Unbiased estimation of log normalizing constants with applications to Bayesian cross-validation

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Abstract

Posterior distributions often feature intractable normalizing constants, called marginal likelihoods or evidence, that are useful for model comparison via Bayes factors. This has motivated a number of methods for estimating ratios of normalizing constants in statistics. In computational physics the logarithm of these ratios correspond to free energy differences. Combining unbiased Markov chain Monte Carlo estimators with path sampling, also called thermodynamic integration, we propose new unbiased estimators of the logarithm of ratios of normalizing constants. As a by-product, we propose unbiased estimators of the Bayesian cross-validation criterion. The proposed estimators are consistent, asymptotically Normal and can easily benefit from parallel processing devices. Various examples are considered for illustration.

1 Setting

Monte Carlo methods address the approximation of intractable integrals of the form
\[ \pi(h) = \int h(x) \pi(dx), \]
where \( \pi \) is a probability distribution on a space \( X \), for instance a subset of \( \mathbb{R}^d \), and \( h \) a test function of interest. In Bayesian inference \( \pi \) is the posterior distribution that combines the prior density \( x \mapsto p(x) \) and the likelihood \( x \mapsto p(y \mid x) \), where the data \( y \) are assumed fixed, through the relation \( \pi(x) = p(x) p(y \mid x) / p(y) \) where \( p(y) = \int_X p(y \mid x) p(x) dx \). Using various Markov chain Monte Carlo methods (Robert and Casella, 2004; Stoltz et al., 2010; Brooks et al., 2011) one can approximate \( \pi(h) \) without having access to the normalizing constant \( p(y) \), which is often intractable. However, the interest is sometimes in the normalizing constant \( p(y) \) itself (Chen et al., 1997), also called the marginal likelihood or evidence, as it can be used for model comparison (e.g. Jeffreys, 1939; Bernardo and Smith, 2009; Dawid, 2011). Below we denote the normalizing constant of \( \pi \) by \( Z \), and the unnormalized density by \( \tilde{\pi}, \) so that \( \pi(x) = \tilde{\pi}(x)/Z \).

In this article we propose a new estimator of \( Z \), which combines unbiased Markov chain Monte Carlo (Jacob et al., 2017) with the path sampling identity (Gelman and Meng (1998); see also Chapter 5 of Chen et al. (2000)), also known as thermodynamic integration (Kirkwood, 1935; Neal, 2005; Calderhead and Girolami, 2009). The specificity of the proposed estimator is its unbiasedness for the logarithm of \( Z \), i.e. the expectation of the proposed estimator is exactly \( \log Z \). Existing estimators based on Markov chain Monte Carlo (Chen et al., 1997) are only asymptotically unbiased, while existing estimators based on annealed importance samplers (Neal, 2001) and sequential Monte Carlo samplers (Del Moral et al., 2006) are unbiased for \( Z \) and not for \( \log Z \).

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Leveraging unbiasedness for $\log Z$, we consider a Bayesian cross-validation (CV) criterion based on the logarithmic scoring rule (e.g. Alqallaf and Gustafson, 2001; Bornn et al., 2010; Vehtari et al., 2017). In cross-validation, one randomly splits the available data into training and validation, then the posterior distribution given the training data is numerically approximated, and finally the predictive performance on the validation data is assessed e.g. with the logarithmic scoring rule (Parry et al., 2012). We propose an estimator that is directly unbiased for these Bayesian cross-validation objectives, which can be averaged over independent copies to obtain consistent estimators and asymptotically exact confidence intervals from the central limit theorem for i.i.d. variables.

The rest of the document is structured as follows. Section 2 introduces the proposed estimators, and their tuning parameters are discussed. Numerical experiments in simple examples can be found in Section 3. Section 4 discusses our findings and future directions. The code to reproduce the experiments of the article is available at https://github.com/pierrejacob/unbiasedpathsampling.

2 Proposed estimators

We propose an unbiased estimator of $\log Z$ in Section 2.1, and obtain an unbiased estimator of a Bayesian cross-validation criterion in Section 2.2. Our implementation relies on the unbiased MCMC estimators of Jacob et al. (2017), which are briefly reviewed in Section 2.3, while Section 2.4 discusses tuning choices.

2.1 Unbiased path sampling

We first recall thermodynamic integration, or path sampling, for the approximation of normalizing constants (Chen et al., 1997; Gelman and Meng, 1998; Calderhead and Girolami, 2009; Cameron et al., 2014), see also Stoltz et al. (2010) for a thorough overview of related methods. We introduce a “path” of distributions: $\pi_\lambda(x) = \exp(-U_\lambda(x))/Z_\lambda$, with $\lambda \in [0,1]$, and $Z_\lambda = \int \exp(-U_\lambda(x)) dx$. We also write $\tilde{\pi}_\lambda(x) = \exp(-U_\lambda(x))$. The path is such that the object of interest is $r_{01} = \log(Z_1/Z_0)$. For instance, it could represent the difference in the logarithm of the marginal likelihood (or evidence) between two models in a Bayesian setting. In settings where $U_0$ and $U_1$ are given, a common example of path is the “geometric” path defined as $U_\lambda : x \mapsto (1 - \lambda)U_0(x) + \lambda U_1(x)$ for all $\lambda \in [0,1]$. The geometric path is not optimal in any way but it can be practical; we will also discuss other choices in the experiments.

The thermodynamic integration or path sampling identity relies on the following interchange between differentiation and integration (Kirkwood, 1935),

$$\nabla_\lambda \log Z_\lambda = \frac{\nabla_\lambda Z_\lambda}{Z_\lambda} = \frac{\nabla_\lambda \left[ \int \tilde{\pi}_\lambda(x) dx \right]}{Z_\lambda} = \int \nabla_\lambda \log \tilde{\pi}_\lambda(x) \pi_\lambda(x) dx,$$

where $\nabla_\lambda$ denotes derivative with respect to $\lambda$. The formula holds under regularity conditions such as: $\lambda \mapsto \nabla_\lambda \tilde{\pi}_\lambda(x)$ is continuous for all $x$, and there exists an integrable function $x \mapsto \tilde{\pi}(x)$ such that $|\nabla_\lambda \tilde{\pi}_\lambda(x)| \leq \tilde{\pi}(x)$ for all $x$ and for all $\lambda$. Denoting by $E_\lambda$ expectations with respect to $\pi_\lambda$, integrating the above expression with respect to $\lambda$ yields

$$r_{01} = \log Z_1 - \log Z_0 = - \int_0^1 E_\lambda[\nabla_\lambda U_\lambda(X)]d\lambda.$$

By introducing an arbitrary density $\lambda \mapsto q(\lambda)$, strictly positive on $(0,1)$, we obtain the path sampling identity:

$$r_{01} = - \int_0^1 \frac{E_\lambda[\nabla_\lambda U_\lambda(X)]}{q(\lambda)} q(\lambda)d\lambda.$$

This is useful if we can approximate integrals with respect to $\lambda$ by Monte Carlo or numerical integration, and if we can approximate the inside expectation $E_\lambda[\nabla_\lambda U_\lambda(X)]$ by Markov chain Monte Carlo (MCMC,
Robert and Casella (2004)), for instance.

For instance, we might discretize \( \lambda \) on \([0, 1]\) by introducing a grid of points \( \lambda^{[1]}, \ldots, \lambda^{[L]} \). Then for each \( l \in \{1, \ldots, L\} \) and \( \lambda = \lambda^{[l]} \), we could approximate each \( \mathbb{E}_{\lambda}[\nabla_\lambda U_\lambda(X)] \) with an MCMC estimator based on \( T_l \) iterations. We could finally aggregate these estimators to obtain a consistent estimator for \( r_{01} = \log(Z_1/Z_0) \), as \( L \to \infty \) and as \( T_l \to \infty \) for all \( l \in \{1, \ldots, L\} \) (Gelman and Meng, 1998). Instead, if we directly define an MCMC algorithm targeting the distribution \( q(d\lambda)\pi_\lambda(dx) \) on the joint space \([0, 1] \times \mathcal{X} \), then we can obtain an estimator of \( r_{01} \) that would be valid in a single asymptotic regime, as the number of iterations goes to infinity.

Here we denote by \( E(\lambda) = -\mathbb{E}_{\lambda}[\nabla_\lambda U_\lambda(X)] \) the inner expectation in (3), and we introduce \( \hat{E}(\lambda) \), an unbiased estimator of \( E(\lambda) \) that we can generate for any \( \lambda \in [0, 1] \); we defer the construction of such estimators to Section 2.3. We can then define an estimator of \( r_{01} = \log(Z_1/Z_0) \) with the following procedure.

