Abstract: The naive importance sampling (IS) estimator generally does not work well in examples involving simultaneous inference on several targets, as the importance weights can take arbitrarily large values, making the estimator highly unstable. In such situations, alternative multiple IS estimators involving samples from multiple proposal distributions are preferred. Just like the naive IS, the success of these multiple IS estimators crucially depends on the choice of the proposal distributions. The selection of these proposal distributions is the focus of this article. We propose three methods: (i) a geometric space filling approach, (ii) a minimax variance approach, and (iii) a maximum entropy approach. The first two methods are applicable to any IS estimator, whereas the third approach is described in the context of Doss’s (2010) two-stage IS estimator. For the first method, we propose a suitable measure of ‘closeness’ based on the symmetric Kullback-Leibler divergence, while the second and third approaches use estimates of asymptotic variances of Doss’s (2010) IS estimator and Geyer’s (1994) reverse logistic regression estimator, respectively. Thus, when samples from the proposal distributions are obtained by running Markov chains, we pro-
vide consistent spectral variance estimators for these asymptotic variances. The proposed methods for selecting proposal densities are illustrated using various detailed examples.

Key words and phrases: Bayes factor, central limit theorem, Markov chain, marginal likelihood, polynomial ergodicity, reverse logistic regression.

1. Introduction

Importance sampling (IS) is a popular Monte Carlo procedure where samples from one distribution are weighted to estimate features of other distributions. Here, we consider IS in the context of the following problem. Let $\Pi$ be the family of target densities on the space $X$ with respect to a measure $\mu$ where $\pi(x) = \nu(x)/\theta \in \Pi$. Here, $\nu(x)$ is known, but the normalizing constant $\theta = \int_X \nu(x) \mu(dx)$ is unknown. Let $f$ be a $\pi$-integrable, real-valued function defined on $X$ for all $\pi \in \Pi$. There are two goals. The first goal is to estimate the normalizing constants $\theta$ up to a constant of proportionality for all $\pi \in \Pi$. The second goal is to estimate the integrals $E_\pi f := \int_X f(x) \pi(x) \mu(dx)$ for all $\pi \in \Pi$. Estimation of normalizing constants plays an important role in both frequentist and Bayesian inference, as well as in other areas, like statistical physics. In Bayesian statistics, the ratio of normalizing constants for two different posteriors is the Bayes factor, which is at the core of Bayesian hypothesis testing and model selection.
The empirical Bayes estimate corresponds to the value of a hyper parameter where the normalizing constant (marginal likelihood) attains its maximum (Doss, 2010; Roy et al., 2016). In latent variable models e.g. generalized linear mixed models, the ratio of the normalizing constants is the likelihood ratio for hypothesis testing (Christensen, 2004). The normalizing constants also need to be estimated in the problems involving intractable likelihoods, e.g., exponential random graph models and autologistic models (Geyer and Thompson, 1992). Similarly, in statistical physics, an important problem is the estimation of some normalizing constants known as the partition function. On the other hand, estimation of (posterior) means of certain functions \( f \) as the posterior density varies is the key issue of Bayesian sensitivity analysis (Buta and Doss, 2011). In Bayesian penalized regression methods, plotting regularization paths boils down to estimating means of regression coefficients as the penalty parameters vary (Roy and Chakraborty, 2017).

The two objectives mentioned above can be accomplished using naive importance sampling. Let \( q_1(x) = \varphi_1(x)/c_1 \) be another density on \( X \) with respect to \( \mu \) such that we are able to generate samples from \( q_1 \), and \( \nu(x) = 0 \) whenever \( \varphi_1(x) = 0 \). Indeed, if \( \{X_i\}_{i=1}^n \) is either independent and identically distributed (iid) samples from \( q_1 \) or a positive Harris recurrent Markov chain
with invariant density $q_1$, then the naive IS estimator is consistent, that is,

$$\frac{1}{n} \sum_{i=1}^{n} \frac{\nu(X_i)}{\varphi_1(X_i)} \xrightarrow{a.s.} \int \frac{\nu(x)}{\varphi_1(x)} q_1(x) \mu(dx) = \frac{\theta}{c_1} \int \frac{\nu(x) / \theta}{\varphi_1(x) / c_1} q_1(x) \mu(dx) = \frac{\theta}{c_1}.$$  \hfill (1.1)

Similarly, $E_{\pi} f$ can be estimated by the ratio of $(1/n) \sum_{i=1}^{n} [f(X_i) \nu(X_i) / \varphi_1(X_i)]$ and the estimator in (1.1). These naive IS estimators suffer from high variance when the target probability density function (pdf) $\pi$ is not ‘close’ to the proposal pdf $q_1$ (Geyer, 2011) because, in that case, the ratio $\nu(X_i) / \varphi_1(X_i)$ takes arbitrarily large values for some samples $X_i$’s.

To alleviate this issue, samples from multiple proposals, properly weighted, can be used, as done in the variants of multiple importance sampling (Veach and Guibas, 1995; Owen and Zhou, 2000; Elvira et al., 2019), umbrella sampling (Geyer, 2011; Doss, 2010), parallel, serial or simulated tempering (George and Doss, 2018; Geyer and Thompson, 1995; Marinari and Parisi, 1992). In IS estimation based on multiple proposal densities, the single density $q_1$ is generally replaced with a linear combination of $k$ densities (Geyer, 2011). In particular, let $q_i(x) = \varphi_i(x) / c_i$, for $i = 1, \ldots, k$, be $k$ densities from the set of potential proposal densities $Q \equiv \{q(x) = \varphi(x) / c\}$, where the $\varphi_i$’s are known but the $c_i$’s may be unknown. Let $a = (a_1, \ldots, a_k)$ be a vector of $k$ positive constants such that $\sum_{i=1}^{k} a_i = 1$, $q \equiv \sum_{i=1}^{k} a_i q_i$, $d_i = c_i / c_1$ for $i = 1, 2, \ldots, k$ with $d_1 = 1$, and $d \equiv (c_2 / c_1, \ldots, c_k / c_1)$. For
$l = 1, \ldots, k$, let $\{X_{i}^{(l)}\}_{i=1}^{n_l}$ be either iid samples from $q_l$ or a positive Harris recurrent Markov chain with invariant density $q_l$. Then as $n_l \to \infty, \forall l$,

$$
\hat{u} \equiv \sum_{l=1}^{k} a_l \sum_{i=1}^{n_l} \frac{\nu(X_{i}^{(l)})}{\sum_{j=1}^{k} a_j \varphi_j(X_{i}^{(l)})/d_j} \xrightarrow{a.s.} \sum_{l=1}^{k} a_l \int_X \frac{\nu(x)}{\sum_{j=1}^{k} a_j \varphi_j(x)/d_j} q_l(x) \mu(dx) \tag{1.2}
$$

Similarly, $E_{\pi} f$ is estimated by $\hat{\eta}[f] \equiv \hat{v}[f]/\hat{u}$ where

$$
\hat{v}[f] := \sum_{l=1}^{k} a_l \sum_{i=1}^{n_l} \frac{f(X_{i}^{(l)}) \nu(X_{i}^{(l)})}{\sum_{j=1}^{k} a_j \varphi_j(X_{i}^{(l)})/d_j}.
$$

Estimation using (1.2) has been considered in several articles (see, e.g., Gill et al., 1988; Kong et al., 2003; Meng and Wong, 1996; Tan, 2004; Vardi, 1985; Buta and Doss, 2011; Geyer, 1994; Tan et al., 2015). There are alternative weighting schemes proposed in the literature, e.g., the population Monte Carlo of Cappé et al. (2004), although none is as widely applicable as (1.2). If the normalizing constants $c_i$’s are known, the estimator (1.2) resembles the balance heuristic estimator of Veach and Guibas (1995), which is discussed in Owen and Zhou (2000) as the deterministic mixture. On the other hand, in several applications of IS methods, $d$ in (1.2) is unknown, which is the case when $Q = \Pi$, that is, when samples from a subset of densities of $\Pi$ are used to estimate the normalizing constants for the entire family via (1.2). Routine applications of IS estimation with $Q = \Pi$ can be
found in Monte Carlo maximum likelihood estimation, Bayesian sensitivity
analysis and model selection (Geyer and Thompson, 1992; Buta and Doss,
2011; Doss, 2010). If $d$ is unknown, Doss (2010) proposed a two-stage
method, where in the first step, using samples from $q_i, i = 1, \ldots, k$, $d$ is
estimated by $\hat{d}$ using Geyer’s (1994) reverse logistic regression estimator or
Meng and Wong’s (1996) bridge sampling method. Then, independent of
step one, new samples are used to calculate (1.2) with $d$ replaced by $\hat{d}$.

The effectiveness of (1.2) depends on the choice of $k$, $a$, $n_l$, and the
importance densities $q = \{q_1, \ldots, q_k\}$. This article focuses on the choice of
the importance densities because it is the most crucial, and the multiple
IS estimator (1.2), just like the naive IS estimator (1.1), is useless if these
densities are ‘off targets’. Although increasing $k$ or $n_l$, may lead to esti-
mators with less variance, it results in higher computational cost, therefore
these are often determined based on the available computational resources.
On the other hand, for fixed $k$, $a$, and $n_l$, efficiency and stability of the
estimator (1.2) can be highly improved by appropriately choosing the $k$
importance densities $q$ from the set $Q$.

This paper is the first where systematic methods of selection of proposal
distributions for IS are developed and tested. We propose three approaches.
(i) Our first approach is based on a geometric spatial design method, called
the space filling (SF) method. In particular, among all subsets \( q \subset Q \) with \(|q| = k\), the one that minimizes the gaps between the elements of \( q \) and those of \( \Pi \) is chosen. The choice of the distance between the elements of \( q \) and \( \Pi \) is crucial, and here we propose the symmetric Kullback-Leibler divergence. (ii) The second approach, called the minimax (MNX) method, chooses \( q \) that minimizes the maximum standard error, or the maximum relative standard error of the estimator \( \hat{u} \) (or \( \hat{\eta}[\ell] \)). (iii) Finally, the third approach is applicable when \( d \) in (1.2) is unknown, and Doss’s (2010) two-stage IS method is used. In this approach, called the maximum entropy (ENT) method, following the maximum entropy criterion of experimental design, \( q \) is chosen by maximizing the determinant of the asymptotic covariance matrix of \( \hat{d} \). We describe and compare these three methods in details in Section 3. Each of the three methods is better suited to different situations. MNX is applicable to any IS estimator for which valid standard errors are available. Implementation of both MNX and ENT needs estimates of asymptotic variances in a central limit theorem. In the absence of such variance estimates, SF can be used. SF does not depend on the form of the particular IS estimator (1.2), thus, the same SF proposal distributions are used for any IS estimator. However, successful implementation of the SF, as shown later, crucially depends on the choice of the metric. Unlike
the MNX design, which depends on the choice of the function $f$, the same SF and ENT proposals work no matter if the goal is to estimate the normalizing constants or the means. Overall, SF is the most straightforward to implement, although SF may not always be ideal, as it is independent of the form of the estimator and the particular estimand of interest, in our experience, with a properly chosen metric, it consistently provides desirable results. The three methods are implemented in the R package geoBayes (Evangelou and Roy, 2022). We illustrate these methods using several detailed examples involving autologistic models, Bayesian regression models and spatial generalized linear mixed models.

Unfortunately, in the literature, there is not much discussion on the choice of the importance densities in multiple IS methods, although given $q$, in the special case when $d$ is known and iid samples are available from the proposals, there are some methods for selecting the weights $a$ (see e.g. Li et al., 2013). One exception is Buta and Doss (2011) who described an ad-hoc method in the important special case of $Q = \Pi$. Buta and Doss (2011) stated that solving the minimax variance design problem, that is, the one that minimizes $\phi(q) = \max_{\pi \in \Pi} \sigma_u^2(\pi; q)$ exactly, where $\sigma_u^2(\pi; q)$ is the asymptotic variance of $\hat{u}$ in (1.2), is ‘hopeless’. Assuming that a consistent estimator $\hat{\sigma}_u^2(\pi; q)$ of $\sigma_u^2(\pi; q)$ is available, Buta and Doss (2011) pro-
posed a procedure where starting from some ‘trial’ proposal pdfs, $\hat{\sigma}^2_u(\pi; q)$ is computed for all $\pi \in \Pi$. Then, proposal densities are either moved to regions of $\Pi$ where $\hat{\sigma}^2_u(\pi; q)$ is large, or new proposal densities from these high variance regions are added increasing $k$. Here, we develop a principled approach, called the sequential method (SEQ), formalizing this procedure and compare its performance with the three proposed methods.

As mentioned above, the MNX and ENT approaches developed here as well as the SEQ method utilize asymptotic standard errors of $\hat{d}$ and $\hat{u}$. Another contribution of this paper is the development of spectral variance (SV) estimators of asymptotic variances for $\hat{d}$ and $\hat{u}$. Availability of consistent estimators is important in its own right as it allows for calculation of asymptotically valid standard errors of the IS estimators. Recently, Roy et al. (2018) provided standard errors estimators of $\hat{d}$ and $\hat{u}$ using the batch means method. In different numerical examples (not shown here), we observe that the proposed SV estimators are generally less variable than the batch means estimators. This observation is in line with Flegal and Jones (2010) who showed that, for estimating means of scalar valued functions, certain SV estimators are less variable than the batch means estimators by a factor of 1.5.

The rest of the paper is organized as follows. In Section 2 we describe
both the multiple IS estimation as well as the reverse logistic regression estimation. The proposed methods of selecting proposal densities for IS estimators are described in Section 3. Some illustrative examples are given in Section 4. Section 5 contains conclusions of the paper. Proofs of theorems and several examples are relegated to the supplementary materials.

2. Multiple IS estimation of normalizing constants and expectations

Recall that \( \Pi = \{ \pi : \pi(x) = \nu(x)/\theta \} \) is a family of target densities on \( X \), and \( f : X \rightarrow \mathbb{R} \) is a function of interest. Given samples \( \Phi_l \equiv \{ X_{i(l)}^{(l)} \}_{i=1}^{n_l}, l = 1, \ldots, k \) from a small number of proposal densities \( \{ q_l = \varphi_l(x)/c_l, l = 1, \ldots, k \} \), one wants to estimate \( \theta \) (or, rather \( \theta/c_1 \)) and \( E_{\pi} f \) for all \( \pi \in \Pi \). Recall that we estimate \( u(\pi, q_1) \equiv \theta/c_1 \) and \( E_{\pi} f \) by \( \hat{u}(d) \equiv \hat{u}(\pi; d) \) defined in (1.2) and \( \hat{\eta}^{[f]} \equiv \hat{\eta}^{[f]}(\pi; d) \), respectively. We also consider the more general setting when \( d \) is unknown, which is the case if \( Q = \Pi \). In such situations, we use the two-stage IS procedure of Doss (2010), where first, \( d \) is estimated using Geyer’s (1994) reverse logistic regression method (described in Section 2.1) based on Markov chain samples \( \tilde{\Phi}_l \equiv \{ \tilde{X}_{i(l)}^{(l)} \}_{i=1}^{N_l} \) with stationary density \( q_l \), for \( l = 1, \ldots, k \). Once \( \hat{d} \) is formed, independent of stage 1, new samples \( \Phi_l \equiv \{ X_{i(l)}^{(l)} \}_{i=1}^{n_l}, l = 1, \ldots, k \) are obtained to estimate \( u(\pi, q_1) \) and \( E_{\pi} f \) by \( \hat{u}(\hat{d}) \) and \( \hat{\eta}^{[f]}(\pi; \hat{d}) \), respectively. Buta and Doss (2011) quantify
2.1 Reverse logistic regression estimator of $d$

Let $N = \sum_{l=1}^{k} N_l$ and $a_l \in [0,1]$ for $l = 1, \ldots, k$ such that $\sum_{l=1}^{k} a_l = 1$. Define

$$
\zeta_l = -\log(c_l) + \log(a_l), \quad l = 1, \ldots, k,
$$

(2.3)

and

$$
p_l(x, \zeta) = \frac{\varphi_l(x)e^{\zeta_l}}{\sum_{s=1}^{k} \varphi_s(x)e^{\zeta_s}}, \quad l = 1, \ldots, k,
$$

(2.4)

where $\zeta = (\zeta_1, \ldots, \zeta_k)$. (Note that, if $a_l = N_l/N$, given that $x$ belongs to the pooled sample $\{\tilde{X}_i^{(l)}, i = 1, \ldots, N_l, l = 1, \ldots, k\}$, $p_l(x, \zeta)$ is the probability that $x$ comes from the $l$th distribution.) Following Doss and Tan (2014), consider the log quasi-likelihood function

$$
\ell_N(\zeta) = \sum_{l=1}^{k} a_l \frac{N_l}{N} \sum_{i=1}^{N_l} \log(p_l(\tilde{X}_i^{(l)}, \zeta)).
$$

(2.5)

Note that adding the same constant to all $\zeta_l$’s leaves (2.5) invariant. Let $\zeta^0 \in \mathbb{R}^k$ denote the true $\zeta$ normalized to add to zero, that is, $\zeta^0_l = \zeta_l - \left(\sum_{j=1}^{k} \zeta_j\right)/k$. Here, $\zeta_l$ denotes the $l$th element of $\zeta$. Note that the function $g: \mathbb{R}^k \rightarrow \mathbb{R}^{k-1}$ that maps $\zeta^0$ into $d$ is given by $g(\zeta) = (e^{\zeta_1-\zeta_2}a_2/a_1, e^{\zeta_1-\zeta_3}a_3/a_1, \ldots, e^{\zeta_1-\zeta_k}a_k/a_1)^\top$. We estimate $\zeta^0$ by $\hat{\zeta}$, where

$$
\hat{\zeta} = \arg\max \ell_N(\zeta) \text{ subject to } \sum_{j=1}^{k} \zeta_j = 0,
$$
and thus, obtain $\hat{d} = g(\hat{\zeta})$.

3. Selection of proposal distributions

In this section we propose three criteria for selecting the proposal distributions $q = \{q_1, \ldots, q_k\} \subset Q$ for efficient use of the multiple IS estimators. For $q \subset Q$, the proposed criterion is generally denoted by $\phi(q)$ and the optimal set is obtained by:

$$\text{Minimize } \phi(q) \text{ over } q \subset Q.$$  

We consider the case where the set $Q$ corresponds to a family of densities parameterized by $\xi \in \Xi$, thus searching over $Q$ is equivalent to searching over $\Xi$. The variable $\xi$ can be multidimensional and the range of $\xi$, in every direction, can be infinite. Thus, for computational purposes, it may be required to narrow down the potential region of search, depending on the application. Evangelou and Roy (2019) considered the problem of maximizing (1.2) with respect to $\xi$, which, as mentioned in the Introduction, is the situation in empirical Bayes methods, so they used Laplace approximations to identify the region where the maximizer may lie. Thus, using Laplace approximations, as in Evangelou and Roy (2019), we can narrow $\Xi$ down to a search set $\tilde{\Xi}$. In Section S10 of the supplement, we demonstrate an alternative approach to choosing $\tilde{\Xi}$ using preliminary samples.
3.1 Space filling approach

Solving the minimization problem is a research problem in its own right. We implemented two algorithms for searching over ˜Ξ, the point-swapping algorithm of Royle and Nychka (1998), and a simulated annealing algorithm. Details about these algorithms are given in Section S7 of the supplementary materials. The point-swapping algorithm generally requires more iterations, so it is more suited to cases where the design criterion \( \phi \) can be computed quickly after a swap, as is often the case for the SF method.

