):1099–1135.
- Cornuet, J. M., Marin, J. M., Mira, A., and Robert, C. P. (2012). Adaptive multiple importance sampling. *Scandinavian Journal of Statistics*, 39(4):798–812.
- Denny, M. (2001). Introduction to importance sampling in rare-event simulations. *European Journal of Physics*, 22(4):403.
- Dong, J. and Glynn, P. (2019). A new approach to sequential stopping for stochastic simulation. *Preprint*.
- Ekvall, K. O. and Jones, G. L. (2014). Markov chain Monte Carlo. *Wiley StatsRef: Statistics Reference Online*, pages 1–9.
- Elvira, V. and Chouzenoux, E. (2022). Optimized population Monte Carlo. *IEEE Transactions on Signal Processing*, 70:2489–2501.
- Elvira, V. and Martino, L. (2021). *Advances in Importance Sampling*, pages 1–14. John Wiley & Sons, Ltd.
- Elvira, V., Martino, L., Luengo, D., and Bugallo, M. F. (2017). Improving population Monte Carlo: Alternative weighting and resampling schemes. *Signal Processing*, 131:77–91.
- Elvira, V., Martino, L., Luengo, D., and Bugallo, M. F. (2019). Generalized multiple importance sampling. *Statistical Science*, 34(1):129–155.

- Elvira, V., Martino, L., and Robert, C. P. (2022). Rethinking the effective sample size. *International Statistical Review*, n/a(n/a).
- Flegal, J. M. and Gong, L. (2015). Relative fixed-width stopping rules for Markov chain Monte Carlo simulations. *Statistica Sinica*, pages 655–675.
- Frey, J. (2010). Fixed-width sequential confidence intervals for a proportion. *The American Statistician*, 64(3):242–249.
- Glynn, P. W. and Whitt, W. (1992). The asymptotic validity of sequential stopping rules for stochastic simulations. *Annals of Applied Probability*, 2:180–198.
- Gómez-Rubio, V. and Rue, H. (2018). Markov chain Monte Carlo with the integrated nested laplace approximation. *Statistics and Computing*, 28(5):1033–1051.
- Kahn, H. (1950a). Random sampling (Monte Carlo) techniques in neutron attenuation problems. i. *Nucleonics (US) Ceased Publication*, 6(See also NSA 3-990).
- Kahn, H. (1950b). Random sampling (Monte Carlo) techniques in neutron attenuation problems. ii. *Nucleonics (US) Ceased Publication*, 6(See also NSA 4-3795).
- Kong, A. (1992). A note on importance sampling using standardized weights. *University of Chicago, Dept. of Statistics, Tech. Rep.*, 348.
- Kuntz, J., Crucinio, F. R., and Johansen, A. M. (2022). Product-form estimators: exploiting independence to scale up Monte Carlo. *Statistics and Computing*, 32:1–22.
- Lehmann, E. L. (2004). *Elements of Large-sample Theory*. Springer Science and Business Media.
- Lindgren, F. and Rue, H. (2015). Bayesian spatial modelling with R-INLA. *Journal of Statistical Software*, 63:1–25.
- Martino, L., Elvira, V., Luengo, D., and Corander, J. (2015). Layered adaptive importance sampling. *Statistics and Computing*, 27(3):599–623.
- Martino, L., Elvira, V., Míguez, J., Artés-Rodríguez, A., and Djurić, P. (2018). A comparison of clipping strategies for importance sampling. In *2018 IEEE Statistical Signal Processing Workshop (SSP)*, pages 558–562. IEEE.
- Miller, C., Corcoran, J. N., and Schneider, M. D. (2021). Rare events via cross-entropy population Monte Carlo. *IEEE Signal Processing Letters*, 29:439–443.
- Mohamed, S., Rosca, M., Figurnov, M., and Mnih, A. (2020). Monte Carlo gradient estimation in machine learning. *J. Mach. Learn. Res.*, 21(132):1–62.
- Nilakanta, H. (2020). *Output analysis of Monte Carlo methods with applications to networks and functional approximation*. PhD thesis, University of Minnesota.
- Owen, A. B. (2013). *Monte Carlo Theory, Methods and Examples*.
- Owen, A. B., Maximov, Y., and Chertkov, M. (2019). Importance sampling the union of rare events with an application to power systems analysis. *Electronic Journal of Statistics*, 13(1):231–254.
- Pal, A., Mitra, S., and Kundu, D. (2021). Bayesian order-restricted inference of a Weibull multi-step step-stress model. *Journal of Statistical Theory and Practice*, 15(2):1–33.

- Park, J. and Haran, M. (2018). Bayesian inference in the presence of intractable normalizing functions. *Journal of the American Statistical Association*, 113:1372–1390.
- Rice, J. A. (2006). *Mathematical Statistics and Data Analysis*. Nelson Education.
- Robert, C. and Casella, G. (2013). *Monte Carlo Statistical Methods*. Springer Science and Business Media.
- Sanz-Alonso, D. (2018). Importance sampling and necessary sample size: an information theory approach. *SIAM/ASA Journal on Uncertainty Quantification*, 6(2):867–879.
- Sanz-Alonso, D. and Wang, Z. (2021). Bayesian update with importance sampling: Required sample size. *Entropy*, 23(1):22.
- SenGupta, A. (1987). Tests for standardized generalized variances of multivariate normal populations of possibly different dimensions. *Journal of Multivariate Analysis*, 23:209–219.
- Vats, D., Flegal, J. M., and Jones, G. L. (2019). Multivariate output analysis for Markov chain Monte Carlo. *Biometrika*, 106(2):321–337.
- Vats, D., Flegal, J. M., and Jones, G. L. (2021). *Monte Carlo Simulation: Are We There Yet?*, pages 1–15. In Wiley StatsRef: Statistics Reference Online.
- Vehtari, A., Simpson, D., Gelman, A., Yao, Y., and Gabry, J. (2015). Pareto smoothed importance sampling. *arXiv preprint arXiv:1507.02646*.
- Wilks, S. S. (1932). Certain generalizations in the analysis of variance. *Biometrika*, pages 471–494.