1. Draw \( \lambda \sim q(d\lambda) \), a distribution supported on \([0, 1] \).
2. Given \( \lambda \), generate a variable \( \hat{E}(\lambda) \) with expectation \( \hat{E}(\lambda) = -\mathbb{E}_{\lambda}[\nabla_\lambda U_\lambda(X)] \).
3. Return \( \hat{r}_{01} = \hat{E}(\lambda)/q(\lambda) \).

The random variable \( \hat{r}_{01} \) has expectation \( r_{01} \) by the law of iterated expectations, and we refer to it as an unbiased path sampling estimator (UPS). Note that sequential Monte Carlo samplers and related methods (Del Moral et al., 2006) would provide unbiased estimators of \( Z \) and not of \( \log Z \). Thus these estimators will not be unbiased for \( r_{01} \). We will now see that the lack of bias on the logarithmic scale can be exploited to propose new estimators of Bayesian cross-validation criteria.

### 2.2 Unbiased Bayesian cross-validation

A number of articles discuss the computational difficulties associated with Bayesian cross-validation, e.g. Alqallaf and Gustafson (2001); Bhattacharya and Haslett (2007); Bornn et al. (2010); Lamnisos et al. (2012); McVinish et al. (2013); Vehtari et al. (2017). We first define the object of interest, before presenting our estimator. Let \( x \) denote an unknown parameter with prior density \( p(x) \), and let \( y_{1:n} = \{y_1, \ldots, y_n\} \) denote the data composed of \( n \) units. The likelihood function is denoted by \( x \mapsto p(y_{1:n} | x) \). Cross-validation is then a measure of accuracy in predicting \( y \) using the training data \( T \). A typical choice is the logarithmic score \( \log p(V | T) \) (see Parry et al., 2012, for a discussion on the choice of scoring rule) where \( p(V | T) = \int p(V | T, x) p(x | T) \, dx \) is the posterior predictive density given \( T \) and evaluated on \( V \). Note that \( p(V | T, x) \) simplifies to \( p(V | x) \) if the data are modeled as conditionally independent given \( x \). The cross-validation objective, “CV” below, is defined as an average over all splits \( (T, V) \) of size \( (n_T, n_V) \).}

\[
CV = -(n \choose n_T)^{-1} \sum_{T,V \in \mathcal{S}} \log p(V | T),
\]

where \( \mathcal{S} \) is the set of partitions of \( \{1, \ldots, n\} \) into \( T, V \) of sizes \( n_T, n_V \). To approximate this criterion, one can sample partitions \( T, V \), and approximate \( \log p(V | T) \) with MCMC estimators. For any fixed \( n_T \), this procedure would give consistent estimates of \( \text{CV} \) as the number of splits and the number of MCMC iterations go to infinity.

Given a split \( T, V \), we can estimate \( \log p(V | T) \) using the path sampling identity and the unbiased estimators of the previous section. Indeed, that quantity is a log-ratio of the normalizing constants \( p(T) \)
and \( p(T, V) \). By introducing the path

\[
\forall \lambda \in [0, 1] \quad \tilde{\pi}_\lambda(x) = p(x) p(T \mid x) p(V \mid T, x)^\lambda,
\]

we have \( Z_0 = \int \tilde{\pi}_0(x) \, dx = p(T) \) and \( Z_1 = \int \tilde{\pi}_1(x) \, dx = p(T, V) \), thus \( \log(Z_1/Z_0) = \log p(V \mid T) \). Other paths can be used, as long as \( Z_0 = p(T) \) and \( Z_1 = p(T, V) \). Assuming that we can perform unbiased MCMC targeting \( \pi_\lambda \) for all \( \lambda \), and that we can evaluate \( \nabla_\lambda \log \tilde{\pi}_\lambda(x) \) for all \( x, \lambda \), then we can obtain unbiased estimators of \( \log p(V \mid T) \).

This motivates the following strategy: sample a split \( T, V \) uniformly from \( \mathcal{S} \), and then obtain an unbiased estimator of \( -\log p(V \mid T) \) given \( T, V \). The resulting estimator is directly unbiased for CV in (4), by the law of iterated expectations. We summarize the procedure below.

1. Sample index sets \( T, V \) uniformly at random over \( \mathcal{S} \), the set of partitions of \( \{1, \ldots, n\} \) into a set of size \( n_T \) and a set of size \( n_V = n - n_T \).
2. Given \( T, V \), introduce a path \((\tilde{\pi}_\lambda)\) with \( \lambda \in [0, 1] \), with constant \( Z_\lambda = \int \tilde{\pi}_\lambda(x) \, dx \) such that \( r_{01} = \log(Z_1/Z_0) = \log p(V \mid T) \). Given the path, obtain an unbiased estimator of \( \log p(V \mid T) \), denoted by \( \tilde{r}_{01} \).
3. Return \(-\tilde{r}_{01}\), an unbiased estimator of CV in (4).

Note how the lack of bias on the logarithmic scale is important for the above procedure to produce an unbiased estimator of CV. We could also extend the above procedure to allow for non-uniform sampling of the partitions from \( \mathcal{S} \).

### 2.3 Reminders on unbiased MCMC

The UPS algorithm of Section 2.1 presupposes the ability to unbiasedly estimate expectations of the form \( \pi(h) := \int h(x) \pi(dx) \), where \( \pi \) is a target distribution, and \( h \) is a test function. In this paper, we use unbiased estimators recently proposed in Jacob et al. (2017), themselves building on those in Glynn and Rhee (2014), though other unbiased estimators could be substituted. We thus briefly recall the estimators proposed in Jacob et al. (2017), and the associated tuning parameters. Introduce a Markov kernel \( P \), i.e. \( P(x, \cdot) \) is a distribution on \( \mathcal{X} \) for all \( x \in \mathcal{X} \), and for any measurable set \( A \), the function \( x \mapsto P(x, A) \) is measurable, and assume that \( P \) is \( \pi \)-invariant. Next, introduce a “coupled” Markov kernel \( \tilde{P} \) on the joint space \( \mathcal{X} \times \mathcal{X} \), such that for all \( x, \tilde{x}, A, B \), \( \tilde{P}((x, \tilde{x}), (A, \mathcal{X})) = P(x, A) \) and \( \tilde{P}((x, \tilde{x}), (\mathcal{X}, B)) = P(\tilde{x}, B) \), i.e. \( \tilde{P} \) couples \( P \) with itself. Furthermore we will construct \( \tilde{P} \) such that, at least for certain pairs \((x, \tilde{x})\), the distribution \( \tilde{P}((x, \tilde{x}), \cdot) \) puts some non-zero mass on the diagonal \( \{(x', \tilde{x}') \in \mathcal{X} \times \mathcal{X} : x' = \tilde{x}'\} \).

With these elements, introduce two Markov chains \((X_n)_{n \geq 0}\) and \((\tilde{X}_n)_{n \geq 0}\) as follows. First, \( X_0 \) and \( \tilde{X}_0 \) are drawn from an initial distribution (for simplicity, independently). Then \( X_1 \) is sampled from \( P(X_0, \cdot) \). At step \( n \geq 1 \), the pair \((X_{n+1}, \tilde{X}_n)\) is sampled from the coupled kernel \( \tilde{P}((X_n, \tilde{X}_{n-1}), \cdot) \). The construction must be such that, for all \( n \geq 0 \), \( X_n \) has the same distribution as \( \tilde{X}_n \), and such that there exists a random variable \( \tau \), referred to as the “meeting time,” such that for all \( n \geq \tau \), \( X_n = \tilde{X}_{n-1} \), almost surely. We then introduce two integers, \( k \geq 0 \) and \( m \geq k \), which will be tuning parameters, and define the estimator

\[
H_{k:m} = \frac{1}{m-k+1} \sum_{n=k}^{m} h(X_n) + \sum_{n=k+1}^{\tau-1} \min\left(1, \frac{n-k}{m-k+1}\right) \left(h(X_n) - h(\tilde{X}_{n-1})\right).
\]

In the above expression, the convention is that the sum \( \sum_{n=k+1}^{\tau-1} \) is equal to zero in the event \( \tau - 1 < k \). The estimator \( H_{k:m} \) is a standard Markov chain average \((m-k+1)^{-1} \sum_{n=k}^{m} h(X_n)\) based on \( m \) iterations and a burn-in of \( k - 1 \) steps, plus another term that is precisely such that \( \mathbb{E}_{MC}[H_{k:m}] = \pi(h) \), where
\( E_{\text{MC}} \) denotes expectation with respect to all random variables involved in the Monte Carlo algorithm; see Jacob et al. (2017) for more precise statements.