3.1 Space filling approach

In this method, among all subsets \( q = \{q_1, \ldots, q_k\} \) of \( Q \), the one that minimizes the gaps between the elements of \( q \) and the elements of \( \Pi \) is chosen. For \( \pi \in \Pi, q \in Q \), let \( \Upsilon(\pi, q) \) be a suitably chosen metric. Define

\[
\psi_p(q, \pi) = \left( \sum_{q \in q} \Upsilon(\pi, q)^p \right)^{1/p},
\]

as a measure of ‘closeness’ of \( q \) to \( \pi \). Note that, for \( p < 0, \psi_p(q, \pi) \to 0 \) if \( \pi \) is let to converge to a point in \( q \). The design criterion is to choose \( q \) to minimize

\[
\phi_{SF}(q) = \Psi_{p, \tilde{p}}(q) = \left( \sum_{\pi \in \Pi} \psi_p(q, \pi)^{\tilde{p}} \right)^{1/\tilde{p}}
\]

over all subsets \( q \) with \( |q| = k \). In the limit \( (p \to -\infty, \tilde{p} \to \infty) \), \( \Psi_{p, \tilde{p}} \) is related to the minimax design. However, as Royle and Nychka (1998) illustrate, keeping \( p \) and \( \tilde{p} \) finite allows us to quickly evaluate \( \phi \) after a
3.1 Space filling approach

swap of the point-swapping algorithm. We use $p = -30$, $\tilde{p} = 30$ in our examples, which allows us to obtain a near-minimax SF design.

The choice of the metric $\Upsilon(\pi, q)$ is crucial. For instance, in the binomial robit model with degrees of freedom parameter $\xi$ (see the example in Section S8 of the supplemental materials), the family of target densities $\Pi \equiv \{\pi_\xi(x) = \nu_\xi(x)/\theta_\xi : \xi \in \Xi\}$ is indexed by the Student’s $t$ degrees of freedom parameter $\xi$. Here, the relevant geometry (with respect to $\xi$) in $\mathbb{R}$ is not Euclidean. Indeed, degrees of freedom $\xi = 10^2$ and $10^3$ are close, but $\xi = 0.5$ and $\xi = 1$ are not. Thus, the SF based on the Euclidean distance metric (SFE) may not be appropriate unless the indexing variable is a location parameter. The Euclidean distance is also sensitive to reparameterizations of the family of proposal distributions. Another choice is the information metric (Kass, 1989; Rao, 1982) which measures the distance between two parametric distributions using asymptotic standard deviation units of the best estimator. The Kullback-Leibler divergence generates the information number through the information metric (Ghosh et al., 2007). In practice, it may be difficult to implement the information metric although it seems to be appropriate for the context. Here, we use the symmetric Kullback-Leibler divergence (SKLD) although it is not a metric, and
3.1 Space filling approach

denote the corresponding method by SFS. Thus,

\[ \Upsilon(\pi, q) = \int_X \pi(x) \log \frac{\nu(x)}{\varphi(x)} \mu(dx) - \int_X q(x) \log \frac{\nu(x)}{\varphi(x)} \mu(dx). \] (3.6)

In the special case when \( \Pi \equiv \{ \pi_\xi(x) = \nu_\xi(x)/c_\xi: \xi \in \Xi \} \), that is, the target family is indexed by some variable \( \xi \), and \( Q = \Pi \), the SKLD between \( \pi_{\xi_1}(x) \) and \( \pi_{\xi_2}(x) \), is

\[ \Upsilon(\xi_1, \xi_2) = \int_X \pi_{\xi_1}(x) \log \frac{\nu_{\xi_1}(x)}{\nu_{\xi_2}(x)} \mu(dx) - \int_X \pi_{\xi_2}(x) \log \frac{\nu_{\xi_1}(x)}{\nu_{\xi_2}(x)} \mu(dx) \] (3.7a)
\[ = \frac{\int_X \nu_{\xi_1}(x) \log \frac{\nu_{\xi_1}(x)}{\nu_{\xi_2}(x)} \mu(dx)}{\int_X \nu_{\xi_1}(x) \mu(dx)} - \frac{\int_X \nu_{\xi_2}(x) \log \frac{\nu_{\xi_1}(x)}{\nu_{\xi_2}(x)} \mu(dx)}{\int_X \nu_{\xi_2}(x) \mu(dx)}. \] (3.7b)

The SKLD (3.6) is generally not available in closed form. We use a modified Laplace method \cite{Evangelou et al., 2011} to approximate (3.7b), and we describe the method in Section S1. The second order approximation described in the supplement is exact when \( \pi_{\xi_1} \) and \( \pi_{\xi_2} \) are any two Gaussian densities. If \( X \) is discrete, or the target distributions are far from Gaussian, a Monte Carlo estimate of (3.7a) can be used with samples from \( \pi_{\xi_1} \) and \( \pi_{\xi_2} \). Indeed, for some examples considered here, we use the Monte Carlo estimate of (3.7a) to implement SFS.

The SF method does not involve the form of any particular IS estimator. When \( Q = \Pi \), the uniform (with respect to the chosen metric) selection of the proposal distributions attempts to guarantee that each target density is close to at least one proposal distribution. Also, the SF method is
3.2 Minimax approach

Our second method is the minimax (MNX) design based on minimizing the maximum SE or relative SE of \( \hat{u}(\pi, \hat{d}) \) or \( \hat{\eta}[f](\pi; \hat{d}) \) over \( \pi \in \Pi \). Consistency and asymptotic normality of \( \hat{d}, \hat{u}(\pi; \hat{d}) \) and \( \hat{\eta}[f](\pi; \hat{d}) \) are described in Theorems 1, 2 and 3, respectively of Roy et al. (2018). Let \( \sigma^2_u(\pi, q) \) denote the asymptotic variance of \( \hat{u}(\pi, \hat{d}) \) when the set of proposal densities is \( q \subset Q \). Then, the standard error is \( \sigma_{u}(\pi, q)/\sqrt{n} \), where \( n = \sum_{l=1}^{k} n_l \). The minimax approach chooses \( q \) to minimize the largest standard error or the relative standard error, given, respectively by

\[
\phi_{\text{MNX}}(q) = \max_{\pi \in \Pi} \sigma_{u}(\pi, q)/\sqrt{n}, \quad \text{and} \quad \phi_{\text{MNX}}(q) = \max_{\pi \in \Pi} \sigma_{u}(\pi, q)/\{\sqrt{n}\hat{u}(\pi, \hat{d})\}.
\]

Similar measures can be derived in the case of \( \hat{\eta}[f](\pi; \hat{d}) \) with variance \( \sigma^2_\eta(\pi, q) \). In the following, we discuss estimation of the asymptotic variances \( \sigma^2_u(\pi, q) \) and \( \sigma^2_\eta(\pi, q) \) of these estimators. Note that the ratios of the normalizing constants \( (\theta/c_1) \) can take large values as \( \pi \) varies in \( \Pi \), especially when \( X \) is multi-dimensional. The standard errors corresponding to the distributions with large ratios tend to be larger, whereas these standard errors for the distributions with small (relative) normalizing constants can potentially be large relative to the value of the estimates. Thus, if the goal is
3.2 Minimax approach

to estimate the parameters corresponding to largest normalizing constants
(as in the empirical Bayes methods, see e.g. Roy et al. (2016)), then the
first criterion can be used, on the other hand, if one wants to estimate θ
for all π ∈ Π, then the second criterion (relative standard error) may be
preferred.

Spectral variance estimation in reverse logistic regression and
multiple IS methods: First, we provide an SV estimator of the asymp-
totic covariance matrix of \( \hat{d} \), as it is needed for the asymptotic variances
of \( \hat{u}(\pi; \hat{d}) \) and \( \hat{\eta}[^{[l]}](\pi; \hat{d}) \). Also, SV estimator of \( \text{Var}(\hat{d}) \) is important in its
own right, and is used in Section 3.3 in our third approach to selection of
proposal distributions.

As in Roy et al. (2018), we assume that the Markov chains \( \Phi_l, \tilde{\Phi}_l \) are
polynomially ergodic for \( l = 1, \ldots, k \). (The definition of polynomial ergodic-
ity of Markov chains can be found in Roy et al. (2018).) They showed that
if the Markov chain \( \tilde{\Phi}_l \) is polynomially ergodic of order \( t > 1 \) for \( l = 1, \ldots, k \),
then \( \hat{\zeta} \) and \( \hat{d} \) defined in section 2.1 are consistent and asymptotically nor-
mal as \( N_1, \ldots, N_k \to \infty \), that is, there exist matrices \( B, \Omega \in \mathbb{R}^{k,k} \) and
\( D \in \mathbb{R}^{k,k-1} \) such that

\[
\sqrt{N}(\hat{\zeta} - \zeta) \xrightarrow{d} \mathcal{N}(0, U) \quad \text{and} \quad \sqrt{N}(\hat{d} - d) \xrightarrow{d} \mathcal{N}(0, V),
\]

where \( U = B^\dagger \Omega B^\dagger \) and \( V = D^\dagger UD \). Here, for a square matrix \( C, C^\dagger \)
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denotes its Moore-Penrose inverse. The matrices \(B\), \(\Omega\) and \(D\) are as defined in (2.7), (2.8), and (2.5) respectively in Roy et al. (2018). Theorem 1 below provides consistent SV estimators of the asymptotic variances of \(\hat{\zeta}\) and \(\hat{d}\).

We now introduce some notations. Assume \(N_l \to \infty\) such that \(\lim N_l/N \in (0, 1)\) for \(l = 1, \ldots, k\). Recall that \(\hat{d} = g(\hat{\zeta})\), and its gradient at \(\hat{\zeta}\) (in terms of \(\hat{d}\)) is

\[
\hat{D} = \begin{pmatrix}
\hat{d}_2 & \hat{d}_3 & \ldots & \hat{d}_k \\
-\hat{d}_2 & 0 & \ldots & 0 \\
0 & -\hat{d}_3 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & -\hat{d}_k
\end{pmatrix}
\]

As in Roy et al. (2018), the \(k \times k\) matrix \(\hat{B}\) is defined by

\[
\hat{B}_{rr} = \sum_{l=1}^{k} a_l \left( \frac{1}{N_l} \sum_{i=1}^{N_l} p_r(\tilde{X}_i^{(l)}, \hat{\zeta}) \left[ 1 - p_r(\tilde{X}_i^{(l)}, \hat{\zeta}) \right] \right) \quad \text{and}
\]

\[
\hat{B}_{rs} = -\sum_{l=1}^{k} a_l \left( \frac{1}{N_l} \sum_{i=1}^{N_l} p_r(\tilde{X}_i^{(l)}, \hat{\zeta}) p_s(\tilde{X}_i^{(l)}, \hat{\zeta}) \right) \quad \text{for } r \neq s,
\]

that is, \(\hat{B}\) denotes the matrix of second derivatives of \(-\ell_N(\zeta)/N\) evaluated at \(\hat{\zeta}\), where \(\ell_N(\zeta)\) is defined in (2.5). Set \(Z_i^{(l)} = \left( p_1(\tilde{X}_i^{(l)}, \hat{\zeta}), \ldots, p_k(\tilde{X}_i^{(l)}, \hat{\zeta}) \right)^\top\) for \(i = 1, \ldots, N_l\) and \(Z^{(l)} = \sum_{i=1}^{N_l} Z_i^{(l)}/N_l\). Define the lag \(j\) sample autocovariance as

\[
\gamma_N^{(l)}(j) = \frac{1}{N_l} \sum_{i \in S_{j,N}} \left[ Z_i^{(l)} - Z^{(l)} \right] \left[ Z_{i+j}^{(l)} - Z^{(l)} \right]^\top \quad \text{for } l = 1, \ldots, k.
\]
where $S_{j,N} = \{1, \ldots, N - j\}$ for $j \geq 0$ and $S_{j,N} = \{(1 - j), \ldots, N\}$ for $j < 0$. Let

$$\hat{\Sigma}^{(l)} = \sum_{j=-(b_{N_l}-1)}^{b_{N_l}-1} w_{N_l}(j) \gamma_N^{(l)}(j),$$

(3.11)

where $w_{N_l}(\cdot)$ is the lag window, $b_{N_l}$'s are the truncation points for $l = 1, \ldots, k$. Finally, define

$$\hat{\Omega} = \sum_{l=1}^{k} \frac{N}{N_l} a_l^2 \hat{\Sigma}^{(l)}.$$  

(3.12)

**Theorem 1.** Assume that the Markov chains $\tilde{\Phi}_1, \ldots, \tilde{\Phi}_k$ are polynomially ergodic of order $t > 1$, and for all $l = 1, \ldots, k$, $w_{N_l}$ and $b_{N_l}$ satisfy conditions 1-4 in Vats et al. (2018, Theorem 2). Let $\hat{D}$, $\hat{B}$ and $\hat{\Omega}$ be the matrices defined by (3.8), (3.9) and (3.12), respectively. Then, as $N_l \to \infty$ for all $l = 1, \ldots, k$, $\hat{U} := \hat{B}^\top \hat{\Omega} \hat{B}^\top$ and $\hat{V} := \hat{D}^\top \hat{U} \hat{D}$ converge almost surely to $U$ and $V$, respectively.

Next, we consider estimation of the asymptotic variances of $\hat{u}(\pi; \hat{d})$ and $\hat{\eta}^{[f]}(\pi; \hat{d})$. Roy et al. (2018) showed that, under certain conditions, there exist $\sigma_u^2, \sigma_\eta^2 > 0$ such that, as $n_1, \ldots, n_k \to \infty$,

$$\sqrt{n}(\hat{u}(\pi; \hat{d}) - u(\pi, q_1)) \xrightarrow{d} N(0, \sigma_u^2) \quad \text{and} \quad \sqrt{n}(\hat{\eta}^{[f]}(\pi; \hat{d}) - E_{\pi} f) \xrightarrow{d} N(0, \sigma_\eta^2).$$

(3.13)

In Theorem 2 we provide consistent SV estimators of $\sigma_u^2$ and $\sigma_\eta^2$. We first
introduce some notations. Let

\[ u^\pi(x; \mathbf{d}) := \frac{\nu(x)}{\sum_{s=1}^{k} a_s \varphi_s(x)/d_s} \quad \text{and} \quad v^{[j]:\pi}(x; \mathbf{d}) := f(x)u^\pi(x; \mathbf{d}). \quad (3.14) \]

Define the vectors \( c(\pi; \mathbf{d}) \) and \( e(\pi; \mathbf{d}) \) of length \( k-1 \) with \((j-1)\)th coordinate as

\[ [c(\pi; \mathbf{d})]_{j-1} = \frac{u(\pi, q_1)}{d_j^2} \int x \frac{a_j \varphi_j(x)}{\sum_{s=1}^{k} a_s \varphi_s(x)/d_s} \pi(x) \mu(dx) \quad (3.15) \]

\[ [e(\pi; \mathbf{d})]_{j-1} = \frac{a_j}{d_j^2} \int [f(x) - E_x f] \varphi_j(x) \pi(x) \mu(dx), \quad (3.16) \]

for \( j = 2, \ldots, k \), and their estimators \( \hat{c}(\pi; \mathbf{d}) \) and \( \hat{e}(\pi; \mathbf{d}) \) as

\[ [\hat{c}(\pi; \mathbf{d})]_{j-1} = \sum_{l=1}^{k} \frac{1}{n_l} \sum_{i=1}^{n_l} \frac{a_j a_l \nu(X_i^{(l)}) \varphi_j(X_i^{(l)})}{(\sum_{s=1}^{k} a_s \varphi_s(X_i^{(l)})/d_s)^2 d_j^2}, \]

\[ [\hat{e}(\pi; \mathbf{d})]_{j-1} = \frac{\sum_{l=1}^{k} \frac{a_l f(X_i^{(l)}) v(X_i^{(l)}) \varphi_j(X_i^{(l)})}{d_j^2 (\sum_{s=1}^{k} a_s \varphi_s(X_i^{(l)})/d_s)^2}}{\hat{\nu}(\pi; \mathbf{d})} - \frac{[\hat{c}(\pi; \mathbf{d})]_{j-1} \hat{v}^{[j]}(\pi; \mathbf{d})}{\hat{\nu}(\pi; \mathbf{d})}. \quad (3.18) \]

Suppose \( b_n \)'s are the truncation points, \( w_n(j) \)'s are lag window, \( u_i \equiv u_i(\mathbf{d}) \equiv u^\pi(X_i^{(l)}; \mathbf{d}) \), \( v_i^{[j]} \equiv v_i^{[j]}(\mathbf{d}) \equiv v^{[j]:\pi}(X_i^{(l)}; \mathbf{d}) \), and \( \bar{u} \equiv \bar{u}(\mathbf{d}) \), \( \bar{v}^{[j]} \equiv \bar{v}^{[j]}(\mathbf{d}) \) are the averages of \( \{u^\pi(X_1^{(l)}; \mathbf{d}), \ldots, u^\pi(X_n^{(l)}; \mathbf{d})\} \) and \( \{v^{[j]:\pi}(X_1^{(l)}; \mathbf{d}), \ldots, v^{[j]:\pi}(X_n^{(l)}; \mathbf{d})\} \), respectively. (Note that, abusing notations, the dependence on \( l \) is ignored in \( u_i, v_i^{[j]}, \bar{u} \) and \( \bar{v}^{[j]} \).) Let

\[ \hat{\tau}_i^2(\pi; \mathbf{d}) = \frac{1}{n_l} \sum_{j=-(b_n-1)}^{b_n-1} w_n(j) \sum_{i \in S_j,n} [u_i - \bar{u}] [u_{i+j} - \bar{u}], \quad (3.19) \]
3.2 Minimax approach

\[ \tilde{\Gamma}_{l}(\pi; \mathbf{d}) = \frac{1}{n_{l}} \sum_{j=-(b_{n_{l}}-1)}^{b_{n_{l}}-1} w_{n_{l}}(j) \sum_{i \in S_{n_{l}} \pi} \left[ \left( \begin{array}{c} v_{i}^{[f]} \\ u_{i} \end{array} \right) - \left( \begin{array}{c} \bar{v}^{[f]} \\ \bar{u} \end{array} \right) \right] \left[ \left( \begin{array}{c} v_{i+j}^{[f]} \\ u_{i+j} \end{array} \right) - \left( \begin{array}{c} \bar{v}^{[f]} \\ \bar{u} \end{array} \right) \right]^{\top}. \]

Finally, let \( \hat{\tau}^{2}(\pi; \mathbf{d}) = \sum_{l=1}^{k} (a_{l}^{2} n_{l}/n_{l}) \hat{\tau}^{2}_{l}(\pi; \mathbf{d}), \tilde{\Gamma}(\pi; \mathbf{d}) = \sum_{l=1}^{k} (a_{l}^{2} n_{l}/n_{l}) \tilde{\Gamma}_{l}(\pi; \mathbf{d}), \)

and

\[ \hat{\rho}(\pi; \mathbf{d}) = \nabla h(\tilde{v}_{l}^{[f]}(\pi; \mathbf{d}), \tilde{u}(\mathbf{d}))^{\top} \tilde{\Gamma}(\pi; \mathbf{d}) \nabla h(\tilde{v}_{l}^{[f]}(\pi; \mathbf{d}), \tilde{u}(\mathbf{d})), \]

where \( \nabla h(x, y) = (1/y, -x/y^{2})^{\top}. \)

**Theorem 2.** Suppose that for \( \tilde{\Phi}_{l}, l = 1, \ldots, k, \) conditions of Theorem 1 hold and \( \tilde{V} \) is the consistent SV estimator of \( V. \) Suppose that \( N_{l}, n_{l} \to \infty \) for all \( l = 1, \ldots, k, \) and there exists \( \varpi \in [0, \infty) \) such that \( n/N \to \varpi. \) In addition, let \( n_{l}/n \to s_{l} \in (0, 1) \) for \( l = 1, \cdots, k. \) Assume that the Markov chains \( \Phi_{1}, \ldots, \Phi_{k} \) are polynomially ergodic of order \( t \geq (1 + \epsilon)(1 + 2/\delta) \) for some \( \epsilon, \delta > 0 \) such that \( E_{q_{l}}|u_{l}^{[f]}(X; \mathbf{d})|^{4+\delta} < \infty, \) and for each \( l = 1, \cdots, k, \)

\( w_{n_{l}} \) and \( b_{n_{l}} \) satisfy conditions 1-4 in Vats et al. (2018, Theorem 2).