### 2.4 Tuning choices

A number of choices have to be made for the proposed estimators to be operational. The first choice is that of a path of distributions. There are generic choices such as the geometric path, and choices motivated by algorithmic considerations on a case-by-case basis. We will discuss the choice of paths through examples, in Section 3.

Given a path of distributions \((\pi_\lambda)\), algorithms approximating expectations \(E_{\lambda}\) with respect to \(\pi_\lambda\) typically involve tuning parameters. We describe the tuning of unbiased MCMC in Section 2.4.1. Then we discuss choices of distribution \(q(d\lambda)\) in Section 2.4.2.

#### 2.4.1 Tuning of unbiased MCMC

The unbiased MCMC estimators described in Section Section 2.3 require the specification of a Markov kernel \(P\), a coupled kernel \(\bar{P}\), and an initial distribution for the chains. Specifying these objects is typically difficult, but not specific to the setting of normalizing constant estimation. Therefore we defer to the large literature on MCMC algorithms (Robert and Casella, 2004; Brooks et al., 2011), as well as the relevant discussions in Jacob et al. (2017) in the context of unbiased MCMC. Ultimately we will care about the expected cost and the variance of the proposed unbiased estimators, in order to maximize the efficiency of the proposed estimators, as discussed in the next section.

We thus discuss the expected cost and variance of unbiased MCMC estimators. Since the meeting time \(\tau\) is a random variable, the cost of generating \(H_{k,m}\) in (6) is random. Neglecting the cost of drawing from the initial distribution, the cost amounts to that of one draw from the kernel \(P\), \(\tau - 1\) draws from the kernel \(\bar{P}\), and \(m - \tau\) draws from \(P\) if \(\tau < m\). Overall that leads to an expected cost of \(C := E_{\text{MC}}[\tau + \max(\tau, m)]\) units, where each unit is the cost of drawing from \(P\), and assuming that one sample from \(\bar{P}\) costs two units. Note that the expected cost is approximately \(m + E_{\text{MC}}[\tau]\) when \(m\) is much larger than typical values of \(\tau\). The guidelines for the choice of \(k\) and \(m\) in Jacob et al. (2017) are to set \(k\) such that the probability of \(\{\tau > k\}\) is small, based on draws of \(\tau\). Then \(m\) can be set to be a multiple of \(k\), such as \(2k\) or \(5k\), so that the proportion of discarded iterations remains small. In Jacob et al. (2017), under further considerations on the Markov kernels, it is shown that the variance of unbiased MCMC estimators is equivalent to the variance of standard MCMC estimators when \(k\) and \(m\) are large enough. Informally this confirms that the increased variance incurred by the removal of the bias can be inconsequential if we choose \(k\) and \(m\) carefully.

For our purposes, the test function \(h\) will be \(x \mapsto -\nabla_\lambda U_\lambda(x)\) and the target distribution \(\pi_\lambda\), for different \(\lambda \in [0, 1]\). We will index the meeting time \(\tau\), the integers \(k\) and \(m\) and the expected cost \(C\) by \(\lambda\). The corresponding estimator is denoted \(\hat{E}(\lambda)\) and has expectation \(E(\lambda) = E_{\lambda}[-\nabla_\lambda U_\lambda(X)]\). We also introduce notation for the second moment of \(\hat{E}(\lambda)\): let \(m_2(\lambda) = E_{\text{MC}}[\hat{E}(\lambda)^2]\) for all \(\lambda \in [0, 1]\). We will assume that the kernels \(P_\lambda\) and \(\bar{P}_\lambda\) corresponding to each target \(\pi_\lambda\) are such that \(m_2(\lambda) < \infty\) and \(C_\lambda < \infty\) for all \(\lambda \in [0, 1]\); see Jacob et al. (2017) and Middleton et al. (2018) for assumptions on the kernels under which the second moment \(m_2(\lambda)\) and the cost \(C_\lambda\) are guaranteed to be finite.

#### 2.4.2 Tuning of the distribution \(q(d\lambda)\)

Given unbiased MCMC estimators \(\hat{E}(\lambda)\) of \(E(\lambda)\) for all \(\lambda\), we move on to the choice of probability density function \(\lambda \mapsto q(\lambda)\). Various choices lead to valid estimators, provided that the support of \(q(d\lambda)\) is the entire interval \([0, 1]\), but we might want to maximize the efficiency of the estimator \(\hat{r}_{01}\) of \(r_{01} = \log(Z_1/Z_0)\). We introduce the inefficiency as the product of expected cost, \(\int C_\lambda q(\lambda) d\lambda\) and variance \(\sqrt{\text{Var}[\hat{r}_{01}]},\) motivated by Glynn and Heidelberger (1991); Glynn and Whitt (1992). The efficiency is defined
as the inverse of the inefficiency. The variance $\mathbb{V}[\hat{r}_{01}]$ is equal to $\mathbb{E}_{MC}[\hat{r}_{01}^2] - r_{01}^2$, and $\hat{r}_{01} = \hat{E}(\lambda)/q(\lambda)$ with $\lambda \sim q(\lambda)$, thus $\mathbb{E}_{MC}[\hat{r}_{01}^2] = \int (m_2(\lambda)/q(\lambda)) \, d\lambda$, which leads to the following optimization program over functions $q$,

$$\min_q \left\{ \int C_\lambda q(\lambda) \, d\lambda \times \left( \int \frac{m_2(\lambda)}{q(\lambda)} \, d\lambda - r_{01}^2 \right) \right\}$$

such that $\int q(\lambda) \, d\lambda = 1$, and $\forall \lambda \in [0,1] \quad q(\lambda) \geq 0$. \hfill (7)

The above program is simpler if the cost $C_\lambda$ is constant over $\lambda$. This can be enforced by an appropriate choice of parameters $m_\lambda$, since $C_\lambda \approx m_\lambda + \mathbb{E}_{MC}[\tau_\lambda]$. Therefore we will choose $m_\lambda$ to make $C_\lambda$ approximately constant, based on preliminary draws of $\tau_\lambda$ on a grid of values of $\lambda$.

If $C_\lambda$ is constant over $\lambda$, then the solution of the above minimization problem is given by $\lambda \mapsto g^*(\lambda) \propto \sqrt{m_2(\lambda)}$. In Gelman and Meng (1998) that solution is given, and then the verification that this is indeed a solution is done via Cauchy-Schwarz. Here we provide an informal derivation of the solution, in the case where $C_\lambda$ is constant over $\lambda$. We write the function to minimize as $\int m_2(\lambda)/q(\lambda) \, d\lambda$, and introduce the Lagrangian

$$\int \frac{m_2(\lambda)}{q(\lambda)} \, d\lambda + \xi \left( \int q(\lambda) \, d\lambda - 1 \right).$$

We would like to differentiate with respect to $q$ and set the derivative to zero. Introduce the directional derivative $\frac{d}{d\varepsilon}(q(\lambda) + \varepsilon v(\lambda))$ where $v(\lambda)$ is a function. Replacing $q(\lambda)$ by $q(\lambda) + \varepsilon v(\lambda)$ and differentiating with respect to $\varepsilon$ in the Lagrangian yields

$$\frac{d}{d\varepsilon} \left\{ \int \frac{m_2(\lambda)}{q(\lambda) + \varepsilon v(\lambda)} \, d\lambda + \xi \left( \int (q(\lambda) + \varepsilon v(\lambda)) \, d\lambda - 1 \right) \right\}$$

$$= \int \frac{d}{d\varepsilon} \left\{ \frac{m_2(\lambda)}{q(\lambda) + \varepsilon v(\lambda)} + \xi (q(\lambda) + \varepsilon v(\lambda)) \right\} \, d\lambda \quad \text{(interchange deriv. and integr.)} \hfill (9)$$

$$= \int \left\{ \frac{-m_2(\lambda)v(\lambda)}{(q(\lambda) + \varepsilon v(\lambda))^2} + \xi v(\lambda) \right\} \, d\lambda.$$

Setting $\varepsilon$ to zero yields $\int \left\{ -m_2(\lambda)/q(\lambda)^2 + \xi v(\lambda) \right\} \, d\lambda$, and trying to set that expression to zero simultaneously for every choice of $v$, we obtain $-m_2(\lambda)/(q(\lambda)^2) + \xi = 0$, i.e. $q(\lambda) \propto \sqrt{m_2(\lambda)}$. This gives the candidate solution.