(a) Then \( \hat{\sigma}_{u}^{2} = (n/N)\hat{c}(\pi; \mathbf{d})^{\top} \hat{V} \hat{c}(\pi; \mathbf{d}) + \hat{\tau}^{2}(\pi; \mathbf{d}) \) converges almost surely to \( \sigma_{u}^{2}. \)

(b) In addition, suppose that \( E_{q_{l}}|v_{l}^{[f]}(X; \mathbf{d})|^{4+\delta} < \infty. \) Then \( \hat{\sigma}_{\eta}^{2} = (n/N)\hat{c}(\pi; \mathbf{d})^{\top} \hat{V} \hat{c}(\pi; \mathbf{d}) + \hat{\rho}(\pi; \mathbf{d}) \)

converges almost surely to \( \sigma_{\eta}^{2}. \)

The estimators \( \hat{V} \) as well as \( \hat{\sigma}_{u}^{2} \) and \( \hat{\sigma}_{\eta}^{2} \) are implemented in the R package geoBayes (Evangelou and Roy, 2022). Since samples are obtained by
running the Markov chains with the stationary densities in $q$, we denote
the corresponding reverse logistic regression estimator of $d \equiv d_q$ by $\hat{d}_q$ and
its asymptotic variance as $V_q$. Similarly, in this case, we denote the SV
estimators of the asymptotic variances (3.13) of $\hat{u}(\pi; \hat{d}_q)$ and $\hat{\eta}^{[f]}(\pi; \hat{d}_q)$ as
$\hat{\sigma}_u^2(\pi; q)$ and $\hat{\sigma}_\eta^2(\pi; q)$, respectively.

When $Q = \Pi$, a less computationally demanding approach is the SEQ
method in which densities are chosen sequentially from $\Pi$ where $\hat{\sigma}_u^2(\pi; q)$ is
the largest. Specifically, starting with an initial density $q_1 = \{\bar{q}\}$, suppose
that we have completed the $i$th step with the set $q_i$ chosen along with
(Markov chain) samples from each density in $q_i$. If $d$ is unknown, part
of this sample (stage 1) is used for calculating the estimator $\hat{d}$, and the
remaining sample is used to compute $\hat{\sigma}_u^2(\pi; q_i)$ for the remaining densities
$\pi \in \Pi \setminus q_i$. Then $q_{i+1} = q_i \cup \{\pi_j\}$ where $\pi_j = \arg\max_{\pi \in \Pi \setminus q_i} \hat{\sigma}_u^2(\pi; q_i)$,
and the existing (Markov chain) sample is augmented with samples from
$\pi_j$. Thus, at each step, the density corresponding to the largest (estimated)
asymptotic variance is chosen. The process is repeated until $k$ densities
have been selected. The initial $\bar{q}$ can be the density where the multiple IS
estimator (1.2) or any other interesting quantity based on samples from a
preliminary SF set is maximized (see Section S10 of the supplement for an
example).
3.3 Maximum entropy approach

The third method uses maximum entropy sampling (Shewry and Wynn, 1987) for selecting \(q\). This method is applicable when \(d\) is unknown and is developed in the context of Doss’s (2010) two-stage IS estimation scheme described before. We use the notation \(\text{Ent}(\cdot)\) to denote the Boltzmann-Shannon entropy of the random variable inside the brackets. The maximum entropy (ENT) approach chooses \(q\) that minimizes

\[
\phi_{\text{ENT}}(q) = -\text{Ent}(\hat{d}_q).
\]

This is interpreted as sampling those elements of \(Q\) that carry the most uncertainty in \(\hat{d}_q\). As we show below, since \(\hat{d}_q\) is used in the calculation of both \(\hat{u}\) and \(\hat{\eta}^{[f]}\), the optimal \(q\) will cause (asymptotically) lower uncertainty in those estimators. Note that since \(\hat{d}_q\) depends on the reference density \(q_1\), it is assumed that \(q_1\) remains fixed, which can be the density \(\tilde{q}\) discussed in Section 3.2. In the following, we assume that the objective is to estimate ratios of normalizing constants. In the supplementary materials, we derive similar results under the objective of estimating means \(E_{\pi}f\).

To derive a formula for \(\text{Ent}(\hat{d}_q)\) we require the asymptotic joint distribution of \(\hat{d}_q\) with \(\hat{u}\) over \(\Pi\). Let \(\hat{u}(\pi; \hat{d}_q)\) be the vector of length \(|\Pi|\) consisting of \(\hat{u}(\pi; \hat{d}_q)\)'s, \(\pi \in \Pi\) in a (any) fixed order. Indeed, we refer to this fixed ordering whenever we write \(\Pi\) in this section. Similarly define
the vector of true (ratios of) normalizing constants \( u(\pi, q_1) \). Let \( C(\pi; d_q) \) be the \(|\Pi| \times (k-1)\) matrix with rows \( c(\pi; d_q) \) (defined in (3.13)), \( \pi \in \Pi \). Similarly, define \( \hat{C}(\pi; d_q) \) with rows \( \hat{c}(\pi; d_q) \) (defined in (3.17)), \( \pi \in \Pi \). Let \( u^\pi(x; d_q) \) be the \(|\Pi|\) dimensional vector consisting of \( u^\pi(x; d_q) \)'s defined in (3.14). Let \( T_l(d_q) \) be the \(|\Pi| \times |\Pi|\) matrix with elements

\[
\tau_l^2(\pi, \pi'; d_q) = \text{Cov}_{q_l}(u^\pi(X_1^{(l)}; d_q), u^{\pi'}(X_1^{(l)}; d_q))
\]

\[
+ \sum_{g=1}^{\infty} \text{Cov}_{q_l}(u^\pi(X_1^{(l)}; d_q), u^{\pi'}(X_1^{(l+g)}; d_q)) + \sum_{g=1}^{\infty} \text{Cov}_{q_l}(u^\pi(X_{1+g}^{(l)}; d_q), u^{\pi'}(X_1^{(l)}; d_q)).
\]

Finally, let

\[
\hat{T}_l(d_q) = \frac{1}{n_l} \sum_{j=-(b_n-1)}^{b_n-1} w_n(j) \sum_{i \in S_{j,n}} \left[ u^\pi(X_i^{(l)}; d_q) - \bar{u}(d_q) \right] \left[ u^{\pi'}(X_{i+j}^{(l)}; d_q) - \bar{u}(d_q) \right]^\top,
\]

where \( b_n \)'s are the truncation points, \( w_n(j) \)'s are the lag windows, and

\[
\bar{u}(d_q) = \sum_{i=1}^{n_l} u^\pi(X_i^{(l)}; d_q) / n_l.
\]

**Theorem 3.** Suppose that \( N_l, n_l \to \infty \) for all \( l = 1, \ldots, k \), and there exists \( \varpi \in [0, \infty) \) such that \( n/N \to \varpi \). In addition, let \( n_l/n \to s_l \in (0, 1) \) for \( l = 1, \ldots, k \).

(a) Assume that the stage 1 Markov chains \( \tilde{\Phi}_l, l = 1, \ldots, k \) are polynomially ergodic of order \( t > 1 \). Further, assume that the stage 2 Markov chains \( \Phi_l, l = 1, \ldots, k \) are polynomially ergodic of order \( t \), and for some \( \delta > 0 \)

\[
E_{q_l}|u^\pi(X; d_q)|^{2+\delta} < \infty \text{ for each } \pi \in \Pi \text{ and } l = 1, \ldots, k
\]
where \( t > 1 + 2/\delta \). Then as \( n_1, \ldots, n_k \to \infty \),

\[
\sqrt{n} \begin{pmatrix} \hat{d}_q - d_q \\ \hat{u}(\pi; \hat{d}_q) - u(\pi, q_1) \end{pmatrix} \xrightarrow{d} N \left( 0, \begin{pmatrix} \varpi V_q & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} \right),
\]

where \( \Sigma_{21} = \varpi C(\pi; d_q)V_q \), \( \Sigma_{12} = \Sigma_{21}^\top \), and \( \Sigma_{22} = \varpi C(\pi; d_q)V_qC(\pi; d_q)^\top + \sum_{l=1}^k (a_l^2/s_l)T_l(d_q) \).

(b) Suppose that the conditions of Theorem 1 hold for the stage 1 Markov chains. Let \( \hat{V}_q \) be the consistent estimator of \( V_q \) given in Theorem 1. Assume that the Markov chains \( \Phi_l, l = 1, \ldots, k \) are polynomially ergodic of order \( t \geq (1 + \epsilon)(1 + 2/\delta) \) for some \( \epsilon, \delta > 0 \) such that \( E_q \|u^\pi(X; d_q)\|^{4 + \delta} < \infty \), (\( \| \cdot \| \) denotes the Euclidean norm) for all \( l = 1, \ldots, k \), and \( w_{n_l} \) and \( b_{n_l} \) satisfy conditions 1-4 in Vats et al. (2018, Theorem 2). Then \( (n/N)\tilde{C}(\pi; \hat{d}_q)\hat{V}_q\tilde{C}(\pi; \hat{d}_q)^\top + \sum_{l=1}^k (a_l^2/s_l)\tilde{T}_l(\hat{d}_q) \) and \( (n/N)\tilde{C}(\pi; \hat{d}_q)\hat{V}_q \) converges almost surely to \( \Sigma_{22} \) and \( \Sigma_{21} \), respectively.

Let \( Y \equiv (Y^T_q, Y^T_{q1})^T \) be a random vector having the normal distribution in (3.22). The Boltzmann-Shannon entropy of \( Y \) is \( \text{Ent}(Y) = \text{constant} + \frac{1}{2} \log \det(\Sigma) \), where \( \Sigma \) is the covariance matrix of \( Y \). Note that

\[
\log \det(\Sigma) = \log \det(\varpi V_q) + \log \det(\Sigma_{22} - \varpi C(\pi; d_q)V_qC(\pi; d_q)^\top),
\]

where the second matrix on the right side is the covariance matrix of the
3.3 Maximum entropy approach

conditional distribution of $Y_{\Pi}|Y_q$. Since Theorem 3 (b) provides a consistent estimator of this conditional covariance matrix, we can minimize the determinant of this estimator matrix to choose $q$.

As mentioned in Shewry and Wynn (1987), great computational benefit can be achieved by converting this conditional problem to an unconditional problem. In particular, as noted in Shewry and Wynn (1987), minimization of the second term is equivalent to maximization of $\log \det(V_q)$. In practice, we would replace $V_q$ by its estimator given in Theorem 1, i.e. $\hat{V}_q$, using Markov chain samples from densities in $q$. In this case, the ENT criterion simplifies to

$$\phi_{ENT}(q) = -\log \det(\hat{V}_q).$$

Unlike the SF, MNX and SEQ methods, the ENT approach is applicable only in the context of Doss’s (2010) two-stage IS estimation scheme. In contrast, if the multiple IS estimator (1.2) is used, since ENT avoids the second stage IS estimation, it needs fewer samples than the MNX and SEQ methods which require enough samples to be used for both stages. Also, ENT avoids computing the target un-normalized densities $\nu$ for $\pi \in \Pi$. However, one advantage of the MNX and SEQ methods is that at the end of the procedure, we already have available samples from densities in $q$ which can be used in the two-stage IS estimation scheme.
4. Examples

**Autologistic model:** Consider the popular autologistic models (Besag, 1974), which are Markov random field models for binary observations. Let $s_i$ denote the $i$th spatial location, and let $\text{nb}_i \equiv \{s_j : s_j \text{ is a neighbor of } s_i\}$ denote the neighborhood set of $s_i, i = 1, \ldots, m$. Markov random field models for $x = \{x(s_i), i = 1, \ldots, m\}$ are formulated by specifying the conditional probabilities $p_i = P(x(s_i) = 1|\{x(s_j) : j \neq i\}) = P(x(s_i) = 1|\{x(s_j) : s_j \in \text{nb}_i\}), i = 1, \ldots, m$. For simplicity, we impose that all neighborhoods have the same size $w = |\text{nb}_i|, i = 1, \ldots, m$. We consider a centered parameterization (Kaiser et al., 2012) given by $\logit(p_i) = \logit(\kappa) + (\gamma/w) \sum_{s_j \in \text{nb}_i} (x(s_j) - \kappa)$, where $\logit(z) = \log(z/[1 - z])$, $\gamma$ is a dependence parameter, and $\kappa$ is the probability of observing one in the absence of statistical dependence. Jointly, the probability mass function (pmf) $\pi(x|\gamma, \kappa)$ of $x$ is given by (see Section S9.1 of the supplementary materials)

$$\pi(x|\gamma, \kappa) \propto \exp \left\{ (\logit(\kappa) - \gamma \kappa) \sum_{i=1}^{m} x(s_i) + \frac{\gamma}{2w} \sum_{i=1}^{m} \sum_{s_j \in \text{nb}_i} x(s_i)x(s_j) \right\}.$$  

The normalizing constant $\theta = \theta(\gamma, \kappa)$ in $\pi(x|\gamma, \kappa)$ is intractable when $\gamma \neq 0$. Sherman et al. (2006) mention that ‘there is no known simple way to approximate this normalizing constant’. Here, we use multiple IS for estimating $\theta$ and then estimate $\xi = (\gamma, \kappa)$ by maximum likelihood method.
We consider a $10 \times 10$ square lattice on a torus, with four-nearest (east-west, north-south) neighborhood structure with the family of autologistic pmfs $\Pi = \{\pi(x|\gamma,\kappa) : \gamma = -4, -3.2, \ldots, 4, \kappa = 0.1, 0.2, \ldots, 0.9\}$. The family of importance densities $Q = \Pi$ in this case, therefore, choosing the importance densities amounts to choosing the parameters $\xi$. We want to choose $k = 5$ densities from $Q$, i.e, $k$ different $\xi$ values, one of which must be $\xi_1 = (0, 0.5)$. We apply the multiple IS based on proposal densities from the five methods, namely, SFE, SFS, MNX, SEQ, and ENT, as well as the naive IS method NIS. MNX and SEQ are based on the relative standard error criterion. Computation of the SFS, MNX, SEQ, and ENT criteria is based on 20,000 stage 1 and 20,000 stage 2 samples produced from each candidate density via Gibbs sampling (except for the case $\gamma = 0$ where independent sampling was used), after a burn in of 4,000 each time. For the computation of the SV estimator we used the Tukey-Hanning window (see Section S9.2). We observe that SEQ chooses a skeleton set on the boundary of the search space for $(\gamma, \kappa)$, while SFS, MNX, and ENT choose some points close to the boundary (see Section S9.2).

To test the performance of the different methods when used to estimate the parameters $\xi$, we simulate from the model for different choices of $\xi$ as shown in Table I and then estimate these parameters using the maximum
likelihood method. As the likelihood is intractable, $\theta(\gamma, \kappa)/\theta(0, 0.5)$ is estimated via (1.2) with the proposal densities derived from each method. To that end, we took 10,000 samples from each density after a burn in of 1,000. For NIS we took 50,000 samples. We generated 125 realisations (data) for each choice of $(\gamma, \kappa)$ parameters. We observed that some realized data resulted in an unbounded likelihood for some methods. NIS was most affected with 39% of the realized values resulting in an unbounded likelihood followed by SEQ with 11% and ENT with 8%. Table 1 shows the root mean squared error for estimating $\gamma$ excluding the cases with unbounded likelihood for each method. The results show that the multiple IS methods perform significantly better than NIS. Between the multiple IS methods, we note that SEQ has in general worse performance than MNX and SFE is worse than SFS. The root mean squared error for estimating $\kappa$ does not show significant differences across the multiple IS methods so it is not shown, although we observed that NIS performed worse. Further comparisons and computational details are given in Section S9.2 in the supplementary materials.
| $\kappa$ | $\gamma$ | NIS  | SFE  | SFS  | MNX  | SEQ  | ENT  |
|---------|---------|------|------|------|------|------|------|
| 0.2     | -1      | 7.55 | 3.68 | 4.14 | 4.62 | 5.19 | 3.65 |
| 0.2     | 1       | 10.91| 3.63 | 1.67 | 1.67 | 1.74 | 1.69 |
| 0.3     | -2      | 8.75 | 1.38 | 1.61 | 1.60 | 9.42 | 1.37 |
| 0.3     | 2       | 5.13 | 1.17 | 1.19 | 1.18 | 1.21 | 1.18 |
| 0.4     | -3      | 4.51 | 5.36 | 1.59 | 1.52 | 9.55 | 1.63 |
| 0.4     | 3       | 3.76 | 1.11 | 1.12 | 1.11 | 1.18 | 1.11 |
| 0.5     | -4      | 10.69| 5.65 | 1.20 | 1.15 | 10.13| 3.61 |
| 0.5     | 4       | 4.83 | 1.04 | 1.04 | 1.03 | 1.06 | 1.02 |
| 0.6     | -3      | 6.71 | 1.33 | 1.21 | 1.22 | 6.16 | 7.59 |
| 0.6     | 3       | 3.65 | 1.12 | 1.12 | 1.12 | 1.22 | 1.12 |
| 0.7     | -2      | 9.62 | 1.62 | 1.93 | 1.79 | 1.80 | 5.97 |
| 0.7     | 2       | 6.09 | 1.27 | 1.27 | 1.26 | 1.35 | 1.48 |
| 0.8     | -1      | 14.84| 5.37 | 4.52 | 3.64 | 4.38 | 5.88 |
| 0.8     | 1       | 11.88| 2.14 | 1.96 | 1.94 | 2.06 | 2.40 |

Table 1: Root mean squared error for estimating $\gamma$ in the autologistic example.

**Bayesian negative binomial regression:** We consider a Bayesian negative binomial regression model with response variable $y_i$, $i = 1, \ldots, 21$,
generated independently from the negative binomial distribution with size parameter $\xi$ and mean for $y_i$, $\mu_i = \exp(\beta_0 + \beta_1 \times w_i)$, $w_i = -1 + 0.1 \times (i - 1)$. Here, $x = (\beta_0, \beta_1)$ are unknown parameters, assigned a bivariate normal prior with mean 0 and covariance matrix $10(W^T W)^{-1}$, where $W$ denotes the design matrix. As $\xi \to \infty$, the negative binomial distribution converges to the Poisson distribution. Let the family of target densities $\Pi$ be the posterior densities for $x$ for $\xi \in (0, \infty]$. Here, $\xi = \infty$ corresponds to the Poisson model. We wish to compute the logarithm of Bayes factor $b_\xi = \log(\theta_\xi / \theta_\infty)$, where $\theta_\xi$ denotes the unknown normalizing constant of the posterior density. The Bayes factor can be used to decide between the models for given data. We estimate $b_\xi$ by multiple IS using (1.2), with the proposal densities chosen from $\Pi$, i.e. $Q = \Pi$, one of which must correspond to $\xi = \infty$ and two more densities chosen from $\hat{\Xi} = \{1, 2, \ldots, 40\}$, i.e., $k = 3$. The choice of the proposal densities for MNX and SEQ are based on the relative standard error of the multiple IS estimator of $\exp(b_\xi)$. For comparison, we also consider the naive IS (NIS) method with proposal at $\xi = \infty$.

We generate data from four models with $\xi = 0.5, 1, 2, \infty$ and $(\beta_0, \beta_1) = (1, 0.5)$, 400 times from each model. For each data set we compute the skeleton set for the 5 criteria: SFE, SFS, MNX, SEQ, and ENT. We
used $N_l = n_l = 3,600$ Monte-Carlo samples from the $l$th proposal, after a burn in of 1,000, $l = 1, 2, 3$, for computing the spectral variance estimates, and the SKLD was also computed using the same samples. The Monte-Carlo algorithm was implemented using the R package rstan (Stan Development Team, 2020). After the skeleton set for each method and data set is found, we generate additional 5,000 Monte Carlo samples from each proposal, discard the first 1,000, and use the remaining 4,000 to compute the estimator of $b_{\xi}$ for all $\xi \in \tilde{\Xi}$ via (1.2). For NIS we used 12,000 samples in total from the proposal density. Alternatively, $\theta_{\xi}$ can be computed by numerical integration. For this, we use the Gauss-Kronrod method as implemented in the R package pracma (Borchers, 2021) with relative error set to $10^{-6}$, from where we can compute $b_{\xi}$. We treat the estimates obtained by numerical integration as the golden standard and compare each IS estimate against it. As the models are very similar for large values of $\xi$, our comparison concentrates in the range $\xi = 1, \ldots, 10$. The average root mean squared difference between the IS estimate of $b_{\xi}$ for each method and the one obtained via numerical integration for the 400 simulations and over $\xi = 1, \ldots, 10$ are given in Table 2. The results show that generally MNX and ENT have better performance than SEQ, both for estimating the Bayes factor and the regression coefficient and that SFS
is better than SFE. NIS performs significantly worse than the multiple IS methods.

|      | 0.5   | 1     | 2     | ∞      |
|------|-------|-------|-------|--------|
| NIS  | 1214.640 | 716.045 | 383.153 | 129.079 |
| SFE  | 2.916  | 2.698  | 2.080  | 2.172  |
| SFS  | 2.337  | 2.343  | 1.712  | 1.850  |
| MNX  | 2.222  | 2.161  | 1.594  | 1.806  |
| SEQ  | 2.293  | 2.307  | 1.745  | 1.810  |
| ENT  | 2.266  | 2.140  | 1.626  | 1.774  |

Table 2: Average root mean squared difference between the estimates obtained by IS and the values obtained via numerical integration for \( b_\xi \). The table shows the original values multiplied by 100.

5. Discussions

We consider situations where one is simultaneously interested in large number of target distributions, as in model selection and sensitivity analysis examples. Multiple IS estimators are particularly useful in this context, however, the choice of proposal distributions for these estimators has not received much attention in the literature. We provide three systematic techniques for addressing this issue. The first method, based on a geomet-
ric space filling criterion, and the second method, based on the minimax asymptotic standard error, can be used for any multiple IS estimators. The third, maximum entropy method, is designed for the two-stage multiple IS estimators of Doss (2010). We compare the performance of these three methods in several examples. Our results show that careful choice of the proposal densities, as produced by our methods, results in more accurate estimates.

The proposed minimax and entropy methods use asymptotic standard errors for the multiple IS and the reverse logistic regression estimators, respectively. We construct consistent SV estimators for these standard errors. These estimators are important in their own right as they are valuable for assessing the quality of the multiple IS estimators and the reverse logistic regression estimator.
S1. A modified Laplace approximation for Kullback-Leibler divergence

In this section, we describe a modified Laplace approximation for the symmetric Kullback-Leibler divergence (SKLD) defined in the paper. Let $X = \mathbb{R}^r$, for some $r \geq 1$, and $\mu$ be the Lebesgue measure. Consider the SKLD between two densities $\pi_{\xi_1}(x) = \nu_{\xi_1}(x)/c_{\xi_1}$ and $\pi_{\xi_2}(x) = \nu_{\xi_2}(x)/c_{\xi_2}$, with the assumption $\log \nu_{\xi_i}(x) = O(M)$ for some $M, i = 1, 2$. Note that

$$
\Upsilon(\xi_1, \xi_2) = \frac{M \int_X J(x) \exp(G(x)) \mu(dx)}{\int_X \exp(G(x)) \mu(dx)} - \frac{M \int_X J(x) \exp(H(x)) \mu(dx)}{\int_X \exp(H(x)) \mu(dx)},
$$

(S1.1)

where $G(x) = \log \nu_{\xi_1}(x)$, $H(x) = \log \nu_{\xi_2}(x)$, and $J(x) = (G(x) - H(x))/M$.

We apply Laplace approximation on each integral in (S1.1) separately. Specifically, we expand the integrals in the first term around $\hat{x} = \arg\max_{x \in X} G(x)$ and the integrals in the second term around $\tilde{x} = \arg\max_{x \in X} H(x)$. Let $\hat{J}$ and $\tilde{J}$ denote $J$ evaluated at $\hat{x}$ and $\tilde{x}$ respectively. We denote $\hat{G}_i = \frac{\partial}{\partial x_i} G(x)|_{x=\hat{x}}$ and similarly $\hat{G}_{ij}$ for second order partial derivatives and so on. We also denote $\hat{G}^{-1}_{ij}$ to be the $(i, j)$th element of the inverse of the matrix with elements $\hat{G}_{ij}$'s. Then by an application of (17) from Evangelou et al. (2011),

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we have
\[
\int_X J(x) \exp(G(x)) \mu(dx) \approx \hat{J} + \frac{1}{2} \hat{J}_{i_1} \hat{G}_{i_2i_3i_4} \hat{G}_{i_1i_2}^{-1} \hat{G}_{i_3i_4}^{-1} - \frac{1}{2} \hat{J}_{i_1i_2} \hat{G}_{i_1i_2}^{-1}
\]
with an implicit summation \(i_1, \ldots, i_4 \in \{1, \ldots, r\}\). A similar approximation is derived for the second term:
\[
\int_X J(x) \exp(H(x)) \mu(dx) \approx \tilde{J} + \frac{1}{2} \tilde{J}_{i_1} \tilde{H}_{i_2i_3i_4} \tilde{H}_{i_1i_2}^{-1} \tilde{H}_{i_3i_4}^{-1} - \frac{1}{2} \tilde{J}_{i_1i_2} \tilde{H}_{i_1i_2}^{-1}.
\]
The first order approximation to \(\text{SKLD}(\xi_1, \xi_2)\) is \(M(\hat{J} - \tilde{J})\), which may be sufficient, but not if \(\hat{x} = \tilde{x}\). Note that, the second order approximation is exact for two Gaussian densities.

**S2. Proof of Theorem 1**

From Roy et al. (2018), we only need to show \(\hat{\Omega} \xrightarrow{a.s.} \Omega\) where the SV estimator \(\hat{\Omega}\) is defined in (3.12) and the \(k \times k\) matrix \(\Omega\), following Roy et al. (2018), is defined through
\[
\Omega_{rs} = \sum_{l=1}^{k} \frac{a_l^2}{s_l} \left[ E_{q_l} \{Y_1^{(r,l)} Y_1^{(s,l)}\} + \sum_{i=1}^{\infty} E_{q_l} \{Y_1^{(r,l)} Y_{1+i}^{(s,l)}\} + \sum_{i=1}^{\infty} E_{q_l} \{Y_{1+i}^{(r,l)} Y_{1}^{(s,l)}\} \right],
\]
for \(r, s = 1, \ldots, k\); where, \(N_l/N \to \tilde{s}_l\) and for \(r, l = 1, \ldots, k\),
\[
Y_i^{(r,l)} \equiv p_r(\tilde{X}_i^{(l)}, \zeta^0) - E_{q_l}(p_r(X, \zeta^0)), \quad i = 1, \ldots, N_l.
\]
As in Roy et al. (2018), this will be proved in couple of steps. First, we consider a single chain \(\tilde{\Phi}_l\) used to calculate \(k\) quantities. We use the results in
Vats et al. (2018) who obtain conditions for the multivariate SV estimator to be strongly consistent. Second, we combine results from the \( k \) independent chains. Finally, we show that \( \hat{\Omega} \) is a strongly consistent estimator of \( \Omega \).

Denote \( \bar{Y}^{(l)} = (\bar{Y}^{(1,l)}, \bar{Y}^{(2,l)}, \ldots, \bar{Y}^{(k,l)})^\top \) where \( \bar{Y}^{(r,l)} = \frac{\sum_{i=1}^{N_l} Y_i^{(r,l)}}{N_l} \). From Roy et al. (2018) we have \( \sqrt{N_l} \bar{Y}^{(l)} \xrightarrow{d} \mathcal{N}(0, \Sigma^{(l)}) \) as \( N_l \to \infty \), where \( \Sigma^{(l)} \) is a \( k \times k \) covariance matrix with
\[
\Sigma^{(l)}_{rs} = E_{q_l} \{ Y_1^{(r,l)} Y_1^{(s,l)} \} + \sum_{i=1}^{\infty} E_{q_l} \{ Y_1^{(r,l)} Y_{1+i}^{(s,l)} \} + \sum_{i=1}^{\infty} E_{q_l} \{ Y_{1+i}^{(r,l)} Y_1^{(s,l)} \}. \tag{S2.2}
\]

The SV estimator of \( \Sigma^{(l)} \) is given in (3.11). We now prove the strong consistency of \( \hat{\Sigma}^{(l)} \). Note that \( \hat{\Sigma}^{(l)} \) is defined using the terms \( \bar{Z}^{(l)}_i \)'s which involve the random quantity \( \hat{\zeta} \). We define \( \hat{\Sigma}^{(l)}(\zeta^0) \) to be \( \hat{\Sigma}^{(l)} \) with \( \zeta^0 \) substituted for \( \hat{\zeta} \), that is,
\[
\hat{\Sigma}^{(l)}(\zeta^0) = \frac{1}{N_l} \sum_{j=-b_{N_l}-1}^{b_{N_l}-1} w_{N_l}(j) \sum_{i \in S_{l,N}} \left[ Y_i^{(l)} - \bar{Y}^{(l)} \right] \left[ Y_{i+j}^{(l)} - \bar{Y}^{(l)} \right]^\top \text{ for } l = 1, \ldots, k,
\]
where \( Y_i^{(l)} = (Y_i^{(1,l)}, \ldots, Y_i^{(k,l)})^\top \). We prove \( \hat{\Sigma}^{(l)} \xrightarrow{a.s.} \Sigma^{(l)} \) in two steps:
(1) \( \hat{\Sigma}^{(l)}(\zeta^0) \xrightarrow{a.s.} \Sigma^{(l)} \) and (2) \( \hat{\Sigma}^{(l)} - \hat{\Sigma}^{(l)}(\zeta^0) \xrightarrow{a.s.} 0 \). Under the conditions of Theorem 1, it follows from Vats et al. (2018) that \( \hat{\Sigma}^{(l)}(\zeta^0) \xrightarrow{a.s.} \Sigma^{(l)} \) as \( N_l \to \infty \). We show \( \hat{\Sigma}^{(l)}_{rs} - \hat{\Sigma}^{(l)}_{rs}(\zeta^0) \xrightarrow{a.s.} 0 \) where \( \hat{\Sigma}^{(l)}_{rs} \) and \( \hat{\Sigma}^{(l)}_{rs}(\zeta^0) \) are the \((r, s)\)th elements of the \( k \times k \) matrices \( \hat{\Sigma}^{(l)}_{rs} \) and \( \hat{\Sigma}^{(l)}_{rs}(\zeta^0) \) respectively. By the mean value theorem (in multiple variables), there exists \( \zeta^* = t\hat{\zeta} + (1-t)\zeta^0 \)
for some $t \in (0, 1)$, such that
\[
\hat{\Sigma}^{(l)}_{rs} - \hat{\Sigma}^{(l)}_{rs}(\zeta^0) = \nabla \hat{\Sigma}^{(l)}_{rs}(\zeta^*) \cdot (\hat{\zeta} - \zeta^0), \tag{S2.3}
\]
where $\cdot$ represents the dot product. Note that
\[
\hat{\Sigma}^{(l)}_{rs}(\zeta) = \frac{1}{N_l} \sum_{j=-(b_{N_l}-1)}^{b_{N_l}-1} w_{N_l}(j) \sum_i \left[ Z^{(r,l)}_i(\zeta) - \bar{Z}^{(r,l)}(\zeta) \right] \left[ Z^{(s,l)}_{i+j}(\zeta) - \bar{Z}^{(s,l)}(\zeta) \right],
\]
where $Z^{(r,l)}_i(\zeta) := p_r(\tilde{X}^{(l)}_i, \zeta)$ and $\bar{Z}^{(r,l)}(\zeta) := \sum_{j=1}^{N_l} p_r(\tilde{X}^{(l)}_j, \zeta)/N_l$. Some calculations show that for $t \neq r$
\[
\frac{\partial Z^{(r,l)}_j(\zeta)}{\partial \zeta_t} = -p_r(\tilde{X}^{(l)}_j, \zeta)p_r(\tilde{X}^{(l)}_j, \zeta)
\]
and
\[
\frac{\partial Z^{(r,l)}_j(\zeta)}{\partial \zeta_r} = p_r(\tilde{X}^{(l)}_j, \zeta)(1 - p_r(\tilde{X}^{(l)}_j, \zeta)).
\]
Simplifying the notations, we denote $U^{(r,t)}_j := \partial Z^{(r,l)}_j(\zeta)/\partial \zeta_t$, $\bar{U}^r := \partial \bar{Z}^{(r,l)}(\zeta)/\partial \zeta_t$
and simply write $Z^{(r,l)}_j$ and $\bar{Z}^{(r,l)}$ for $Z^{(r,l)}_j(\zeta)$ and $\bar{Z}^{(r,l)}(\zeta)$ respectively. Thus we have
\[
\frac{\partial \hat{\Sigma}^{(l)}_{rs}(\zeta)}{\partial \zeta_t} = \frac{1}{N_l} \sum_{j=-(b_{N_l}-1)}^{b_{N_l}-1} w_{N_l}(j) \sum_i \left[ (Z^{(r,l)}_i - \bar{Z}^{(r,l)})(U^{(s,t)}_{i+j} - \bar{U}^{(s,t)}) + (U^{(r,t)}_i - \bar{U}^{(r,t)})(Z^{(s,l)}_{i+j} - \bar{Z}^{(s,l)}) \right]
\]
\[
= \frac{1}{N_l} \sum_{j=-(b_{N_l}-1)}^{b_{N_l}-1} w_{N_l}(j) \sum_i \left[ (Z^{(r,l)}_i - \bar{Z}^{(r,l)})(U^{(s,t)}_{i+j} - \bar{U}^{(s,t)}) \right] \tag{S2.4}
\]
\[
+ \frac{1}{N_l} \sum_{j=-(b_{N_l}-1)}^{b_{N_l}-1} w_{N_l}(j) \sum_i \left[ (U^{(r,t)}_i - \bar{U}^{(r,t)})(Z^{(s,l)}_{i+j} - \bar{Z}^{(s,l)}) \right], \tag{S2.5}
\]
Let $V_i^{(l)} := (Z_i^{(r,l)}, U_i^{(s,t)})^T$ and
\[
\hat{\Sigma}_V^{(l)}(\zeta) = \frac{1}{N_l} \sum_{j=-b_N-1}^{b_N-1} w_{N_l}(j) \sum_i \left[ V_i^{(l)} - \bar{V}^{(l)} \right] \left[ V_{i+j}^{(l)} - \bar{V}^{(l)} \right]^T.
\]

Since $p_r(X, \zeta)$ is uniformly bounded by 1 and $\hat{\Phi}_l$ is polynomially ergodic of order $m > 1$, from Vats et al. (2018) we know that
\[
\hat{\Sigma}_V^{(l)}(\zeta) \xrightarrow{\text{a.s.}} \Sigma_V^{(l)}(\zeta)
\]
where $\Sigma_V^{(l)}(\zeta)$ is the covariance matrix of the asymptotic distribution of $\sqrt{N_l}(\bar{V}^{(l)} - E_q V)$. Since the expression in (S2.4) is the off-diagonal elements of $\hat{\Sigma}_V^{(l)}(\zeta)$, it is bounded with probability one. We can similarly see that the expression in (S2.5) is bounded with probability one. Note that, the proof to show that $\partial \hat{\Sigma}_V^{(l)}(\zeta) / \partial \zeta_t$ is bounded with probability one is quite different from the proof in Roy et al. (2018).