### 2.4.3 Proposed tuning procedure

We now combine the above sections into practical guidelines for the proposed estimators.

1. Set up path, $\tilde{\pi}_\lambda$ for $\lambda \in [0,1]$, such that $\int \tilde{\pi}_0(x) \, dx = Z_0$ and $\int \tilde{\pi}_1(x) \, dx = Z_1$, and such that the object of interest is $\log(Z_1/Z_0)$.

2. For $\lambda$ in a grid of $L + 1$ values $0 = \lambda[0] \leq \ldots \leq \lambda[L] = 1$, construct and tune an unbiased MCMC (initial distribution, Markov kernel $P$, and coupled kernel $\tilde{P}$) targeting $\pi_\lambda$, and draw independent samples of the associated meeting times $\tau_\lambda$.

3. Based on the distribution of meeting times at each $\lambda$, choose $k_\lambda$ and $m_\lambda$, to complete the tuning of the unbiased estimator $\hat{E}(\lambda)$. The choice of $m_\lambda$ can be made such that the expected cost $C_\lambda = \mathbb{E}_{MC}[\tau_\lambda - 1 + \max(\tau_\lambda, m_\lambda)]$ is approximately constant over $\lambda$.

4. Draw independent samples of $\hat{E}(\lambda)$ using the chosen $k_\lambda$ and $m_\lambda$, and estimate $m_2(\lambda) = \mathbb{E}_{MC}[\hat{E}(\lambda)^2]$ for $\lambda$ in the grid $\lambda[0] \leq \ldots \leq \lambda[L]$.

5. Use these estimates to define a distribution $q(\lambda)$, such that $q(\lambda)$ is approximately proportional to $\sqrt{m_2(\lambda)}$ for all $\lambda$ in $[0,1]$. 

6
We describe a concrete way of performing step 5, for completeness. Given a grid of values $0 = \lambda^{[0]} \leq \ldots \leq \lambda^{[L]} = 1$ and associated estimates $(\hat{m}_2(\lambda^{[l]}))^1/2$ of $(m_2(\lambda^{[l]}))^1/2$ for $l \in \{0, \ldots, L\}$ obtained in step 4, we can define a distribution $q(d\lambda)$ that is piecewise uniform on the intervals $[\lambda^{[l]}, \lambda^{[l+1]}]$, and such that
\[
\forall l \in \{0, \ldots, L - 1\} \quad \int_{\lambda^{[l]}}^{\lambda^{[l+1]}} q(d\lambda) \propto (\lambda^{[l+1]} - \lambda^{[l]}) \times \frac{\sqrt{\hat{m}_2(\lambda^{[l]})} + \sqrt{\hat{m}_2(\lambda^{[l+1]})}}{2}.
\]

Sampling from such a distribution can be done in order $O(\log L)$ operations, by first selecting an interval $[\lambda^{[l]}, \lambda^{[l+1]}]$ with probability $\int_{\lambda^{[l]}}^{\lambda^{[l+1]}} q(d\lambda)$, and then sampling uniformly from that interval.

After the preliminary phase described in the five steps above, the generation of estimators $\hat{r}_{01}$ can proceed as follows. First, $\lambda$ is drawn from $q(d\lambda)$ obtained in step 5 above. We then find the nearest value $\lambda^{[l]}$ in the grid, with index $l \in \{0, \ldots, L\}$. We can look up tuning parameters corresponding to $\lambda^{[l]}$ for the unbiased MCMC estimators, stored during step 2 above, and the values of $k_{\lambda^{[l]}}$ and $m_{\lambda^{[l]}}$ stored during step 3 above. Using these tuning values we can generate an unbiased estimator $\hat{E}(\lambda)$ of $E(\lambda) = -\mathbb{E}_\lambda[\nabla_\lambda U_\lambda(X)]$. The estimator $\hat{r}_{01} = \hat{E}(\lambda)/q(\lambda)$ is finally returned.

3 Numerical experiments

The numerical experiments are structured as follows. Section 3.1 contains toy examples of unbiased path sampling estimators. Section 3.2 considers logistic regressions with different choices of paths and of unbiased MCMC estimators, and an example taken from Epifani et al. (2008); Vehari et al. (2017). Section 3.3 considers linear regressions with examples taken from Alqallaf and Gustafson (2001); Peruggia (1997); Vehari et al. (2017). Throughout the experiments, 95% confidence intervals for an estimand $\mu$ are obtained as $\hat{\mu} \pm 1.96s/\sqrt{M}$, where $\hat{\mu}$ is the mean of $M$ independent unbiased estimators of $\mu$ and $s$ is their sample standard deviation. These confidence intervals are justified asymptotically as $M \to \infty$ by the central limit theorem for i.i.d. random variables, provided that the variance of the unbiased estimators is finite. On parallel machines and under budget constraints, valid confidence intervals can be constructed following Glynn and Heidelberger (1991); see also related remarks in Jacob et al. (2017).

3.1 Toy examples of normalizing constant estimation

3.1.1 Normal example

We start with the example of Section 4.4 in Gelman and Meng (1998). Consider $\tilde{\pi}_\lambda(\beta) = \exp(-(\beta - \lambda D)^2/2)$, with $D = 4$, which corresponds to a sequence of distributions $\pi_\lambda$ that interpolates between $\mathcal{N}(0,1)$ and $\mathcal{N}(D,1)$. The normalizing constants are $Z_\lambda = \sqrt{2\pi}$ for all $\lambda$, so that $r_{01} = 0$. Here we have $\nabla_\lambda \log \tilde{\pi}_\lambda : x \mapsto D(\beta - \lambda D)$. To estimate expectations $\mathbb{E}_\lambda$, we consider a Metropolis–Hastings (MH) algorithm, starting from an initial distribution $\mathcal{N}(-1,2^2)$, and with Normal random walk proposals with variance 1. We couple this algorithm by maximally coupling the proposal distributions (Jacob et al., 2017).

We start with a grid of values of $\lambda$: $\lambda^{[l]} = l/L$ for $l \in \{0, \ldots, L\}$, with $L = 10$. For each $\lambda^{[l]}$, we run coupled MH chains until they meet, 100 times independently. We obtain a distribution of meeting times $\tau$ for each $\lambda$, represented on Figure 1a. The overlaid full line represents the 99% quantiles, which we denote by $k_0, \ldots, k_L$. We also compute the average meeting times for each $\lambda^{[l]}$, which we denote $\bar{\tau}_0, \ldots, \bar{\tau}_L$. We then define
\[
\forall l \in \{0, \ldots, L\} \quad m_l = 5 \times \max_j (k_j) + \max_j (\bar{\tau}_j) - \bar{\tau}_l.
\]

This ensures that the expected cost $C_\lambda$, which is approximately equal to $m_\lambda + \mathbb{E}_{MC}[\tau_\lambda]$, is constant over $\lambda$, while also ensuring that $m_\lambda \geq 5k_\lambda$ for all $\lambda$. 

7
meeting times
second
moment
10
20
40
50
0.00 0.25 0.50 0.75 1.00
λ
meeting times
(a) Meeting times for different λ.

(b) Estimates of $\sqrt{m_2(\lambda)}$.

(c) Estimators $\hat{E}(\lambda)/q(\lambda)$.

Figure 1: Normal target example of Section 3.1.1. Left: distribution of meeting times for $\lambda \in \{0/L, 1/L, \ldots, L/L\}$ and $L = 10$, in violin plots. The 99% quantiles are shown as a full line. Middle: estimates of $\sqrt{m_2(\lambda)}$ on a grid of values of $\lambda$, used to define a proposal distribution $q(d\lambda)$. Right: estimators $\hat{E}(\lambda)/q(\lambda)$ plotted against $\lambda$, where $\lambda$ is drawn from $q(d\lambda)$.

Given values of $k_l$ and $m_l$, for each $\lambda[l]$ in the grid of $L + 1$ values defined above, we approximate the first and second moments of $\pi_\lambda$ with 100 independent estimators. We use these moments to redefine the initial distribution of the Markov chains, which we set to a Normal distribution adapted to $\pi_\lambda$, and to tune the proposal standard deviation, which we set to be the estimated standard deviation of $\pi_\lambda$. At this point we could sample meeting times again and choose new values for $k_\lambda$ and $m_\lambda$, but we omit this here. Next, we estimate $\sqrt{m_2(\lambda)}$ for each $\lambda[l]$ in the grid, and define $q(d\lambda)$ accordingly, following step 5 in Section 2.4. The estimates of $\sqrt{m_2(\lambda)}$ are shown in Figure 1b. This completes the tuning phase, and we can now generate unbiased estimators $\hat{r}_{01} = \hat{E}(\lambda)/q(\lambda)$ of $r_{01} = \log(Z_1/Z_0)$. We show these estimates against $\lambda$ in Figure 1c. These are generated 5,000 times independently. Concretely, they yield the confidence interval $[-0.11, 0.12]$ for the estimand $r_{01} = 0$ at level 95%.

3.1.2 Double-well example

We perform similar experiments on a path of two-dimensional distributions linking the potential $U_0 : x \mapsto (x_1 + 2)^2 + (x_2^2/2)$, corresponding to a Normal distribution centered at $(-2, 0)$ and with diagonal variances $(1/2, 1)$, to the potential $U_1 : x \mapsto (1/10)(((x_1 - 1)^2 - x_2^2)^2 + 10(x_1^2 - 5)^2 + (x_1 + x_2)^4 + (x_1 - x_2)^4)$. The latter is a double-well potential, with modes around $(-2, 0)$ and $(2, 0)$. By numerical integration we find $\log(Z_1/Z_0)$ to be approximately $-6.9$. We introduce the geometric path $U_\lambda(x) = (1 - \lambda)U_0(x) + \lambda U_1(x)$.

For each $\lambda$, we start chains from a Normal centered at $(-2, -2)$ and with covariance matrix $I_2$, the identity matrix of size $2 \times 2$. We consider random walk MH schemes with Normal proposal, with covariance $2I_2$; the coupled version relies on maximal couplings of the proposals, as in the previous section.

We draw 1,000 meeting times independently, for $\lambda[l] = l/L$ with $l \in \{0, \ldots, L\}$ and $L = 10$. The distributions are shown in violin plots in Figure 2a. We observe much larger meeting times for $\lambda$ close to one, which corresponds to the MH chains struggling to explore both modes of the double-well potential.

We thus conservatively set $k_l$ to be twice the 99% quantiles of the meeting times, instead of the quantiles themselves.

We follow the same heuristics as in Section 3.1.1 for the choice of $m_l$. Without modifying the initial distribution nor the proposal distribution of the MH chains, we estimate $\sqrt{m_2(\lambda)}$ for each $\lambda[l]$ in the grid, based on 100 independent copies, and define $q(d\lambda)$ following again step 5 in Section 2.4. The estimates of $\sqrt{m_2(\lambda)}$ are shown in Figure 2b. Finally we generate unbiased estimators $\hat{r}_{01} = \hat{E}(\lambda)/q(\lambda)$ of $r_{01} = \log(Z_1/Z_0)$, and represent these estimates against $\lambda$ in Figure 2c. These are generated 1,000 times independently and result in the 95% confidence interval $[-7.55, -6.37]$ for the estimand $r_{01} \approx -6.9$. 
Figure 2: Double-well potential example of Section 3.1.2. Left: distribution of meeting times for \( \lambda \in \{0/L, 1/L, \ldots, L/L\} \) and \( L = 10 \), in violin plots. Twice the 99\% quantiles are shown as a full line. Middle: estimates of \( \sqrt{m_2(\lambda)} \) on a grid of values of \( \lambda \), used to define a proposal distribution \( q(d\lambda) \). Right: estimators \( \hat{E}(\lambda)/q(\lambda) \) plotted against \( \lambda \), where \( \lambda \) is drawn from \( q(d\lambda) \).

3.2 Logistic regression

We consider a logistic regression setting, where a tuning-free Gibbs sampler can be used to estimate \( E(\lambda) \) conditional on each \( \lambda \), provided the path is chosen appropriately. Let us consider the regression of \( Y = (y_1, \ldots, y_n) \in \{0, 1\}^n \) on covariates \( D = (d_1, \ldots, d_n) \in \mathbb{R}^{n \times p} \). Throughout all the probability statements are conditioned on \( D \), which we sometimes omit from the notation. The logistic regression model assumes \( p(y_i = 1 \mid \beta) = \expit(d_i^\top \beta) \), where \( \expit : z \mapsto 1/(1 + \exp(-z)) \). The parameters \( \beta \in \mathbb{R}^p \) are the regression coefficients of interest, filling the role of the target parameters \( x \in X \) in the presentation of Section 2. The prior on \( \beta \) is Normal \( \mathcal{N}(b, B) \), with mean \( b \) and covariance matrix \( B \), and density denoted by \( \beta \mapsto \varphi(\beta; b, B) \). The posterior distribution has unnormalized probability density function:

\[
p(\beta \mid Y) \propto \varphi(\beta; b, B) \prod_{i=1}^n \left( \expit(d_i^\top \beta)^{y_i} (1 - \expit(d_i^\top \beta))^{1-y_i} \right). \tag{12}
\]

With basic manipulations this is equivalent to the following simpler form

\[
p(\beta \mid Y) \propto \varphi(\beta; b, B) \prod_{i=1}^n \frac{\exp(d_i^\top \beta y_i)}{1 + \exp(d_i^\top \beta)}. \tag{13}
\]

The Pólya-Gamma Gibbs (PGG) sampler (Polson et al., 2013; Choi and Hobert, 2013) is a Gibbs sampler that targets \( p(\beta \mid Y) \) through the introduction of auxiliary variables \( W \). First, we recall that the Pólya-Gamma distribution with parameters \((1, c)\), denoted by \( \text{PG}(1, c) \), has a density \( x \mapsto \text{pg}(x; c) \) defined for all \( c \geq 0 \), \( x > 0 \) as

\[
\text{pg}(x; c) = \cosh \left( \frac{c}{2} \right) \exp \left( -\frac{c^2 x}{2} \right) \sum_{k=0}^\infty (-1)^k \frac{(2k + 1)^2}{\sqrt{2^k k!}} \exp \left( -\frac{(2k + 1)^2}{8x} \right). \tag{14}
\]

Introduce \( n \) auxiliary variables \( W = (W_1, \ldots, W_n) \), independent of each other given \( \beta \), such that \( W_i \) follows \( \text{PG}(1, |d_i^\top \beta|) \) for all \( 1 \leq i \leq n \). An extended target distribution is defined as \( p(\beta, \omega \mid Y) \propto p(\beta \mid Y)g(\omega \mid \beta) \), where \( \omega \) denotes a realization of \( W \), and \( g(\omega \mid \beta) = \prod_{i=1}^n \text{pg}(\omega_i; |d_i^\top \beta|) \). The appeal of this extension is that we can write the target as

\[
p(\beta, \omega \mid Y) \propto \varphi(\beta; b, B)g(\omega \mid \beta) \prod_{i=1}^n \frac{\exp(d_i^\top \beta y_i)}{1 + \exp(d_i^\top \beta)}, \tag{15}
\]
and therefore the conditional of $\beta$ given $\omega, Y$ simplifies to

$$p(\beta \mid \omega, Y) \propto \varphi(\beta; b, B) \prod_{i=1}^{n} \exp \left( y_i d_i^T \beta - \frac{d_i^T \beta}{2} - \frac{(d_i^T \beta)^2}{2} \right).$$ (16)

Noting that the prior on $\beta$ is Normal, we find a Normal distribution for $\beta$ given $\omega, Y$, with mean $\mu(\omega)$ and covariance matrix $\Sigma(\omega)$ with $\Sigma(\omega) = (D^T \text{diag}(\omega) D + B^{-1})^{-1}$, and $\mu(\omega) = \Sigma(\omega)(D^T \hat{Y} + B^{-1} b)$ where $\hat{Y} = (y_1 - \frac{1}{2}, \ldots, y_n - \frac{1}{2})$. To summarize, the PGG sampler generates a chain $(\beta(t), W(t))_{t \geq 0}$ in two steps:

1. given $(\beta(t), W(t))$, draw $\beta(t+1) \sim \mathcal{N}(\mu(W(t)), \Sigma(W(t)))$.

2. draw $W_{i(t+1)} \sim \text{PG}(1, |d_i^T \beta(t+1)|)$, independently for all $i \in \{1, \ldots, n\}$.