Note that the terms $Z_i^{(r,l)}, U_i^{(s,t)}$, etc., above actually depends on $\zeta$, and we are indeed concerned with the case where $\zeta$ takes on the value $\zeta^*$, lying between $\hat{\zeta}$ and $\zeta^0$. Since, $\hat{\zeta} \xrightarrow{\text{a.s.}} \zeta^0$, we have $\zeta^* \xrightarrow{\text{a.s.}} \zeta^0$ as $N_l \to \infty$. Let $\|u\|_{L_1}$ denotes the $L_1$ norm of a vector $u \in \mathbb{R}^k$. So from (S2.3), and the fact that $\partial \hat{\Sigma}_V^{(l)}(\zeta) / \partial \zeta_t$ is bounded with probability one, we have
\[
|\hat{\Sigma}_{rs}^{(l)} - \hat{\Sigma}_{rs}^{(l)}(\zeta^0)| \leq \max_{1 \leq i \leq k} \left\{ \left| \frac{\partial \hat{\Sigma}_{rs}^{(l)}(\zeta^*)}{\partial \zeta_t} \right| \right\} \| \hat{\zeta} - \zeta^0 \|_{L_1} \xrightarrow{\text{a.s.}} 0 \text{ as } n \to \infty.
\]

Let
\[
\hat{\Sigma} = \begin{pmatrix}
\hat{\Sigma}^{(1)} & 0 \\
0 & \hat{\Sigma}^{(k)}
\end{pmatrix}.
\]
Since \( \hat{\Sigma}^{(l)} \xrightarrow{a.s.} \Sigma^{(l)} \), for \( l = 1, \ldots, k \), it follows that \( \hat{\Sigma} \xrightarrow{a.s.} \Sigma \) where \( \Sigma \) is the corresponding \( k^2 \times k^2 \) covariance matrix, that is, \( \Sigma \) is a block diagonal matrix as \( \hat{\Sigma} \) with \( \Sigma^{(l)} \) substituted for \( \hat{\Sigma}^{(l)} \), \( l = 1, \ldots, k \). Define the following \( k \times k \) matrix
\[
A_N = \begin{pmatrix}
-\sqrt{\frac{N}{N_1}} a_1 I_k & -\sqrt{\frac{N}{N_2}} a_2 I_k & \cdots & -\sqrt{\frac{N}{N_k}} a_k I_k
\end{pmatrix},
\]
where \( I_k \) denotes the \( k \times k \) identity matrix. Then we have \( \hat{\Omega} \equiv A_N \hat{\Sigma} A_N^T \xrightarrow{a.s.} \Omega \) as \( N \to \infty \).

### S3. Proof of Theorem 2 (a)

From Roy et al. (2018) we know that \( \sigma^2_u = \varphi c(\pi; \hat{d})^\top V c(\pi; \hat{d}) + \tau^2(\pi; \hat{d}) \), where \( \tau^2(\pi; \hat{d}) = \sum_{i=1}^{k} (a_i^2 / s_i) \tau_i^2(\pi; \hat{d}) \), and
\[
\tau_i^2(\pi; \hat{d}) = \text{Var}_{q_i}(u^\pi(X_i^{(l)}; \hat{d})) + 2 \sum_{g=1}^{\infty} \text{Cov}_{q_i}(u^\pi(X_i^{(l)}; \hat{d}), u^\pi(X_{1+g}^{(l)}; \hat{d})).
\]

To prove Theorem 2 (a), note that, we already have a consistent SV estimator \( \hat{V} \) of \( V \). From Roy et al. (2018) it follows that \( \hat{c}(\pi; \hat{d})^\top \hat{V} c(\pi; \hat{d}) \xrightarrow{a.s.} c(\pi; \hat{d})^\top V c(\pi; \hat{d}) \).

We now show \( \hat{\tau}_i^2(\pi; \hat{d}) \) is a consistent estimator of \( \tau_i^2(\pi; \hat{d}) \) where \( \hat{\tau}_i^2 \) is defined in (3.19). Since the Markov chains \( \{X_i^{(l)}\}_{i=1}^{n_l}, l = 1, \ldots, k \) are independent, it then follows that \( \tau^2(\pi; \hat{d}) \) is consistently estimated by \( \hat{\tau}_i^2(\pi; \hat{d}) \) completing the proof of Theorem 2 (a).
If \( \mathbf{d} \) is known from the assumptions of Theorem 2 and the results in Vats et al. (2018), we know that \( \hat{\tau}_l^2(\pi; \mathbf{d}) \) is consistently estimated by its SV estimator \( \hat{\tau}_l^2(\pi; \mathbf{d}) \). Note that, \( \hat{\tau}_l^2(\pi; \mathbf{d}) \) is defined in terms of the quantities \( u^\pi(X_i^{(l)}; \mathbf{d})'s \). We now show that \( \hat{\tau}_l^2(\pi; \hat{\mathbf{d}}) - \hat{\tau}_l^2(\pi; \mathbf{d}) \xrightarrow{a.s.} 0 \).

Let \( \partial U^m_i(z) := \frac{\partial u_i(z)}{\partial z_m} = \frac{a_m}{z_m^2} \frac{\nu(X_i^{(l)})\varphi_m(X_i^{(l)})}{\left( \sum_s a_s \varphi_s(X_i^{(l)})/z_s \right)^2} \), and \( \bar{\partial U}^m(z) \) be the averages of \( \{ \partial U^m_i(z), i = 1, \ldots, n_l \} \). Denoting \( \hat{\tau}_l^2(\pi; \mathbf{z}) \) by \( G(z) \), by the mean value theorem (in multiple variables), there exists \( \mathbf{d}^* = t\hat{\mathbf{d}} + (1 - t)\mathbf{d} \) for some \( t \in (0, 1) \), such that \( G(\hat{\mathbf{d}}) - G(\mathbf{d}) = \nabla G(\mathbf{d}^*) \cdot (\hat{\mathbf{d}} - \mathbf{d}) \). For any \( m \in \{ 2, \ldots, k \} \), and \( z \in \mathbb{R}^{k-1} \),

\[
\frac{\partial G(z)}{\partial z_m} = \sum_{j=-(b_m-1)}^{b_m-1} w_{n_l}(j) \sum_i \left[ u_i(z) - \bar{u}(z) \right] \left[ \partial U^m_{i+j}(z) - \bar{\partial U}^m(z) \right] + \sum_{j=-(b_m-1)}^{b_m-1} w_{n_l}(j) \sum_i \left[ \partial U^m_i(z) - \partial U^m(z) \right] \left[ u_{i+j}(z) - \bar{u}(z) \right]
\]

Then using similar arguments as in the proof of Theorem 1, it can be shown that \( \partial G(z)/\partial z_m \) is bounded with probability one. Then it follows that

\[
|G(\hat{\mathbf{d}}) - G(\mathbf{d})| \leq \max_{1 \leq m \leq k-1} \left\{ \left| \frac{\partial G(\mathbf{d}^*)}{\partial z_m} \right| \right\} \| \hat{\mathbf{d}} - \mathbf{d} \|_{L_1} \xrightarrow{a.s.} 0.
\]
S4. Proof of Theorem 2 (b)

From Roy et al. (2018) we know that

\[ \sigma^2 = e(\pi; d)^\top V e(\pi; d) + \rho(\pi; d), \]

where

\[ \rho(\pi; d) = \nabla h \left( E_{\pi} f u(\pi, \pi_1), u(\pi, \pi_1) \right) \nabla h \left( E_{\pi} f u(\pi, \pi_1), u(\pi, \pi_1) \right)^\top, \]

\[ \Gamma(\pi; d) = \sum_{l=1}^k \frac{a_l^2}{s_l} \Gamma_l(\pi; d); \Gamma_l(\pi; d) = \begin{pmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{pmatrix}, \]

with

\[ \gamma_{11} = \gamma_{11}(\pi; d) = \text{Var}_{q_l}(v^{[j], \pi}(X^{(l)}_1; d)) + 2 \sum_{g=1}^{\infty} \text{Cov}_{q_l}(v^{[j], \pi}(X^{(l)}_1; d), v^{[j], \pi}(X^{(l)}_{1+g}; d)), \]

\[ \gamma_{12} = \gamma_{12}(\pi; d) = \gamma_{21} = \gamma_{21}(\pi; d) \]

\[ = \text{Cov}_{q_l}(v^{[j], \pi}(X^{(l)}_1; d), u^{\pi}(X^{(l)}_1; d)) \]

\[ + \sum_{g=1}^{\infty} \left[ \text{Cov}_{q_l}(v^{[j], \pi}(X^{(l)}_1; d), u^{\pi}(X^{(l)}_{1+g}; d)) + \text{Cov}_{q_l}(v^{[j], \pi}(X^{(l)}_{1+g}; d), u^{\pi}(X^{(l)}_1; d)) \right] \]

\[ \gamma_{22} = \gamma_{22}(\pi; d) = \text{Var}_{q_l}(u^{\pi}(X^{(l)}_1; d)) + 2 \sum_{g=1}^{\infty} \text{Cov}_{q_l}(u^{\pi}(X^{(l)}_1; d), u^{\pi}(X^{(l)}_{1+g}; d)). \]

From Roy et al. (2018) we know that \( \hat{e}(\pi; \hat{d})^\top \hat{V} \hat{e}(\pi; \hat{d}) \overset{a.s.}{\rightarrow} e(\pi; d)^\top V e(\pi; d). \)

Thus, to prove Theorem 2 (b), we only need to show that \( \hat{\Gamma}_l(\pi; \hat{d}) \overset{a.s.}{\rightarrow} \)
\[ \Gamma_l(\pi; d). \] Note that,

\[
\hat{\Gamma}_l(\pi; d) = \frac{1}{n_l} \sum_{j=-b_{n_l}}^{b_{n_l}-1} w_{n_l}(j) \sum_{i \in S_{n_l}} \left( \begin{bmatrix} v_i[f] - \bar{v}[f] & v_i[f] - \bar{v}[f] & u_i[j] - \bar{u} \\ v_i[f] - \bar{v}[f] & u_i - \bar{u} & u_i - \bar{u} \\
 & & u_i + j - \bar{u} \end{bmatrix} \right),
\]

\[
= \begin{pmatrix} \hat{\gamma}_{11}^l(\pi; d) & \hat{\gamma}_{12}^l(\pi; d) \\ \hat{\gamma}_{21}^l(\pi; d) & \hat{\gamma}_{22}^l(\pi; d) \end{pmatrix}.
\]

If \( d \) is known, from the assumptions of Theorem 2 (b) and the results in Vats et al. (2018), we know that \( \Gamma_l(\pi; d) \) is consistently estimated by its SV estimator \( \hat{\Gamma}_l(\pi; d) \). We now show that \( \hat{\Gamma}_l(\pi; \hat{d}) - \hat{\Gamma}_l(\pi; d) \overset{a.s.}{\longrightarrow} 0. \)

From Theorem 2 (a), we know that \( \hat{\gamma}_{22}^l(\pi; \hat{d}) - \hat{\gamma}_{22}^l(\pi; d) \overset{a.s.}{\longrightarrow} 0 \) as \( \gamma_{22}^l \) is the same as \( \tau_2^l(\pi; d) \) defined in (S3.6). We now show \( \hat{\gamma}_{11}^l(\pi; \hat{d}) - \hat{\gamma}_{11}^l(\pi; d) \overset{a.s.}{\longrightarrow} 0. \)

Let

\[ \partial V_i^{[f],m}(z) := \frac{\partial V_i^{[f]}(z)}{\partial z_m} = \frac{a_m f(X_i^{(l)}) \nu(X_i^{(l)}) \varphi_m(X_i^{(l)})}{z_m^2 \left( \sum_s a_s \varphi_s(X_i^{(l)}) / z_s \right)^2}, \]

and \( \bar{\partial} V_i^{[f],m}(z) \) be the averages of \( \{ \partial V_i^{[f],m}(z), i = 1, \ldots, n_l \} \).

Letting \( \hat{\gamma}_{11}^l(\pi; z) \) by \( H(z) \), by the mean value theorem, there exists \( d^* = t\hat{d} + (1-t)d \) for some \( t \in (0, 1) \), such that \( H(\hat{d}) - H(d) = \nabla H(d^*) \cdot (\hat{d} - d) \).
For any \( m \in \{2, \ldots, k\} \), and \( z \in R^{+k-1} \),
\[
\frac{\partial H(z)}{\partial z_m} = \sum_{j = -(b_{n_l} - 1)}^{b_{n_l} - 1} w_{n_l}(j) \sum_i \left[ v_i^m(z) - \bar{v}^m(z) \right] \left[ \partial V_{i+j}^m(z) - \bar{\partial V}^m(z) \right] 
+ \sum_{j = -(b_{n_l} - 1)}^{b_{n_l} - 1} w_{n_l}(j) \sum_i \left[ \partial V_{i+j}^m(z) - \bar{\partial V}^m(z) \right] \left[ v_i^m(z) - \bar{v}^m(z) \right]
\]

The rest of the proof is analogous to Theorem 2 (a) and thus we have \( \hat{\gamma}_{l}^{11}(\pi; \hat{d}) - \hat{\gamma}_{l}^{11}(\pi; d) \xrightarrow{a.s.} 0 \). Finally, using similar arguments as before we can show \( \hat{\gamma}_{l}^{12}(\pi; \hat{d}) - \hat{\gamma}_{l}^{12}(\pi; d) \xrightarrow{a.s.} 0 \).

S5. Proof of Theorem 3

Since the Markov chains used in stage 1 are polynomially ergodic of order \( m > 1 \), from Roy et al. (2018, Theorem 1), we have \( N^{1/2}(\hat{d}_q - d_q) \xrightarrow{d} \mathcal{N}(0, V_q) \). Since \( n/N \to r \), it follows that \( \sqrt{n}(\hat{d}_q - d_q) \xrightarrow{d} \mathcal{N}(0, \sigma V_q) \).

Following Roy et al. (2018, Proof of Theorem 2) we write
\[
\sqrt{n}(\hat{u}(\pi; \hat{d}_q) - u(\pi, q_1)) = \sqrt{n}(\hat{u}(\pi; \hat{d}_q) - \hat{u}(\pi; d_q)) + \sqrt{n}(\hat{u}(\pi; d_q) - u(\pi, q_1)).
\]

(S5.7)

Note that the 2nd term involves randomness only from the 2nd stage Markov chains. Since \( \sum_{l=1}^k a_l E_{q_l} u^\pi(X_l; d_q) = u(\pi, q_1) \), we have
\[
\sqrt{n}(\hat{u}(\pi; d_q) - u(\pi, q_1)) = \sum_{l=1}^k a_l \sqrt{n} \sum_{i=1}^n \frac{(u^\pi(X_i^{(l)}; d_q) - E_{q_l} u^\pi(X_l; d_q))}{\sqrt{n_l}}.
\]

Since \( \Phi_t \) is polynomially ergodic of order \( m \) and \( E_{q_l} |u^\pi(X_l; d_q)|^{2+\delta} \) is finite for each \( \pi \in \Pi \) where \( m > 1 + 2/\delta \), it follows that \( \sum_{i=1}^n (u^\pi(X_i^{(l)}; d_q) - \)}
\[ E_q u^\pi(X; d_q)/\sqrt{n_l} \xrightarrow{d} N(0, T_i(d_q)) \] where \( T_i(d_q) \) is the matrix with elements defined in (3.20). As \( n_l/n \to s_l \) and the Markov chains \( \Phi_l \)'s are independent, it follows that \( \sqrt{n}(\hat{u}(\pi; d_q) - u(\pi, q_1)) \xrightarrow{d} N(0, \sum_{l=1}^k (a_l^2/s_l)T_l(d_q)). \)

Next by Taylor series expansion of \( F(d) \equiv \hat{u}(\pi; d) \) about \( d_q \), we have

\[
\sqrt{n}(F(\hat{d}_q) - F(d_q)) = \sqrt{n} \nabla F(d_q)^\top (\hat{d}_q - d_q) + \frac{\sqrt{n}}{2}(\hat{d}_q - d_q)^\top \nabla^2 F(d^*)(\hat{d}_q - d_q),
\]

where \( d^* \) is between \( d_q \) and \( \hat{d}_q \). As in Roy et al. (2018), we can then show that

\[
\sqrt{n}(\hat{u}(\pi; \hat{d}_q) - \hat{u}(\pi; d_q)) = \sqrt{q}c(\pi; d_q)\sqrt{N}(\hat{d}_q - d_q) + o_p(1).
\]

Accumulating the terms for all \( \pi \in \Pi \), we have

\[
\sqrt{n}(\hat{u}(\pi; \hat{d}_q) - \hat{u}(\pi; d_q)) = \sqrt{q}C(\pi; d_q)\sqrt{N}(\hat{d}_q - d_q) + o_p(1).
\]

Thus for constant vectors \( t_1 \) and \( t_2 \) of dimensions \( k - 1 \) and \( |\Pi| \) respectively, we have

\[
t_1^\top \sqrt{n}(\hat{d}_q - d_q) + t_2^\top \sqrt{n}(\hat{u}(\pi; \hat{d}_q) - u(\pi, q_1))
= \sqrt{\omega}(t_1^\top + t_2^\top C(\pi; d_q))\sqrt{N}(\hat{d}_q - d_q) + \sum_{l=1}^k a_l \sqrt{\frac{n_l}{n}} \sum_{i=1}^{n_l} t_2^\top (u^\pi(X_i^{(l)}; d_q) - E_q u^\pi(X; d_q))\sqrt{\frac{n_l}{n_l}} + o_p(1)
\]

\[
\xrightarrow{d} N(0, \omega(t_1^\top + t_2^\top C(\pi; d_q))V_q(t_1 + C(\pi; d_q)^\top t_2) + \sum_{l=1}^k (a_l^2/s_l)T_l(d_q)t_2),
\]

(S5.8)
where the last step follows from the independence of the Markov chains involved in the two stages. Note that the variance in \((S5.8)\) is the same as
\[
(t_1^T, t_2^T) \begin{pmatrix}
\varpi V_q & \Sigma_{12} \\
\Sigma_{21} & \Sigma_{22}
\end{pmatrix} (t_1^T, t_2^T)^T.
\]
Hence the Cramér-Wold device implies the joint central limit theorem (CLT) in (3.22). Thus Theorem 3 (a) is proved.

From the proofs of Theorems 1 and 2 (a), we know that
\[
\hat{\varpi} \hat{C}(\pi; \hat{d}_q) \hat{V}_q \hat{C}(\pi; \hat{d}_q)^T
\]
is a consistent estimator of \(\varpi C(\pi; d_q)V_q C(\pi; d_q)^T\). If \(d_q\) is known from the assumptions of Theorem 3 (b) and the results in Vats et al. (2018), we know that \(T_i(d_q)\) is consistently estimated by its SV estimator \(\hat{T}_i(d_q)\) defined in (3.21). Then using similar arguments as in the proof of Theorem 2 (a), we can show that every element of \(\hat{T}_i(d_q) - \hat{T}_i(\hat{d}_q)\) converges to zero (a.e.). Hence Theorem 3 (b) is proved.

**S6. Entropy decomposition for multiple IS estimators of means**

In this section, we prove a result similar to Theorem 3 for \(\hat{\eta}^{[f]}(\pi; \hat{d})\). Let \(\hat{\eta}^{[f]}(\pi; \hat{d}_q)\) be the vector of length \(|\Pi|\) consisting of \(\hat{\eta}^{[f]}(\pi; \hat{d}_q)\)'s, \(\pi \in \Pi\) in a fixed order. Similarly define \(\hat{v}^{[f]}(\pi; \hat{d}_q)\) and the vector of true means \(E_{\pi f}\).