In the experiments below, we initialize the chains from the prior distribution $\mathcal{N}(b, B)$.

### 3.2.1 Normalizing constant estimation

We first remark that the above reasoning holds when replacing the covariates $D$ by $\lambda D$ for any $\lambda \in [0, 1]$. This corresponds to the likelihood $\beta \mapsto \prod_{i=1}^{n} \exp(\lambda d_i^T \beta y_i)/(1 + \exp(\lambda d_i^T \beta))$, for $\lambda \in [0, 1]$. In the case $\lambda = 0$, the likelihood is equal to $2^{-n}$ for all $\beta$, while with $\lambda = 1$, we retrieve the original likelihood. For all $\lambda$, we can introduce Polya-Gamma variables $W_i$ following $\text{PG}(1, |\lambda d_i^T \beta|)$ for all $1 \leq i \leq n$, and obtain a corresponding PGG sampler.

This enables normalizing constant estimators for the logistic regression model with little tuning, since the PGG sampler itself has no tuning parameters. Here, for all $\lambda, \beta$, we define

$$\hat{\pi}_\lambda(\beta) = \varphi(\beta; b, B) \prod_{i=1}^{n} \exp(\lambda d_i^T \beta y_i) / (1 + \exp(\lambda d_i^T \beta)),$$ (17)

so that,

$$\log \hat{\pi}_\lambda(\beta) = \log \varphi(\beta; b, B) + \sum_{i=1}^{n} \{ \lambda d_i^T \beta y_i - \log(1 + \exp(\lambda d_i^T \beta)) \},$$ (18)

and thus

$$\nabla_\lambda \log \hat{\pi}_\lambda(\beta) = \sum_{i=1}^{n} \left\{ d_i^T \beta y_i - \frac{d_i^T \beta \exp(\lambda d_i^T \beta)}{1 + \exp(\lambda d_i^T \beta)} \right\},$$ (19)

which can be used to carry out the path sampling calculations. Note also that $Z_0 = 2^{-n}$, so the proposed estimator $\hat{r}_{01}$ will have expectation $\log Z_1 + n \log 2$. Finally, notice that the function $\beta \mapsto \nabla_\lambda \log \hat{\pi}_\lambda(\beta)$ is linear in $\beta$ far away from $\beta = 0$, while $\pi_\lambda$ has at most the Gaussian tails of the prior $\mathcal{N}(b, B)$ (by crudely upper-bounding the likelihood by a constant). Therefore, any power of $\nabla_\lambda \log \hat{\pi}_\lambda(\beta)$ has finite expectation under $\pi_\lambda(d\beta)$, for any $\lambda$, and thus we can check that path sampling estimators have a finite variance.

We consider a synthetic data set with $n = 1000$ rows and $p = 7$ columns. The covariates are generated from a standard Normal distribution and the outcome is generated from the model with $\beta^* = (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6)$. The prior mean $b$ is set to zero and the covariance $B$ to a diagonal matrix with entries equal to 10. We start by gridding the interval $[0, 1]$, and for each value $\lambda^{[t]} = l/L$ with $L = 10$, we set $k$ as the 99% quantile of the meeting times for the coupled PGG sampler, based on 1000 independent runs. We set $m$ as in the previous sections, to make the average cost approximately constant over $\lambda$. Next we estimate the second moments of $\hat{E}(\lambda)$ on the grid of values of $\lambda$, we design a proposal $q(d\lambda)$ following step 5 in Section 2.4, and obtain the estimates of Figure 3a.

We obtain the 1,000 independent estimators $\hat{E}(\lambda)/q(\lambda)$ shown in Figure 3b, leading to a 95% confidence interval of $[63, 89]$ on $r_{01} = \log(Z_1/Z_0)$. The actual value is found to be close to 70 using importance sampling based on a Laplace approximation to the posterior, accurate in the present example (see below,
and also related discussions in Bardenet et al. (2017)). We can see from Figure 3b that the estimates take very large values for λ close to zero. This suggests that, instead of choosing an equispaced grid of values of λ on [0, 1] when designing q(dλ), we could aim at a higher resolution towards the left end of the interval [0, 1].

Therefore we consider a grid of values of λ equispaced on the logarithmic scale: \( \lambda^{[l]} = \exp(-L + l) \) for \( l = 0, \ldots, L \) with \( L = 10 \). Going through the exact same tuning steps, we obtain the 1,000 estimators of Figure 3c, leading to the narrower confidence interval \([64.7, 74.7] \) at level 95% (with a width of 10 instead of 36 for the previous one). This illustrates the potential gains obtained by carefully choosing the distribution \( q(d\lambda) \).

We conclude this section by noting that more dramatic gains can be obtained by changing the path of distributions. In the context of logistic regression with \( n \gg p \), the Laplace approximation of the posterior, defined as \( \mathcal{N}(\hat{\beta}_{\text{MLE}}, \hat{V}) \) where \( \hat{\beta}_{\text{MLE}} \) is the maximum likelihood estimator and \( \hat{V} \) is the inverse of minus the Hessian of the log-likelihood evaluated at \( \hat{\beta}_{\text{MLE}} \), seems to be very accurate. We thus introduce a geometric path (\( \pi_\lambda \)) between the Laplace approximation and the posterior distribution. We use a random walk MH algorithm to target \( \pi_\lambda \) for all \( \lambda \in [0, 1] \), with proposal covariance matrix equal to \( \hat{V}/p \) where the dimension \( p \) is equal to 7. To couple the MH algorithms, we use strategy that combines reflection and maximal couplings, as described in Jacob et al. (2017). The initial distribution of the chains is chosen to be the Laplace approximation. For \( \lambda = 0 \), we obtain \( k = 127 \) as the 99\% quantile of the meeting times, and we set \( m = 5k \). We use these values of \( k \) and \( m \) for all \( \lambda \), and we choose \( q(d\lambda) \) to be uniform on \([0, 1]\). With 100 independent estimators we obtain a confidence interval of \([70.24, 70.26] \) at 95\% for \( \log Z_1 + n \log 2 \). This is orders of magnitude narrower than the previous intervals, for a smaller computational cost. The choice of paths can thus play a critical role in the efficiency of the proposed estimators, and approximations of the posterior distribution can be used to construct such paths.

### 3.2.2 Cross-validation

We now consider the approximation of CV in (4). We consider a leave-one-out criterion, with \( n_T = n - 1 \) and \( n_V = 1 \). We thus construct paths between the posterior given the training data \( T \), with normalizing constant \( p(T) \), and the posterior given all the data \( (T, V) \), with normalizing constant \( p(T, V) \).

Our first path follows the reasoning of the previous section: we can multiply the covariates in the validation set by \( \lambda \in [0, 1] \) to preserve the original structure of the likelihood and thus to enable a similar
Figure 4: Cross-validation (leave-one-out) objective of (4) for the logistic regression of Section 3.2. Left: unbiased estimators of CV obtained with coupled PGG samplers, 1000 times independently. Right: unbiased estimators of CV obtained with a path linking partial posteriors to the full posterior by tempering, and using coupled random walk MH.

PGG sampler. The unnormalized densities are then

\[ \forall \lambda \forall \beta \bar{\pi}_\lambda(\beta) = \varphi(\beta; b, B) \left\{ \prod_{d,y \in T} \frac{\exp(d^T \beta y)}{1 + \exp(d^T \beta)} \right\} \left\{ \prod_{d,y \in V} \frac{\exp(\lambda d^T \beta y)}{1 + \exp(\lambda d^T \beta)} \right\}. \tag{20} \]

Note that \( Z_0 \) is here equal to \(-n_V \log(2) + \log p(T)\), and that the derivative of \( \log \bar{\pi}_\lambda(\beta) \) is easily computed as

\[ \nabla_\lambda \log \bar{\pi}_\lambda(\beta) = \sum_{d,y \in V} \left\{ d^T \beta y - \frac{d^T \beta \exp(\lambda d^T \beta)}{1 + \exp(\lambda d^T \beta)} \right\}. \tag{21} \]

Again we see that this is essentially a linear function of \( \beta \) and thus its moments under \( \pi_\lambda \) are finite for all \( \lambda \).

To tune the procedure, we obtain meeting times for the coupled PGG sampler based on the full data set, and choose \( k \) as a 99% quantile (here equal to 8), and \( m = 5k = 40 \). Recall that the PGG sampler itself has no tuning parameters. Then, drawing a validation set at random 1,000 times independently, generating \( \lambda \) uniformly on \([0, 1]\) and obtaining the associated estimator \( \hat{E}(\lambda) \), we obtain unbiased estimators of CV in (4). We plot a histogram of these estimators in Figure 4a. A 95% confidence interval for the CV objective is obtained as \([-0.62, -0.56]\).

Alternatively, we introduce a geometric path between the posterior given \( T \) and given \( T, V \), which corresponds to the unnormalized densities

\[ \forall \lambda \forall \beta \bar{\pi}_\lambda(\beta) = \left\{ \prod_{d,y \in T} \frac{\exp(d^T \beta y)}{1 + \exp(d^T \beta)} \right\} \left\{ \prod_{d,y \in V} \frac{\exp(\lambda d^T \beta y)}{1 + \exp(\lambda d^T \beta)} \right\}^{\lambda} \varphi(\beta; b, B), \tag{22} \]

with associated gradient of logarithm,

\[ \nabla_\lambda \log \bar{\pi}_\lambda(\beta) = \sum_{d,y \in V} \left\{ d^T \beta y - \log(1 + \exp(d^T \beta)) \right\}. \tag{23} \]

As with the previous path, we can check that powers of \( \nabla_\lambda \log \bar{\pi}_\lambda(\beta) \) have finite expectation under \( \pi_\lambda \) for all \( \lambda \).

For this path, we use random walk MH as in the previous section, with initial distribution and proposal covariance tuned using a Laplace approximation of the posterior distribution. We obtain a
Figure 5: Cross-validation (leave-one-out) objective of (4) for the logistic regression on the leukemia data of Section 3.2.3, using coupled PGG samplers. Left: meeting times against the index of left-out observation. Middle: CV objective against the index of left-out observation. Right: Histogram of all the 10,000 CV estimates combined.

99% quantile of meetings at $k = 135$ and set $m = 5k$. Over 1,000 independent experiments we obtain unbiased estimators of the CV objective shown in Figure 4b. The associated 95% confidence interval for CV is $[-0.60, -0.56]$. Thus, this second approach appears to be marginally more efficient than the first one; the cost comparison is made slightly difficult by the fact that PGG and MH have different costs per iteration.

3.2.3 Leukemia survival data

We follow Vehtari et al. (2017) and consider the leukemia data presented in Feigl and Zelen (1965) and used as illustration in Epifani et al. (2008). We use the data formatted as in the package BGPhazard, see Garcia-Bueno and Nieto-Barajas (2016). The outcome is taken to be one if the survival time (column time of leukemiaFZ) is larger or equal to 50 weeks, zero otherwise, and the two covariates are the columns wbc and AG, corresponding to counts of white blood cells and the outcome of a test related to white blood cell characteristics. There are 31 patients in the sample, so $n = 31$, and we consider leave-one-out cross-validation, i.e. $n_T = n - 1$ and $n_V = 1$.

We introduce a path of distributions amenable to PGG sampling, as in the previous sections. Sampling uniformly the index of the observation to be left out, then sampling $\lambda$ uniformly in $[0, 1]$, and finally running coupled PGG chains targeting $\pi_\lambda$, we record the meeting times. We do so 1,000 times independently, and show the results as a function of the index of the observation left out in Figure 5a.

Based on this plot we select $k = 100$, conservatively, and $m = 5k = 500$ for all runs. We then generate 10,000 unbiased estimators of CV. We plot the estimators against the index of the left-out observation in Figure 5b, and we note that the values are very different for one particular index, here equal to 17. In Figure 5c we plot a histogram of the estimates of the CV objective, putting all the indices together. From these estimates we obtain a 95% confidence interval $[-0.72, -0.66]$ for the leave-one-out CV objective. Thus we see that the proposed estimators can have a larger variance for certain splits of the data compared to others. Investigating further the behavior of the estimators for certain splits, one might be able to reduce the variance, for instance by tuning the proposal distribution $q(d\lambda)$, or by changing the path. Our estimators of CV might also be considered satisfactory as they stand. In any case, they do not suffer from infinite variance issues typically associated with importance sampling, when using a proposal distribution that has lighter tails than the target distribution.
3.3 Linear regressions

We next consider linear regressions, which have been used to illustrate Bayesian cross-validation e.g. in Alqallaf and Gustafson (2001); Peruggia (1997); Vehtari et al. (2017).

3.3.1 Mammal weight data

The first example is taken from Alqallaf and Gustafson (2001). The data comprise of \( n = 62 \) observations, each corresponding to an animal (arctic fox, owl monkey, etc). For each animal, the data set contains the body weight and the brain weight. The covariate \( d_i \) of animal \( i \) is a vector, with first entry equal to 1 and second entry equal to the logarithm of body weight, while the outcome \( y_i \) is the logarithm of brain weight. As before we write \( Y \) for the vector of outcomes and \( D \) for the matrix of covariates, on which we condition throughout. The model is given by

\[
\forall \ i \in \{1, \ldots, n\} \quad y_i \mid d_i, \beta, \sigma^2 \sim N(d_i^T \beta, \sigma^2), \quad p(\beta, \sigma^2) \propto \sigma^{-2},
\]

where \( \sigma \) is a variance parameter, and \( \beta \in \mathbb{R}^2 \) is the regression coefficient. The training size is taken as \( n_T = n/2 = 31 \). Exact posterior sampling on \( x = (\beta, \sigma) \) is possible but we use Gibbs sampling instead for illustration purposes following Alqallaf and Gustafson (2001). We initialize the chain by drawing \( \beta_0, \beta_1 \sim N(0,1) \) independently and \( \sigma^2 \sim \text{Exp}(1) \). To obtain the full conditionals, we write the joint posterior density,

\[
p(\beta, \sigma^2 \mid Y) \propto (\sigma^2)^{-1-n/2} \exp \left( -\frac{1}{2\sigma^2} \|Y - D\beta\|^2 \right).
\]

To get the conditional distribution of \( \beta \) given \( \sigma^2 \) under the posterior distribution, note that

\[
\|Y - D\beta\|^2 = (\beta - \hat{\beta})^T(D^T D)(\beta - \hat{\beta}) + \text{constant},
\]

where \( \hat{\beta} = (D^T D)^{-1} D^T Y \). Thus, the conditional distribution is Normal with mean \( \hat{\beta} \) and covariance matrix \( \sigma^2 (D^T D)^{-1} \). The distribution of \( \sigma^2 \) given \( \beta \) is inverse Gamma, where recall that

\[
\forall \ z \geq 0 \quad IG(z; a, b) = \frac{b^a}{\Gamma(a)} z^{-a-1} \exp \left( -\frac{b}{z} \right).
\]

Then \( \sigma^2 \) given \( \beta \) is inverse Gamma with \( a = n/2 \) and \( b = \|Y - D\beta\|^2/2 \). Coupling this algorithm can be done by maximal coupling of each of the conditional update of a Gibbs sampler.

In Alqallaf and Gustafson (2001), the predictive performance in this example is measured by the mean squared error, defined conditional on a split as

\[
r(\beta, \sigma^2) = \mathbb{E} \left[ \|Y_V - Y_{V}^{\text{pred}}\|^2 \mid Y_T, \beta, \sigma^2 \right],
\]

where \( (T, V) \) denotes a data split, and \( T = (D_T, Y_T), V = (D_V, Y_V) \), recalling that there is an implicit conditioning on \( D_T, D_V \) throughout this section. Above, \( Y_{V}^{\text{pred}} \) is the predicted outcome, and the expectation is taken with respect to the predictive distribution of \( Y_{V}^{\text{pred}} \) given \( Y_T, \beta, \sigma^2 \). In this example this expectation is equal to \( n_V \sigma^2 + \|D_V \beta - Y_V\|^2 \). Then one of the methods described in Alqallaf and Gustafson (2001) averages \( r(\beta, \sigma^2) \) over MCMC draws approximating \( p(\beta, \sigma^2 \mid Y_T) \). Finally they average the results across different random splits \( (T, V) \). We do not need unbiased path sampling to obtain an unbiased version of the above procedure: we can readily use unbiased MCMC with the test function \( h : (\beta, \sigma^2) \mapsto n_V \sigma^2 + \|D_V \beta - Y_V\|^2 \). The proposed procedure reads: draw a partition \( (T, V) \) randomly, and then obtain an unbiased estimator of \( \pi(h) \) where \( \pi \) is the posterior distribution given \( D_T, Y_T \), and where \( h \) is as above.