Let \(p^* \equiv |\Pi|\). Let \(E(\pi; d_q)\) be the \(p^* \times (k - 1)\) matrix with rows \(e(\pi; d_q)\) (defined in Section 3.2 of the paper), \(\pi \in \Pi\). Similarly, define \(\hat{E}(\pi; d_q)\)
with rows $\hat{e}(\pi; d_q)$, $\pi \in \Pi$. Let $v^{[f],\pi}(x; d_q)$ be the $p$ dimensional vector consisting of $v^{[f],\pi}(x; d_q)$'s defined in (3.14) of the paper, $\pi \in \Pi$. Define the $2p^* \times 2p^*$ matrix
\[
\Lambda_i(d_q) = \begin{pmatrix}
\Lambda_{i11}(d_q) & \Lambda_{i12}(d_q) \\
\Lambda_{i21}(d_q) & T_i(d_q)
\end{pmatrix},
\]
(S6.9)
where the elements of $\Lambda_{i11}(d_q)$ are given by
\[
\lambda_{i11}(\pi, \pi'; d_q) = \text{Cov}_q(v^{[f],\pi}(X_1^{(l)}; d_q), v^{[f],\pi'}(X_1^{(l)}; d_q)) + \sum_{g=1}^{\infty} \text{Cov}_q(v^{[f],\pi}(X_1^{(l)}; d_q), v^{[f],\pi'}(X_1^{(l)}; d_q))
\]
\[
+ \sum_{g=1}^{\infty} \text{Cov}_q(v^{[f],\pi}(X_1^{(l)}; d_q), v^{[f],\pi'}(X_1^{(l)}; d_q)),
\]
and the elements of $\Lambda_{i12}(d_q)$ are given by
\[
\lambda_{i12}(\pi, \pi'; d_q) = \text{Cov}_q(v^{[f],\pi}(X_1^{(l)}; d_q), u^{\pi'}(X_1^{(l)}; d_q)) + \sum_{g=1}^{\infty} \text{Cov}_q(v^{[f],\pi}(X_1^{(l)}; d_q), u^{\pi'}(X_1^{(l)}; d_q))
\]
\[
+ \sum_{g=1}^{\infty} \text{Cov}_q(v^{[f],\pi}(X_1^{(l)}; d_q), u^{\pi'}(X_1^{(l)}; d_q)).
\]
Also $\Lambda_{i21}(d_q) = \Lambda_{i12}(d_q)^\top$ and let $\Lambda(d_q) = \sum_{i=1}^{k}(a_i^2/s_i)\Lambda_i(d_q)$. Define a function $h: \mathbb{R}^{2p^*} \rightarrow \mathbb{R}^{p^*}$ where
\[
h(x_1, \ldots, x_{2p^*}) = \left(\frac{x_1}{x_{p^*+1}}, \frac{x_2}{x_{p^*+2}}, \ldots, \frac{x_{p^*}}{x_{2p^*}}\right)
\]
with its gradient given by

\[
\nabla h(x) = \begin{pmatrix}
1/x_{p^*+1} & 0 & \ldots & 0 & -x_1/x_{p^*+1} & 0 & \ldots & 0 \\
0 & 1/x_{p^*+2} & \ldots & 0 & 0 & -x_2/x_{p^*+2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 1/x_{2p^*} & 0 & 0 & \ldots & -x_{p^*}/x_{2p^*}
\end{pmatrix}.
\]

Define the \( p^* \times p^* \) matrix

\[
\rho(d_q) = \nabla h(E_\pi f \odot u(\pi, q_1), u(\pi, q_1))^{\top} \Lambda(d_q) \nabla h(E_\pi f \odot u(\pi, q_1), u(\pi, q_1)^{\top},
\]

where \( \odot \) denotes element-wise multiplication. Let

\[
\hat{\Lambda}(d_q) = \frac{1}{n_l} \sum_{j=-(b_{n_l}-1)}^{b_{n_l}-1} w_{n_l}(j) \sum_{i \in S_{n_l}} \begin{pmatrix}
v[f](X_i^{(l)}; d_q) - \bar{v}(d_q) \\
u(\pi(X_i^{(l)}; d_q) - \bar{u}(d_q)
\end{pmatrix}^{\top},
\]

where \( b_{n_l}'s \) are the truncation points, \( w_{n_l}(j)'s \) are lag window, and \( \bar{v}(d_q) = \sum_{i=1}^{n_l} v[f](X_i^{(l)}; d_q)/n_l \). Let \( \hat{\Lambda}(d_q) \equiv \sum_{l=1}^{k} (a_l^2 n_l / n_l) \hat{\Lambda}(d_q) \). Finally, let

\[
\tilde{\rho}(\hat{d}_q) = \nabla h(\bar{v}(d_q), \bar{u}(\pi; d_q))^{\top} \hat{\Lambda}(d_q) \nabla h(\bar{v}(d_q), \bar{u}(\pi; d_q))^{\top},
\]

**Theorem 4** Suppose that \( N_l, n_l \to \infty \) for all \( l = 1, \ldots, k \), and there exists \( \varpi \in [0, \infty) \) such that \( n/N \to \varpi \). Here, \( N \equiv \sum_{l=1}^{k} a_l^2 n_l / n_l \) and \( n = \sum_{l=1}^{k} n_l \) are the total sample sizes for stages 1 and 2, respectively. In addition, let \( n_l/n \to s_l \) for \( l = 1, \ldots, k \).
(a) Assume that the stage 1 Markov chains are polynomially ergodic of order \( m > 1 \). Further, assume that the stage 2 Markov chains \( \Phi_1, \ldots, \Phi_k \) are polynomially ergodic of order \( m \), and for some \( \delta > 0 \) \( E_q |u_\pi(X; \hat{d}_q)|^{2+\delta} < \infty \) and \( E_q |v^{[f]}; \pi(X; \hat{d}_q)|^{2+\delta} < \infty \) for each \( \pi \in \Pi \) and \( l = 1, \ldots, k \) where \( m > 1 + 2/\delta \). Then as \( n_1, \ldots, n_k \to \infty \),

\[
\sqrt{n} \begin{pmatrix}
\hat{d}_q - d_q \\
\tilde{\eta}^{[f]}(\pi; \hat{d}_q) - E_\pi f
\end{pmatrix} \xrightarrow{d} \mathcal{N} \left( 0, \begin{pmatrix}
\varpi V_q & \Delta_{12} \\
\Delta_{21} & \Delta_{22}
\end{pmatrix} \right), \quad (S6.11)
\]

where \( \Sigma_{21} = \varpi E(\pi; d_q)V_q, \Sigma_{12} = \Sigma_{21}^T, \) and \( \Sigma_{22} = \varpi E(\pi; d_q)V_q E(\pi; d_q)^T + \rho(\hat{d}_q) \).

(b) Suppose that the conditions of Theorem 1 hold for the stage 1 Markov chains. Let \( \hat{V}_q \) be the consistent estimator of \( V_q \) given in Theorem 1. Assume that the Markov chains \( \Phi_1, \ldots, \Phi_k \) are polynomially ergodic of order \( m \geq (1 + \epsilon)(1 + 2/\delta) \) for some \( \epsilon, \delta > 0 \) such that \( E_q \|u_\pi(X; d)\|^{4+\delta} < \infty \) and \( E_q \|v^{[f]}; \pi(X; d)\|^{4+\delta} < \infty \), \( \| \cdot \| \) denotes the Euclidean norm) for all \( l = 1, \ldots, k \), and \( w_{nl} \) and \( b_{nl} \) satisfy conditions 1-4 in (Vats et al., 2018, Theorem 2). Then \((n/N)\hat{E}(\pi; \hat{d}_q)\hat{V}_q \hat{E}(\pi; \hat{d}_q)^T + \hat{\rho}(\hat{d}_q)\) is a strongly consistent estimator of \( \Delta_{22} \) and \((n/N)\hat{E}(\pi; \hat{d}_q)\hat{V}_q \hat{E}(\pi; \hat{d}_q)^T \) is a consistent estimator of \( \Delta_{21} \).

Using similar arguments as in Section 3.3 of the paper, the joint entropy of \( \tilde{\eta}^{[f]}(\pi; \hat{d}_q) \) and \( \hat{d}_q \) is sum of the entropy of \( \hat{d}_q \), and the conditional entropy
of $\eta^{[f]}(\pi; \hat{d}_q)$ given $\hat{d}_q$. Thus the maximum entropy selection of skeleton points boils down to choosing $q$ by maximizing $\log \det(\hat{V}_q)$.

**Proof of Theorem 4.** Since the Markov chains used in stage 1 are polynomially ergodic of order $m > 1$, from Roy et al. (2018, Theorem 1), we have $N^{1/2}(\hat{d}_q - d_q) \xrightarrow{d} \mathcal{N}(0, V_q)$. Since $n/N \to \varpi$, it follows that $\sqrt{n}(\hat{d}_q - d_q) \xrightarrow{d} \mathcal{N}(0, \varpi V_q)$. Following Roy et al. (2018, Proof of Theorem 3) we write

$$\sqrt{n}(\hat{\eta}^{[f]}(\pi; \hat{d}_q) - \mathbf{E}_\pi f) = \sqrt{n}(\hat{\eta}^{[f]}(\pi; \hat{d}_q) - \hat{\eta}^{[f]}(\pi; d_q)) + \sqrt{n}(\hat{\eta}^{[f]}(\pi; d_q) - \mathbf{E}_\pi f).$$

(S6.12)

The 2nd term involves randomness only from the 2nd stage Markov chains.

Note that

$$\hat{v}(\pi; d_q) \overset{a.s.}{\to} \sum_{l=1}^{k} a_l \mathbf{E}_{\pi^l} v^{[f],\pi}(X; d_q) = \mathbf{E}_\pi f \odot u(\pi, q_1).$$

Since $\sum_{l=1}^{k} a_l \mathbf{E}_{\pi^l} u^\pi(X; d_q) = u(\pi, q_1)$, we have

$$\sqrt{n} \left( \begin{array}{c} \hat{v}(\pi; d_q) - \mathbf{E}_\pi f \odot u(\pi, q_1) \\ \hat{u}(\pi; d_q) - u(\pi, q_1) \end{array} \right) = \sum_{l=1}^{k} a_l \sqrt{n} \frac{1}{n_l} \sum_{i=1}^{n_l} \left( \begin{array}{c} v^{[f],\pi}(X_i^{(l)}; d_q) - \mathbf{E}_{q_l} v^{[f],\pi}(X; d_q) \\ u^\pi(X_i^{(l)}; d_q) - \mathbf{E}_{q_l} u^\pi(X; d_q) \end{array} \right).$$

(S6.13)

Since $\Phi_l$ is polynomially ergodic of order $m$ and $E_{q_l}|u^\pi(X; d_q)|^{2+\delta}$ and $E_{q_l}|v^{[f],\pi}(X; d_q)|^{2+\delta} < \infty$ are finite for each $\pi \in \Pi$ where $m > 1 + 2/\delta$,
it follows that
\[
\frac{1}{\sqrt{n_t}} \sum_{i=1}^{n_t} \left( \begin{array}{c}
v^{[f], \pi}(X_i; d_q) - E_{q_i} v^{[f], \pi}(X; d_q) \\
u^{\pi}(X_i; d_q) - E_{q_i} u^{\pi}(X; d_q)
\end{array} \right) \xrightarrow{d} N(0, \Lambda_t(d_q))
\]
where \(\Lambda_t(d_q)\) is defined in (S6.9). As \(n_t/n \to s_t\) and the Markov chains \(\Phi_t's\) are independent, it follows that
\[
\sqrt{n} \left( \begin{array}{c}
vild^f(\pi; d_q) - E_{\pi} f \odot u(\pi, q_1) \\
uild(\pi, q_1; d_q) - u(\pi, q_1)
\end{array} \right) \xrightarrow{d} N(0, \Lambda(\d_q)).
\]
Then applying the delta method to the function \(h\) we have a CLT for the estimator \(\hat{\eta}^{[f]}(\pi; d_q)\), that is, we have \(\sqrt{n}(\hat{\eta}^{[f]}(\pi; d_q) - E_{\pi} f) \xrightarrow{d} N(0, \rho(d_q))\).

Next by Taylor series expansion of \(L(d) = \hat{\eta}^{[f]}(\pi; d)\) about \(d_q\), we have
\[
\sqrt{n}(L(\hat{d}_q) - L(d_q)) = \sqrt{n} \nabla L(d_q) \top (\hat{d}_q - d_q) + \frac{\sqrt{n}}{2} (\hat{d}_q - d_q) \top \nabla^2 L(d^*) (\hat{d}_q - d_q),
\]
where \(d^*\) is between \(d_q\) and \(\hat{d}_q\). As in Roy et al. (2018), we can then show that
\[
\sqrt{n}(\hat{\eta}^{[f]}(\pi; \hat{d}_q) - \hat{\eta}^{[f]}(\pi; d_q)) = \sqrt{\omega} e(\pi; d_q) \sqrt{N}(\hat{d}_q - d_q) + o_p(1).
\]
Accumulating the terms for all \(\pi \in \Pi\), we have
\[
\sqrt{n}(\hat{\eta}^{[f]}(\pi; \hat{d}_q) - \hat{\eta}^{[f]}(\pi; d_q)) = \sqrt{\omega} E(\pi; d_q) \sqrt{N}(\hat{d}_q - d_q) + o_p(1).
\]
Thus for constant vectors \(t_1\) and \(t_2\) of dimensions \(k - 1\) and \(p\) respectively,
we have
\[
t_1^T \sqrt{n}(\hat{d}_q - d_q) + t_2^T \sqrt{n}(\hat{\eta}^{[f]}(\pi; \hat{d}_q) - \hat{\eta}^{[f]}(\pi; d_q)) \\
\xrightarrow{d} N(0, \varpi(t_1^T + t_2^T E(\pi; d_q))V_q(t_1 + E(\pi; d_q)^T t_2) + t_2^T \rho(d_q)t_2),
\]
(S6.14)
where the last step follows from the independence of the Markov chains involved in the two stages. Note that the variance in (S6.14) is the same as
\[
\begin{pmatrix}
\varpi V_q & \Delta_{12} \\
\Delta_{21} & \Delta_{22}
\end{pmatrix}
\begin{pmatrix}
t_1^T \\
t_2^T
\end{pmatrix}
\]
Hence the Cramér-Wold device implies the joint CLT in (S6.11). Thus Theorem 4 (a) is proved.

From the proofs of Theorem 1 and Theorem 2 (b), we know that
\[
\varpi \hat{E}(\pi; \hat{d}_q)\hat{V}_q \hat{E}(\pi; \hat{d}_q)^\top
\]
is a consistent estimator of \(\varpi E(\pi; d_q)V_q E(\pi; d_q)^\top\). Also, \(\nabla h(\hat{v}^{[f]}(\pi; \hat{d}_q), \hat{u}(\pi; \hat{d}_q)) \xrightarrow{a.s.} \nabla h(E_{\pi} f \odot u(\pi, q_1), u(\pi, q_1))\). If \(d_q\) is known from the assumptions of Theorem 4 (b) and the results in Vats et al. (2018), we know that \(\Lambda_l(d_q)\) is consistently estimated by its SV estimator \(\hat{\Lambda}_l(d_q)\) defined in (S6.9). Then using similar arguments as in the proof of Theorem 3, we can show that every element of \(\hat{\Lambda}_l(d_q) - \hat{\Lambda}_l(\hat{d}_q)\) converges to zero (a.e.). Thus \(\hat{\rho}(\hat{d}_q)\) is a consistent estimator of \(\rho(d_q)\). Hence Theorem 5 (b) is proved. \(\square\)
S7. Algorithms for computing the optimal skeleton set

In many cases, searching over the whole space $Q$ to find the optimal set of proposal densities is computationally hard. Often, $Q$ comprises of a parametric family of densities parameterized by $\xi \in \Xi$ so the problem becomes choosing the skeleton set $\xi = \{\xi_1, \xi_2, \ldots, \xi_k\}$ corresponding to the parameter values of the proposal densities that minimizes an optimality criterion $\phi(\xi)$.

For convenience we work with a discretized version $\tilde{\Xi}$ of $\Xi$ and the skeleton set $\xi$ is constrained to be $\xi \subset \tilde{\Xi}$. Finding the optimal skeleton set in this context has been studied in the sampling design and computer experiments literature (Ko et al., 1995; Royle and Nychka, 1998; Fang et al., 2006). Here we present the two algorithms we used in this paper, a point-swapping algorithm and a simulated annealing algorithm. Further details for these algorithms can be found in Royle and Nychka (1998) and Bélisle (1992) respectively.

S7.1 Point-swapping algorithm

This algorithm performs many iterations, so it is mostly suited in cases where the optimality criterion is fast to compute. We used the point-swapping algorithm for computing the space-filling proposal distributions
S7.2 Simulated annealing algorithm

because in these cases the criterion depends only on pairwise distances of
the proposal distributions which are fast to compute.

The algorithm proceeds as follows:

**Initialization:** Initialize the skeleton set at $\xi^{(0)}$ with $|\xi^{(0)}| = k$.

**Iterations:** Repeat for $i = 1, 2, \ldots$:

For $j = 1, \ldots, k$: Swap the $j$th element of $\xi^{(i-1)}$ with the element $\xi_j' \in \tilde{\Xi} \setminus \xi^{(i-1)}$ such that the new set $\xi^{(i)} = \xi^{(i-1)} \setminus \{\xi_j\} \cup \{\xi_j'\}$ produces the biggest drop in the value of the optimality criterion. If no such $\xi_j'$ exists, i.e., if $\phi(\xi^{(i-1)}) < \phi(\xi^{(i-1)} \setminus \{\xi_j\} \cup \{\xi_j'\})$ for all $\xi_j' \in \tilde{\Xi} \setminus \xi^{(i-1)}$, then $\xi^{(i)} = \xi^{(i-1)}$.

**Termination:** Stop if, after looping over all elements in $\xi^{(i)}$, the skeleton set remains unchanged. Return the final skeleton set.

We used the implementation in the R package *fields* (Nychka et al., 2017) to compute the optimal skeleton set in our paper.

S7.2 Simulated annealing algorithm

We use simulated annealing to compute the optimal set of proposal distributions for MNX and ENT. The criterion for these methods is based on the SV estimate of the asymptotic SE of the multiple IS estimator which
Simulated annealing algorithm is computed from Monte Carlo samples. In this case, if samples from a particular proposal distribution in the skeleton set already exist, then they are reused, otherwise they are generated and stored for a possible future use.

The algorithm proceeds as follows:

**Initialization:** Initialize the skeleton set at $\xi^{(0)}$ with $|\xi^{(0)}| = k$ and an initial temperature at $T_0$.

**Iterations:** Repeat for $i = 1, 2, \ldots$:

(a) Set $T = T_0 / \log((i - 1)/B + \exp(1))$, where $B$ is a parameter of the algorithm denoting the number of iterations before the temperature is lowered.

(b) Randomly select $\xi \in \xi^{(i-1)}$ and $\xi' \in \tilde{\Xi} \setminus \xi^{(i-1)}$. Form the candidate set $\xi' = \xi^{(i-1)} \setminus \{\xi\} \cup \{\xi'\}$.