We implement this procedure and draw 1,000 independent coupled chains. We observe meeting times
between 1 and 5. Thus we set $k = 10$, $m = 25$, and draw 1,000 independent unbiased estimators of CV. We obtain a 95% confidence interval of $[32.79, 33.03]$, and standard error of 0.06. By comparison, Alqallaf and Gustafson (2001) use 200 splits, and run 125 iterations of MCMC for each split, discarding the first 100. The total number of Gibbs iterations performed is approximately the same, and Alqallaf and Gustafson (2001) obtain standard errors that are similar. An advantage of our method is in its simplicity: if we want more precise results, we simply generate more independent estimators.

We now consider the criterion $- \log p(Y_V \mid Y_T)$, instead of the point-prediction mean squared error as above. The sequence of distributions defined in (5) is still amenable to a Gibbs sampling strategy and we need to work out the conditional distributions. The joint posterior density is

$$
\pi_\lambda(\beta, \sigma^2) \propto (\sigma^2)^{-1-n_T/2-\lambda n_V/2} \exp \left( -\frac{1}{2\sigma^2} \| Y_T - D_T \beta \|^2 - \frac{\lambda}{2\sigma^2} \| Y_V - D_V \beta \|^2 \right). \tag{29}
$$

Note that

$$
- \frac{1}{2\sigma^2} \| Y_T - D_T \beta \|^2 - \frac{\lambda}{2\sigma^2} \| Y_V - D_V \beta \|^2 \\
= -\frac{1}{2} (\beta - \mu) ^\top \Lambda_\lambda (\beta - \mu) + \text{constant}, 
$$

with

$$
\Lambda_\lambda = \sigma^{-2} D_T ^\top D_T + \lambda \sigma^{-2} D_V ^\top D_V \\
\mu_\lambda = \Lambda_\lambda^{-1} (\sigma^{-2} D_T ^\top Y_T + \lambda \sigma^{-2} D_V ^\top Y_V), \tag{31}
$$

so that $\beta$ given the rest is $N(\mu_\lambda, \Lambda_\lambda^{-1})$. On the other hand $\sigma^2$ given the rest is inverse Gamma $(a, b)$ with

$$
a = (n_T + \lambda n_V)/2, \quad b = \| Y_T - D_T \beta \|^2/2 + \lambda \| Y_V - D_V \beta \|^2/2. \tag{32}
$$

This enables a Gibbs sampler targeting $\pi_\lambda$ for any $\lambda \in [0, 1]$. Next, we compute $\nabla_\lambda \log \tilde{\pi}_\lambda$ as a function of $\beta, \sigma^2$, which we need to obtain UPS estimators. We write

$$
\nabla_\lambda \log \tilde{\pi}_\lambda(\beta, \sigma^2) = \log p(Y_V \mid D_V, \beta, \sigma^2) = \sum_{j=1}^{n_V} \log \varphi(y_{V,j}; d_{V,j} ^\top \beta, \sigma^2), \tag{33}
$$

where $y_{V,j}$ refers to the $j$-th outcome in the validation set, $d_{V,j}$ to the $j$-th row vector of corresponding covariates, and $\varphi(z; \mu, \sigma^2)$ is the Normal pdf evaluated at $z$, with mean $\mu$ and variance $\sigma^2$. We observe that $\nabla_\lambda \log \tilde{\pi}_\lambda(\beta, \sigma^2)$ and powers of it are integrable with respect to $\pi_\lambda$, noting that $\pi_\lambda$ is here a Normal-inverse-Gamma distribution.

This enables unbiased estimators of $- \log p(Y_V \mid Y_T)$, and thus of CV in (4). Running 1,000 independent estimators, we observe meeting times all less than 5, and setting $k = 10$ and $m = 25$, we obtain an estimated CV criterion of 33.97 with a standard error of 0.1.

### 3.3.2 Stack loss data

We consider the stack loss data example, which was considered in Peruggia (1997); Vehtari et al. (2017). In the former article, it is shown that importance sampling from the posterior given all the data to the posterior leaving one point out can lead to infinite variance estimators. Here we use the stackloss data set of (R Core Team, 2015), with the outcome set to be the column stack.loss, and the covariates Air.Flow, Water.Temp, Acid.Conc., and a column of ones. The data are shown in Figure 6a. We consider leave-one-out cross-validation, with $n_T = n - 1 = 20$ here. For simplicity we use the same model as in the previous section, with a flat prior on $\beta$ given $\sigma^2$, instead of the proper prior given in Peruggia (1997).
(a) Stack loss data; stack.loss is the outcome, the other variables (b) CV objective against index of are covariates.

Figure 6: Cross-validation (leave-one-out) for the linear regression on the stack loss data of Section 3.3.2. Data on the left, and CV objective against left-out observation on the right.

Using the coupled Gibbs sampler described in the previous section, we find meeting times to be less than 10 with large probability, thus we set $k = 10$ and $m = 25$. We obtain the CV estimators shown in Figure 6b, based on 10,000 independent replicates, plotted against the index of the left-out observation. As in Section 3.2.3, we can see that the variance of the CV estimators varies across the different ways of partitioning the data into training and validation sets. These CV estimators yield the 95% confidence interval [2.78, 2.82].

4 Discussion

Further work will be needed to compare the proposed estimators with state-of-the-art methods such as sequential Monte Carlo samplers for normalizing constant estimation (e.g. Lee and Whiteley, 2015; Zhou et al., 2016; Andrieu et al., 2016), with alternative approaches such as the ones described in Chen et al. (1997); Johnson (1999); Neal (2005); Salomone et al. (2018) and references therein, and with the different existing approaches for Bayesian cross-validation (e.g. Alqallaf and Gustafson, 2001; Bornn et al., 2010; Vehtari et al., 2017).

Our estimators combine the path sampling identity with unbiased estimators of intractable integrals. As such, they are expected to break if either path sampling or the unbiased estimators break. Path sampling can give poor results if the path of distributions is ill-chosen, thus the design of these paths remains crucial. We have seen in Section 3.2 that different paths can give orders of magnitude differences in efficiencies. We have also seen that the paths can benefit from approximations of the posterior distribution, such as Laplace approximations. Mixtures of distributions fitted on MCMC samples or variational approximations could also be considered. Conditional on a path, the choice of distribution $q(d\lambda)$ is also important and can be guided by preliminary runs. Unbiased MCMC estimators themselves break either if the underlying MCMC algorithms mix poorly, or if the coupling strategy is ineffective; we defer to Jacob et al. (2017) for related discussions, and to Heng and Jacob (2018) for the case of Hamiltonian Monte Carlo algorithms.

We note that the path sampling identity (3) is an instance of a nested Monte Carlo (MC) problem, as defined and discussed in Rainforth et al. (2016). The target of nested MC is an expectation $I$ of the form

$$I = \mathbb{E}_{\lambda \sim p(\lambda)}[f(\lambda, E(\lambda))],$$

with

$$E(\lambda) = \mathbb{E}_{X \sim p(x|\lambda)}[\phi(\lambda, X)],$$

where the functions $f$, $\phi$ and the joint distribution of $(x, \lambda)$ are problem-dependent choices. In the case
of path sampling, we obtain $I = r_{01}$ by choosing:

\begin{align*}
  p(\lambda) &= q(\lambda), \\
  p(x | \lambda) &= \pi(x) \\
  \phi(\lambda, x) &= \nabla_{\lambda} \log \tilde{\pi}_{\lambda}(x), \ 	ext{and} \\
  f(\lambda, E(\lambda)) &= E(\lambda)/q(\lambda). \tag{35}
\end{align*}

In this case $f(\lambda, E(\lambda))$ is linear in its second argument, thus, given $\lambda$, unbiased estimators of $E(\lambda)$ directly translate into unbiased estimators of $f(\lambda, E(\lambda))$. We remark that unbiased estimators could also be obtained for functions $f$ that are nonlinear in the second argument. For instance we can get an unbiased estimator of $\{E(\lambda)\}^k$, by sampling $k$ independent estimators of $\tilde{E}(\lambda)$ and taking their product. More generally we can obtain unbiased estimators of $f(\lambda, E(\lambda))$ given $\lambda$ for functions $f$ that are polynomials in the second argument.

Finally it is possible to adapt the proposed approach to estimate the Bayesian cross-validation objective associated with some other scoring rules, such as the one proposed in Hyvärinen (2005), and considered in the setting of model comparison in e.g. Dawid and Musio (2015); Shao et al. (2018).

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