(c) With probability $\min\{1, \exp[(\phi(\xi^{(i-1)}) - \phi(\xi'))/T]\}$ set $\xi^{(i)} = \xi'$, otherwise set $\xi^{(i)} = \xi^{(i-1)}$.

**Termination:** Stop if $i > i_{\text{max}}$, a predetermined number of iterations. Return the skeleton set found among all iterations which corresponds to the lowest value of the optimality criterion.
S8. Finney’s (1947) vasoconstriction data analysis using robit model

Finney’s (1947) vasoconstriction data consist of 39 binary responses denoting the presence or absence, \( y \), of vasoconstriction on the subject’s skin after he or she inhaled air of volume \( V \) at rate \( R \). We consider a binomial generalized linear model (GLM) where the probability of presence for the \( i \)th subject, \( \alpha_i \), is modeled using a robit link function with degrees of freedom (df) \( \xi \),

\[
F_{\xi}^{-1}(\alpha_i) = \beta_0 + \beta_1 \log V_i + \beta_2 \log R_i, \quad \text{for} \quad i = 1, \ldots, 39.
\]

Here, \( F_{\xi}(\cdot) \) denotes the distribution function of the standard Student’s \( t \) distribution with df \( \xi \). As in Roy (2014), we consider a Bayesian analysis of the data with robit model. The prior for \( \beta \) is \( \beta \sim t_3(0, 10^4(W^\top W)^{-1}, 3) \), where \( W \) is the design matrix.

Roy (2014) estimates the df parameter \( \xi \) by maximizing the marginal likelihood, that is, \( \hat{\xi} = \arg\max_{\xi} \theta_{\xi}(y) \). In particular, Roy (2014) uses the multiple IS estimator (1.2) to estimate the (ratios of) marginal likelihoods, which in turn provides the estimate \( \hat{\xi} \). Our objective is to choose the importance sampling distributions from the family of posterior densities \( \Pi = \{ \pi_{\xi}(\beta|y) : \xi > 0 \} \) for the estimation of (1.2). We consider this in section S8.1. Whereas in section S8.2 we analyze this problem with proposal densities from the multivariate normal family.
S8.1 Selection of proposals for multiple IS

In this section, we consider $Q = \Pi$, thus, choosing proposal distributions is the same as choosing appropriate $\xi$ values. Because $\xi$ represents the df parameter, we consider a wide range of points $\tilde{\Xi} = \{0.1, 0.2, \ldots, 20\}$ from where we choose the skeleton sets for the different methods. The reference density corresponds to $\tilde{\xi}$, where $\tilde{\xi} = 10$ is at the middle of this range. For the multiple IS methods we choose $k = 5$ points, one of which must be $\tilde{\xi}$.

The computation is done in two phases. In the first phase we find the optimal skeleton set, $\xi$, for each method. In the second phase we compare the relative standard errors of the naive and multiple IS estimators using the skeleton sets computed in the first phase. The total number of samples used for each method in the second phase is kept the same. The required Markov chain samples were generated by Hamiltonian Monte Carlo implemented in the stan language (Stan Development Team, 2020). In all calculations involving the asymptotic variance of the IS estimator, the SV estimate with the Tukey-Hanning window,

$$w_n(j) = 0.5[1 + \cos(\pi |j|/b_n)]I(|j| < b_n),$$

was used, where $b_n = \sqrt{n}$.

**Phase 1: Finding the optimal set of proposal densities**
• **NIS:** This is not required because the proposal density in the naive importance sampling (NIS) is fixed at $\xi_{nis} = \{10\}$.

• **SFE:** This method is based on the Euclidean distance between the parameters. Therefore, $\xi_{sfe} = \{2, 6, 10, 14, 18\}$.

• **SFS:** This method requires the SKLD between two densities corresponding to two $\xi$ values. Figure 1 shows the logarithm of pairwise SKLD between densities corresponding to two different values of $\xi$. The SKLD is computed using the approximation of Section S1. It can be seen that the distance is non-Euclidean. For example, the densities corresponding to $\xi_1 = 1$ and $\xi_2 = 5$ are further apart than the densities corresponding to $\xi_1 = 16$ and $\xi_2 = 20$. Using the algorithm of Section S7.1 we select $\xi_{sfs} = \{0.3, 1.1, 1.9, 3.3, 10\}$. It is noted that the points concentrate more on the low values in $\tilde{\Xi}$.

• **SEQ:** In this case the optimal set is computed by starting at $\xi^{(1)} = \xi_{nis}$. Then, given that at the $i$th iteration, $i = 2, \ldots, k$ we are at $\xi^{(i-1)}$, we obtain $\xi^{(i)} = \xi^{(i-1)} \cup \{\xi'\}$, where $\xi'$ corresponds to the point in $\tilde{\Xi} \setminus \xi^{(i-1)}$ with the highest relative standard error. The relative standard error is again computed using 2,000 samples for stage 1 and 2,000 new samples for stage 2, after a burn in of 400. We find
\[ \xi_{\text{seq}} = \{0.1, 0.2, 0.3, 0.7, 10\} \].

- **MNX**: The optimal set is found by simulated annealing (Section S7.2).

  We start the simulated annealing algorithm at \( \xi_{\text{sfs}} \), and perform \( i_{\text{max}} = 250 \) iterations with \( T_0 = 0.1 \) and \( B = 10 \). The optimality criterion is computed as follows. Using 2,000 Markov chain samples for stage 1 and 2,000 samples for stage 2, we compute

  \[ \hat{\nu}_1^2(\xi) := \hat{c}(\pi; \hat{d})^\top \hat{V} \hat{c}(\pi; \hat{d}) \]

  and

  \[ \hat{\nu}_2^2(\xi) := \hat{\tau}^2(\pi; \hat{d}) \]

  given in Theorem 2(a) for each \( \xi \in \tilde{\Xi} \) as well as \( \hat{u}(\xi) = \hat{u} \) given in equation (1.2) of the main paper. Then, given stage 1 sample size of \( N \) and stage 2 sample size of \( n \), the relative standard error estimate is given by

  \[ \text{RelSE}(\xi, N, n) := \frac{\hat{\nu}_1(\xi)/\sqrt{N} + \hat{\nu}_2(\xi)/\sqrt{n}}{\hat{u}(\xi)}. \]  

  (S8.15)

  Assuming that the total sample size \( M = N + n \) is fixed, the objective becomes choosing \( \xi_{\text{mnx}} \) in order to minimize

  \[ \min_{N \in (0, M)} \max_{\xi \in \Xi} \text{RelSE}(\xi, N, M - N). \]  

  (S8.16)

  We find \( \xi_{\text{mnx}} = \{0.1, 0.4, 1.6, 3.3, 10\} \). One can also impose a constraint that \( N \) is at least some number and at most some other number while finding \( \xi_{\text{mnx}} \) minimizing (S8.16).

- **ENT**: The optimal set is found by simulated annealing (Section S7.2).

  We start the simulated annealing algorithm at \( \xi_{\text{sfs}} \), and perform \( i_{\text{max}} = \)
Figure 1: Contour plot of the logarithm of the SKLD between the densities corresponding to $\xi_1$ and $\xi_2$ for the vasoconstriction example.

250 iterations with $T_0 = 1$ and $B = 10$. The optimality criterion used for this method is $-\log \det(U)$ where $U$ is the matrix with $(i, j)$th element $U_{ij} = (\hat{V}_q)_{ij}/(\hat{d}_i\hat{d}_j)$. The estimates $\hat{d}$ and $\hat{V}_q$ are computed from 2,000 Markov chain samples. In this example, the ENT skeleton set turns out to be the same as the MNX set, thus $\xi_{ent} = \xi_{mnx} = \{0.1, 0.4, 1.6, 3.3, 10\}$.

**Phase 2: Estimation of the ratio of marginal densities**

After the skeleton sets are found, we generate a total of $M = 50,000$ samples from the proposal densities, equally divided among all densities in the set. The total sample size $M$ is generally determined by available
computational resources. Since we have derived consistent SV estimators of the asymptotic variance of \( \hat{u} \), the sample size \( M \) can be chosen such that the overall SE of \( \hat{u} \) is smaller than a pre-determined level of accuracy. For NIS we simply take \( M \) Gibbs samples from the density corresponding to \( \xi_{\text{nis}} \), and for the multiple IS methods we take \( M/k \) samples from each density in the corresponding \( \xi \) set. However, the total of \( M/k \) samples must be split into stage 1, for estimating the ratio of marginals within \( \xi, d \), and stage 2, for estimating the ratio of marginals over the whole set \( \tilde{\Xi} \). To determine the optimal split we use equation (S8.15) where \( \hat{\upsilon}_1(\xi) \) and \( \hat{\upsilon}_2(\xi) \) are calculated from 2,000 stage 1 and 2,000 stage 2 Markov chain samples.

For MNX, SEQ, and ENT the existing samples from Phase 1 are reused but for the space-filling methods, new samples are generated. We take an equal number of samples from each density, thus we take \( \hat{N}/k \) stage 1 samples from each density in the skeleton set where \( \hat{N} \) is the integer that minimizes \( \max_{\xi \in \tilde{\Xi}} \text{RelSE}(\xi, N, M - N) \), and \( \hat{n}/k \) stage 2 samples, where \( \hat{n} = M - \hat{N} \). This corresponds to stage 1 sample sizes of 1500, 6500, 8500, 9000, 9000 and stage 2 sample sizes of 8500, 3500, 1500, 1000, 1000 from each density for SFE, SFS, SEQ, MNX, ENT, respectively.

The estimates of the relative standard error of (1.2) and the value of the logarithm of (1.2) across all \( \xi \) values in \( \tilde{\Xi} \) corresponding to the different
S8.2 Multiple IS using a mixture of multivariate normal proposals

skeleton sets, \(\xi\), chosen are plotted in Figure 2. It can be seen that the relative standard error is larger when \(\xi\) is small. NIS has the lowest relative standard error at \(\check{\xi}\) but results in much higher standard errors at low values of \(\xi\). Indeed, at \(\xi = 0.5\), the SV estimate of the relative standard error for NIS method is about four times larger than that for the MNX and ENT methods. It can also be seen that SFE does not have as good performance as SFS, again because it avoids sampling from densities corresponding to low values of \(\xi\) which are the ones that produce the largest relative standard error. SEQ also does not have good performance because it concentrates all points in a very narrow region while, evidently, it is more beneficial to spread the points to cover a wider area as MNX and ENT do.

**S8.2 Multiple IS using a mixture of multivariate normal proposals**

The proposed methods of choosing reference distributions are applicable to IS estimators in the situations where \(Q\) can be different from \(\Pi\). To demonstrate this, in this section we analyze the vasoconstriction data using the model and method discussed in Section S8.1 with the difference that the proposal densities are now chosen from the multivariate normal family instead of the family of the posterior density of \(\beta\). Thus we are now able to
Figure 2: Vasoconstriction example: The left and right panels show the values of \( \log \hat{u}(\hat{d}_\xi) \) and estimates of the relative standard error of \( \hat{u}(\hat{d}_\xi) \) across \( \xi \) values for different skeleton sets, respectively. Points included in the skeleton sets are indicated by +.

draw independent and identically distributed (iid) samples from the importance sampling distributions which is not the case when these are posterior densities of \( \beta \) which require Markov chain Monte-Carlo sampling. Since \( d \) is known, the reverse logistic regression estimation is not needed here. The space filling, minimax and sequential approaches developed in the main paper can be used for selecting multivariate normal proposals as we describe below.

If \( n_i \) iid samples, \( X_i^{(l)}, i = 1, \ldots, n_i \), are drawn from the density \( q_l(x) \) (a
S8.2 Multiple IS using a mixture of multivariate normal proposals

normal density described later), \( l = 1, \ldots, k \), then the normalizing constant, \( \theta_\xi \), of the posterior density \( \pi_\xi(x) \equiv \nu_\xi(x)/\theta_\xi \), is estimated by

\[
\hat{\theta}_\xi = \frac{1}{n} \sum_{l=1}^{k} \sum_{i=1}^{n_l} \frac{\nu_\xi(X_i^{(l)})}{\bar{q}(X_i^{(l)})}, \tag{S8.17}
\]

where \( n = n_1 + \ldots + n_k \) and \( \bar{q}(x) = (n_1/n)q_1(x) + \ldots + (n_k/n)q_k(x) \). The variance of this estimator is estimated by

\[
\hat{\text{Var}}(\hat{\theta}_\xi) = \frac{1}{n} \sum_{l=1}^{k} \sum_{i=1}^{n_l} \left( \frac{\nu_\xi(X_i^{(l)})}{\bar{q}(X_i^{(l)})} - \hat{\theta}_\xi \right)^2. \tag{S8.18}
\]

To choose the proposal densities corresponding to a skeleton set \( \xi \), for \( \xi \in \xi \), let \( \tilde{\beta}_\xi \) denote the maximizer of \( \ell_\xi(\beta|y)\pi(\beta) \) and let \( \tilde{H}_\xi \) denote the Hessian matrix of \( -\log\{\ell_\xi(\beta|y)\pi(\beta)\} \) evaluated at \( \tilde{\beta}_\xi \). Then the normal approximation to \( \pi_\xi(\beta|y) \) is taken to be the multivariate normal with mean \( \tilde{\beta}_\xi \) and variance \( \tilde{H}_\xi^{-1} \). Thus, \( q_l \) is the normal approximation to the posterior density \( \pi_\xi(\beta|y) \), where \( \xi = \xi_l \) is a skeleton point.

Unlike in Section S8.1, where we used Hamiltonian Monte Carlo to obtain approximate samples from the proposal (posterior) densities, here we draw iid samples from the proposal distributions. We use (S8.17) to estimate \( \theta_\xi \) for all \( \xi \) values in the range \( \tilde{\Xi} \) identified previously. We set \( k = 5 \) and generate \( n_l = 10000 \) samples from each of the proposal densities \( q_l, l = 1, \ldots, 5 \). We also use naive importance sampling by drawing \( 5 \times 10000 \) samples from the normal approximation to the posterior for \( \beta \) corresponding to \( \xi_{nis} = \{\xi = 10\} \).
For the two space filling methods, the sets $\xi_{sfe}$ and $\xi_{sfs}$ are obtained as described in Section S8.1, thus the skeleton sets are the same as in that section: $\xi_{sfe} = \{2, 6, 10, 14, 18\}$ and $\xi_{sfs} = \{0.3, 1.1, 1.9, 3.3, 10\}$.

For SEQ, we aim to select the set $\xi_{seq}$ sequentially, starting with $\xi^{(1)} = \{\tilde{\xi}\}$. At the $j$th iteration, we obtain the set $\xi^{(j)} = \xi^{(j-1)} \cup \{\xi_j\}$. Then, we draw samples from the normal approximation to the posterior density corresponding to this $\xi_j$, as described in the previous paragraph. Using these samples, together with existing samples from $\xi^{(j-1)}$, we compute, using (S8.17) and (S8.18), the relative standard error of $\hat{\theta}_\xi$ for $\xi \in \tilde{\Xi}$. The value of $\xi$ corresponding to the highest relative standard error, denoted by $\xi_{j+1}$, is added to the set. The final set obtained using this method is $\xi_{seq} = \{0.6, 0.7, 0.8, 0.9, 10\}$.

For MNX, we run the simulated annealing algorithm with $T_0 = 10$, $B = 10$, $i_{max} = 250$, starting from $\xi_{sfs}$. For every new density added to the skeleton set we generate 4000 samples from the corresponding normal approximation, if not already available. These samples, along with the existing samples from the other densities previously added are used to calculate the relative standard error, using (S8.17) and (S8.18), for all $\xi \in \tilde{\Xi}$. The objective of the simulated annealing is to minimize the maximum relative standard error across $\tilde{\Xi}$. The optimal skeleton set is
$\xi_{\text{mnx}} = \{0.2, 0.3, 0.7, 2.6, 10\}$.

Plots of the estimator (S8.17) using the different methods are shown in the left panel of Figure 3. It can be seen that NIS and SFE are significantly different from the other methods. The plots of the relative standard error estimates using (S8.18) are shown in the right panel of Figure 3. It can be seen that the NIS, SFE, and SEQ methods lead to significantly higher relative standard error compared to the proposed methods for low values of $\xi$. For example, at $\xi = 0.5$, the relative standard error for NIS, SFE, and SEQ are 2.5, 7, and 3.8 times higher respectively than MNX.

S9. Further details on the autologistic example used in the main paper

S9.1 Derivation of the autologistic pmf

We start with the conditional pmf of $x(s_i) | x_{-s_i}$ given by

$$\pi_i(x(s_i) | x_{-s_i}) = p_i^{x(s_i)} (1 - p_i)^{1 - x(s_i)},$$

where, as in the main paper,

$$p_i = \frac{\exp\{\logit(\kappa) + (\gamma/w) \sum_{s_j \in \text{nb}_i} (x(s_j) - \kappa)\}}{1 + \exp\{\logit(\kappa) + (\gamma/w) \sum_{s_j \in \text{nb}_i} (x(s_j) - \kappa)\}}.$$
Figure 3: Logarithm of the IS estimates of the marginal density for Finney’s vasoconstriction data using normal proposal densities (left); and estimates of the relative standard error of the marginal density estimates (right). Points included in the skeleton sets are indicated by +.

Letting $\pi(x|\gamma, \kappa) \propto \exp(A(x|\theta))$, since only pairwise dependencies are considered, it is known that (Kaiser and Cressie, 2000)

$$A(x|\theta) = \sum_{1 \leq i \leq m} \log \frac{\pi_i(x(s_i)|x^*-s_i)}{\pi_i(x^*(s_i)|x^*-s_i)} + \sum_{1 \leq i < j \leq m; s_j \in nb_i} \log \frac{\pi_i(x(s_i)|x(s_j), x^*_{-\{s_i,s_j\}})}{\pi_i(x^*(s_i)|x^*_{-\{s_i,s_j\}})}\pi_i(x(s_i)|x^*_s).$$

for a suitably chosen $x^*$. Choosing $x^* = 0$, simple calculations show that

$$A(x|\theta) = (\text{logit}(\kappa) - \gamma \kappa) \sum_{i=1}^{m} x(s_i) + \frac{\gamma}{2w} \sum_{i=1}^{m} \sum_{s_j \in nb_i} x(s_i)x(s_j).$$
Here we give more details on how we produced the results for the autologistic example in the Section 4 of the main paper. We also present the case where $\kappa$ remains fixed at 0.5 and only $\gamma$ is allowed to vary. The parameter set where we search over is

$$\gamma \in \{-4, -3.9, \ldots, 4\},$$

in the case where $\kappa$ is set fixed at $\kappa = 0.5$, and

$$(\gamma, \kappa) \in \{-4, -3.2, \ldots, 4\} \times \{0.1, 0.2, \ldots, 0.9\},$$

in the case where both parameters are assumed unknown. In both cases we denote the parameters by $\xi$ and the parameter set by $\tilde{\Xi}$.

The computation is done in two phases. In the first phase we find the optimal skeleton set, $\xi$, for each method. In the second phase we compare the relative standard error of the naive and multiple IS estimators using the skeleton sets computed in the first phase. The total number of samples used for each method in the second phase is kept the same. The required Markov chain samples were generated by Gibbs sampling from the conditional distribution of each component of $\mathbf{x}$ given its neighbors. In all calculations involving the asymptotic variance of the IS estimator, the SV
estimate with the Tukey-Hanning window,

\[ w_n(j) = 0.5[1 + \cos(\pi |j|/b_n)]I(|j| < b_n), \]

was used, where \( b_n = \sqrt{n} \).

**Phase 1: Finding the optimal set of proposal densities**

- **NIS**: This is not required because the proposal density is fixed at \( \xi_{nis} = \{0\} \) and \( \xi_{nis} = \{(0,0.5)\} \) for the cases \( \kappa \) fixed and \( \kappa \) varying, respectively.

- **SFE**: This method is based on the Euclidean distance between the parameters. Each component of the parameter set \( \tilde{\Xi} \) is scaled to vary between 0 and 1 before the optimal set is computed. We find \( \xi_{sfe} = \{-3.2, -1.6, 0.0, 1.6, 3.2\} \) and \( \xi_{sfe} = \{(0,0.5), (-2.4,0.3), (-2.4,0.7), (2.4,0.3), (2.4,0.7)\} \) for the cases \( \kappa \) fixed and \( \kappa \) varying, respectively.

- **SFS**: This method requires the SKLD between two pairs \( \xi_1, \xi_2 \). We compute the integrals in (3.7a) of the main paper by Monte Carlo using 3,000 Gibbs samples after a burn-in of 400 from each distribution for the \( \kappa \) known case, and 20,000 samples after a burn-in of 4,000 for the \( \kappa \) estimated case. The point-swapping algorithm of Section S7.1 is used to find the optimal set. We find \( \xi_{sfs} = \)
S9.2 Computational details

\{-3.36, -1.68, 0.00, 1.68, 3.28\} and \(\xi_{sfs} = \{(0, 0.5), (-3.2, 0.5), (-1.6, 0.8), (-1.6, 0.2), (3.2, 0.5)\}\) for the cases \(\kappa\) fixed and \(\kappa\) varying, respectively.

- **MNX:** The optimal set is found by simulated annealing (Section S7.2).
  We start the simulated annealing algorithm at \(\xi_{sfs}\) and perform \(i_{\text{max}} = 250\) iterations with \(T_0 = 10\) and \(B = 10\). The SV estimates were calculated using 3,000 Gibbs samples for stage 1 and 3,000 new samples for stage 2 for the \(\kappa\) known case, and 20,000 samples for stage 1 and 20,000 samples for stage 2 for the \(\kappa\) estimated case. We find \(\xi_{mnx} = \{-3.20, -1.60, 0.00, 1.68, 3.20\}\) and \(\xi_{mnx} = \{(0, 0.5), (-3.2, 0.5), (-1.6, 0.2), (-0.8, 0.8), (4.0, 0.4)\}\) for the cases \(\kappa\) fixed and \(\kappa\) varying, respectively.

- **SEQ:** In this case the optimal set is computed by starting at \(\xi^{(1)} = \xi_{nis}\). Then, given that at the \(i\)th iteration, \(i = 2, \ldots, k\) we are at \(\xi^{(i-1)}\), we obtain \(\xi^{(i)} = \xi^{(i-1)} \cup \{\xi'\}\), where \(\xi'\) corresponds to the point in \(\tilde{\Xi} \setminus \xi^{(i-1)}\) with the highest relative standard error. The relative standard error is again computed using 3,000 Gibbs samples for stage 1 and 3,000 new samples for stage 2 for the \(\kappa\) known case, and 20,000 samples for stage 1 and 20,000 samples for stage 2 for the \(\kappa\) estimated case. We find \(\xi_{seq} = \{-4.00, -3.92, 0.00, 3.92, 4.00\}\) and \(\xi_{seq} = \{(0, 0.5), (-4.0, 0.8), (-2.4, 0.9), (-0.8, 0.1), (3.2, 0.2)\}\) for the cases \(\kappa\) fixed and \(\kappa\) varying respectively.
• **ENT:** The optimal set is found by simulated annealing (Section S7.2). We start the simulated annealing algorithm at $\xi_{sfs}$ and perform $i_{\text{max}} = 250$ iterations with $T_0 = 10$ and $B = 10$. The optimality criterion used for this method is $-\log \det(U)$ where $U$ is the matrix with $(i,j)$th element $U_{ij} = (\hat{V}_q)_{ij}/(\hat{d}_i\hat{d}_j)$. The estimates $\hat{d}$ and $\hat{V}_q$ are computed from 3,000 Gibbs samples for the $\kappa$ known case, and 20,000 samples for the $\kappa$ estimated case. We find $\xi_{\text{ent}} = \{-4, -2.08, 0.00, 2.32, 3.52\}$ and $\xi_{\text{ent}} = \{(0, 0.5), (-4.0, 0.3), (-1.6, 0.9), (-0.8, 0.1), (4.0, 0.4)\}$ for the cases $\kappa$ fixed and $\kappa$ varying respectively.

**Phase 2: Estimation of the ratio of marginal densities**

For the case where only $\gamma$ varies, after the skeleton sets are found, we generate a total of $M = 100,000$ samples from the proposal densities, equally divided among all densities in the set. Thus, for NIS we simply take $M$ Gibbs samples from the density corresponding to $\xi_{\text{nis}}$ and for the multiple IS methods we take $M/k$ samples from each density in the corresponding $\xi$ set. However, the total of $M/k$ samples must be split into stage 1, for estimating the ratio of marginals within $\xi$, $d$, and stage 2, for estimating the ratio of marginals over the whole set $\tilde{\Xi}$. To determine the optimal split we use equation (S8.15) where $\hat{v}_1(\xi)$ and $\hat{v}_2(\xi)$ are calculated from 3,000 stage 1 and 3,000 stage 2 Gibbs samples. For MNX, SEQ,
S9.2 Computational details

and ENT the existing samples from Phase 1 are reused but for the space-filling methods, new samples are generated. We take $\hat{N}/k$ stage 1 samples from each density in the skeleton set where $\hat{N}$ is the integer that minimizes $\max_{\xi \in \tilde{\Xi}} \text{RelSE}(\xi, N, M - N)$, and $\hat{n}/k$ stage 2 samples, where $\hat{n} = M - \hat{N}$. In the case where $\kappa$ is fixed, this corresponds to stage 1 sample sizes of $11000, 13000, 12000, 18000, 15000$ and stage 2 sample sizes of $9000, 7000, 8000, 2000, 5000$ from each density for SFE, SFS, MNX, SEQ, ENT, respectively. In the case where $\kappa$ also varies, the stage 1 sample sizes were $5000, 11667, 13889, 25000, 31667$, and the stage 2 sample sizes were $45000, 38333, 36111, 25000, 18333$ for SFE, SFS, MNX, SEQ, ENT, respectively.

Finally, we study the performance of the different methods over repeated simulations. Figure 4 provides relative standard error plots based on 100 replications of the autologistic model with $\kappa = 0.5$ fixed and $\gamma$ varying. Each time a skeleton set is chosen and the standard error is computed based on the Monte Carlo samples. (Naive IS suffers from high variability when $\gamma$ is away from the origin and is not considered in Figure 4.) From the plots we see that the SF methods are the least variable. SFE does not require samples from the autologistic models to choose the skeleton points. On the other hand, SFS requires samples to compute the SKLD but even then it does not increase the variability compared to SFE. MNX and ENT
Figure 4: Relative standard error plots based on 100 replications of the autologistic model with $\kappa = 0.5$ fixed and $\gamma$ varying. The bold line provides the average of the relative standard errors. 

It seems to be the most variable, but shape of the relative standard error curve mostly remains the same. The SEQ method consistently resulted in the highest standard errors. Indeed, the maximum and the minimum of the ratios of the (average) relative standard errors of SEQ to that of MNX are 2.4 and 1.3, respectively.

**S10. Analysis of radionuclide concentrations using spatial GLMM**

The dataset consists of spatial measurements of $\gamma$-ray counts $y_i$ observed during $\ell_i$ seconds at the $i$th coordinate on the Rongelap island, $i = 1, \ldots, 157$. These data were analyzed by Diggle et al. (1998) and Evangelou and Roy (2019) among others using a spatial generalized linear mixed model (SGLMM).

We consider a Poisson SGLMM using a parametric link function for the $\gamma$-ray counts, that is, we assume $y_i|\mu_i \sim \text{Po}(\ell_i \mu_i)$ with $g(\mu_i) = z_i$ for $i =$
where $g_{\lambda}(\cdot)$ is a modified Box-Cox link given in Evangelou and Roy (2019) with parameter $\lambda$, and $z_i$’s are the latent variables. Let $y$ and $\mu$ denote the vectors of $y_i$’s and $\mu_i$’s, respectively. Then $z = (z_1, \ldots, z_{157})$ is modeled by a multivariate Gaussian distribution corresponding to a Gaussian random field (GRF) $Z$ at the sampled locations. In particular, we assume $Z|\beta, \sigma^2 \sim \text{GRF}(\beta, \sigma^2, \phi, \omega, \kappa)$, the GRF with constant mean $\beta$, Matérn correlation, variance $\sigma^2$, range $\phi$, relative nugget $\omega$ and smoothness $\kappa$. The partial sill parameter $\sigma^2$ is assigned a scaled-inverse-chi-square prior ($\text{ScInvX}^2(1, 1)$), and conditioned on $\sigma^2$, the mean parameter $\beta \sim N(0, 100\sigma^2)$. Let $\xi = (\lambda, \phi, \omega, \kappa)$. We consider estimating the marginal likelihood for $\xi$ (relative to an arbitrary reference point $\xi_1 = \tilde{\xi}$ to be defined later) by (1.2) in the main paper. Note that, the empirical Bayes estimate of $\xi$ is the point where the marginal likelihood function is maximized (see e.g. Roy et al., 2016). Since $\beta, \sigma^2$ can be analytically integrated out, one can work with the posterior density of $z$, $\pi_\xi(z|y)$. Here, we consider multiple IS estimator (1.2) in the main paper based on samples from the (transformed) density $\pi_\xi(\mu|y)$ (see Evangelou and Roy, 2019, for the reasons for considering the transformed samples). Thus, here $Q = \Pi = \{\pi_\xi(\mu|y), \xi \in \Xi\}$ for some $\Xi$ defined later.

In order to narrow down the potential region of search, we initially
choose a wide range of values for each component of $\xi$, and form a large grid, denoted by $\Xi$, by combining discrete points within these ranges. This gives us the set consisting of the following $9^4$ points:

$$\Xi = \{0, 0.5, \ldots, 4\} \times \{100, 425, \ldots, 2700\} \times \{0, 0.75, \ldots, 6\} \times \{0.1, 0.35, \ldots, 2.1\}. $$

The SFE method, after each range is scaled in $[0, 1]$, was applied to choose $k = 5$ points from $\Xi$. Markov chain samples from the $k$ densities $\pi_{\xi_i}(\mu|y)$, $i = 1, \ldots, k$ corresponding to this preliminary skeleton set are generated. We evaluate (1.2) in the main paper with $N_l = 1000$, $n_l = 1000$, $l = 1, \ldots, 5$ for all points in $\Xi$, and retain only those points for which the value of (1.2) in the main paper is not less than 60% of the maximum value. The maximum value is attained at $\tilde{\xi} = (1, 425, 2.25, 0.6)$ and there are 33 points satisfying this criterion. These points form the search set $\tilde{\Xi}$ which is a subset of

$$\tilde{\Xi} \subset \{1\} \times \{100, 425, \ldots, 1400\} \times \{1.50, 2.25, \ldots, 4.50\} \times \{0.35, 0.60, \ldots, 2.10\}. $$

Our aim is to choose $k = 5$ elements from $\tilde{\Xi}$, one of which must be $\tilde{\xi}$, to form the skeleton sets, using the methods discussed in Section 3 of the main paper, with the objective of estimating the ratios of marginal densities in $\Xi$ relative to $\tilde{\xi}$. The naive IS method with samples from the posterior density $\pi_{\xi}(\mu|y)$ is considered for comparison.

The SFE optimal set is computed on $\tilde{\Xi}$ after each dimension is scaled in $[0, 1]$. For SFS, we write (3.7b) in the main paper as an integral over
\((z, \log \sigma^2)\), because the prior for \(z\) is multivariate normal and \(\sigma^2 > 0\), and use the approximation given in Section S1 of the supplementary materials. The SEQ, MNX, and ENT optimal sets are computed iteratively. At each iteration, an estimate of the asymptotic relative standard error is computed using Theorem 2(a) based on 1000 samples for the first stage and 1000 samples for the second stage. We use different empirical convergence diagnostics (Roy, 2020) to check mixing of the Markov chains. Further computational details about our implementation are provided in Section S10.1 of this supplementary materials.

Finally, for each obtained skeleton set, we generate new samples which we use to estimate the ratio of the marginal likelihoods and its relative standard error for all \(\xi \in \Xi\). We generate a total of 50,000 samples which are equally divided between each proposal density (see Section S10.1 for further details). The maximum relative standard error estimates corresponding to one component of \(\xi\) fixed across the other components are shown in Figure 5. It can be seen that across all parameters, naive IS and SEQ have the highest variance, and that SFS, MNX, ENT have the lowest maximum variance.
Figure 5: Profile relative standard errors estimates for the Rongelap data.

One parameter is fixed and the maximum relative standard error across the other parameters is plotted against the fixed parameter. The crosses indicate points included in the skeleton set.

S10.1 Computational details

Here we give more details on how we produced the results in this Section. The computation is done in two phases. In the first phase we find the optimal skeleton set, $\xi$, for each method. In the second phase we compare the relative standard error of the naive and multiple IS estimators using the skeleton sets computed in the first phase. The total number of samples used for each method in the second phase is kept fixed and the same. In all calculations involving the asymptotic variance of the IS estimator, the SV estimate with the Tukey-Hanning window,

$$w_n(j) = 0.5[1 + \cos(\pi |j|/b_n)]I(|j| < b_n),$$
S10.1 Computational details

was used, where \( b_n = \sqrt{n} \). Markov chain samples are generated using the algorithm of Diggle et al. (1998).

Phase 1: Finding the optimal set of proposal densities

- **NIS**: This is not required because the proposal density is fixed at
  \( \xi_{\text{nis}} = \{\tilde{\xi}\} = \{(1, 425, 2.25, 0.6)\} \).

- **SFE**: This method is based on the Euclidean distance between the parameters. Each component of the parameter set \( \tilde{\Xi} \) is scaled to vary between 0 and 1 before the optimal set is computed. The point-swapping algorithm of Section S7.1 is used to find the optimal set. We find
  \( \xi_{\text{sfe}} = \{\tilde{\xi}, (1, 100, 3, 1.85), (1, 425, 3.75, 0.6), (1, 750, 3, 0.35), (1, 1075, 1.5, 0.35)\} \).

- **SFS**: This method requires the SKLD between two densities corresponding to two values of \( \xi \). We first write the integrals in (3.7a) of the main paper in terms of \( (z, \log \sigma^2) \), because the prior for \( z \) is multivariate normal and \( \sigma^2 > 0 \). Each ratio of integrals is approximated using the Laplace’s method given in Section S1. The point-swapping algorithm of Section S7.1 is used to find the optimal set. We find
  \( \xi_{\text{sfs}} = \{\tilde{\xi}, (1, 425, 3, 0.6), (1, 425, 3.75, 1.1), (1, 425, 4.5, 0.6), (1, 750, 1.5, 0.35)\} \).

- **SEQ**: In this case the optimal set is computed by starting at \( \xi^{(1)} = \)}
ξ_{nis}. Then, given that at the \( i \)th iteration, \( i = 2, \ldots, k \) we are at \( \xi^{(i-1)} \), we obtain \( \xi^{(i)} = \xi^{(i-1)} \cup \{ \xi' \} \), where \( \xi' \) corresponds to the point in \( \tilde{\Xi} \setminus \xi^{(i-1)} \) with the highest relative standard error. The relative standard error is again computed using 1,000 Gibbs samples for stage 1 and 1,000 new samples for stage 2. We find
\[
\xi_{seq} = \{ \tilde{\xi}, (1, 100, 2.25, 1.35), (1, 100, 2.25, 1.6), (1, 425, 3, 1.1), (1, 425, 3.75, 1.1) \}.
\]

- **MNX:** The optimal set is found by simulated annealing (Section S7.2). We start the simulated annealing algorithm at \( \xi_{sfs} \) and perform \( i_{\text{max}} = 250 \) iterations with \( T_0 = 0.001 \) and \( B = 10 \). The SV estimates were calculated using 1,000 Gibbs samples for stage 1 and 1,000 new samples for stage 2. We find
\[
\xi_{mnx} = \{ \tilde{\xi}, (1, 100, 2.25, 1.85), (1, 425, 1.5, 0.6), (1, 425, 2.25, 1.1), (1, 1075, 3, 0.35) \}.
\]

- **ENT:** The optimal set is found by simulated annealing (Section S7.2). We start the simulated annealing algorithm at \( \xi_{sfs} \) and perform \( i_{\text{max}} = 250 \) iterations with \( T_0 = 10 \) and \( B = 10 \). The optimality criterion used for this method is \( -\log \det(U) \) where \( U \) is the matrix with \((i, j)\)th element \( U_{ij} = (\hat{V}_q)_{ij}/(\hat{d}_i \hat{d}_j) \). The estimates \( \hat{d} \) and \( \hat{V}_q \) are computed from 1,000 Gibbs samples. We find
\[
\xi_{ent} = \{ \tilde{\xi}, (1, 100, 2.25, 1.35), (1, 425, 3, 1.1), (1, 750, 3.75, 0.35), (1, 1075, 1.5, 0.35) \}.
\]
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Phase 2: Estimation of the ratio of marginal densities

After the skeleton sets are found, we generate a total of $M = 50,000$ samples from the proposal densities, equally divided among all densities in the set. Thus, for NIS we simply take $M$ samples from the density corresponding to $\xi_{nis}$ and for the multiple IS methods we take $M/k$ samples from each density in the corresponding $\xi$ set. However, the total of $M/k$ samples must be split into stage 1, for estimating the ratio of marginals within $\xi$, $d$, and stage 2, for estimating the ratio of marginals over the whole set $\Xi$. To determine the optimal split we use equation (S8.15) where $\hat{v}_1(\xi)$ and $\hat{v}_2(\xi)$ are calculated from 1,000 stage 1 and 1,000 stage 2 samples.

For MNX, SEQ, and ENT the existing samples from Phase 1 are reused but for the space-filling methods, new samples are generated. We take $\hat{N}/k$ stage 1 samples from each density in the skeleton set where $\hat{N}$ is the integer that minimizes $\max_{\xi \in \Xi} \text{RelSE}(\xi, N, M - N)$, and $\hat{n}/k$ stage 2 samples, where $\hat{n} = M - \hat{N}$. This corresponds to stage 1 sample sizes of 500 and stage 2 sample sizes of 9,500 from each density for all methods.

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