Regularised Zero-Variance Control Variates for High-Dimensional Variance Reduction

L. F. South†, C. J. Oates††, A. Mira††† and C. Drovandi†

†School of Mathematical Sciences, Queensland University of Technology, Australia, ARC Centre of Excellence for Mathematical & Statistical Frontiers (ACEMS)
††School of Mathematics, Statistics and Physics, Newcastle University, UK, Alan Turing Institute, UK
†††Institute of Computational Science, Università della Svizzera italiana and University of Insubria

January 24, 2019

Abstract

Zero-variance control variates (ZV-CV) are a post-processing method to reduce the variance of Monte Carlo estimators of expectations using the derivatives of the log target. Once the derivatives are available, the only additional computational effort is solving a linear regression problem. Significant variance reductions have been achieved with this method in low dimensional examples, but the number of covariates in the regression rapidly increases with the dimension of the target. We propose to exploit penalised regression to make the method more flexible and feasible, particularly in higher dimensions. Connections between this penalised ZV-CV approach and control functionals are made, providing additional motivation for our approach. Another type of regularisation based on using subsets of derivatives, or a priori regularisation as we refer to it in this paper, is also proposed to reduce computational and storage requirements. Methods for applying ZV-CV and regularised ZV-CV to sequential Monte Carlo (SMC) are described and a new estimator for the normalising constant of the posterior is developed to aid Bayesian model choice. Several examples showing the utility and limitations of regularised ZV-CV for Bayesian inference are given. The methods proposed in this paper are accessible through the R package ZVCV available at [https://github.com/LeahPrice/ZVCV](https://github.com/LeahPrice/ZVCV).

Keywords: variance reduction, Stein’s method, evidence, sequential Monte Carlo, power posteriors

1 Introduction

Our focus in this paper is on calculating the expectation of a square integrable function \( \varphi(\theta) \) with respect to a distribution with (Lebesgue) density \( p(\theta) \), \( \theta \in \Omega \subseteq \mathbb{R}^d \). Given samples \( \{\theta_i\}_{i=1}^N \sim p(\theta) \), the standard Monte Carlo estimator,

\[
\hat{E}_p[\varphi(\theta)] = \frac{1}{N} \sum_{i=1}^{N} \varphi(\theta_i),
\]

is an unbiased estimator of \( E_p[\varphi(\theta)] := \int_{\Omega} \varphi(\theta)p(\theta)d\theta \). The variance of this estimator is of order \( 1/N \) if the samples are independent and identically distributed (iid) according to \( p(\theta) \). Reducing the
Recent control variate methods have focused on reducing the variance of $\nabla_\theta \log p(\theta)$, or some unbiased estimator of this quantity. Zero-variance control variates (ZV-CV) [Assaraf and Caffarel, 1999; Mira et al., 2013] and control functionals (CF) [Oates et al., 2017b] are two such methods. ZV-CV amounts to solving a linear regression problem and CF is a non-parametric alternative. These methods can be used as post-processing procedures for Markov chain Monte Carlo (MCMC) [Metropolis et al., 1953] output and they require only the availability of (approximate) samples from the target and evaluations of $\nabla_\theta \log p(\theta)$ and $\varphi(\theta)$ for each of the samples. Often $\nabla_\theta \log p(\theta)$ is already available because derivative-based methods like Metropolis adjusted Langevin algorithm (MALA) [Roberts and Stramer, 2002; Girolami and Calderhead, 2011] or Hamiltonian Monte Carlo (HMC) [Duane et al., 1987; Girolami and Calderhead, 2011] have been used in the sampling algorithm.

Existing derivative-based control variates suffer from either mediocre performance or high computational cost. The parametric approximation in ZV-CV is based on a polynomial in $\theta$ so the number of coefficients to estimate rapidly increases both with $d$ and with the polynomial order. ZV-CV methods are fast to perform but, as a result of restricting to low polynomial order, they tend to offer less substantial improvements than CF when the distribution $p(\theta)$ or the function $\varphi(\theta)$ is complex. CF, on the other hand, can be highly effective in these scenarios and has good statistical properties which are described in Oates et al. (2017a) and Barp et al. (2018). Oates et al. (2017b) show that CF outperforms existing ZV-CV methods for some low-dimensional examples when few ($N < 100$) samples are available. However, CF has an $O(N^3)$ computational cost and it also suffers from the curse of dimensionality with respect to $d$ due to the use of non-parametric methods. Some results in Oates et al. (2017b), shown mainly in the appendices, suggest that the performance of CF compared to ZV-CV may deteriorate in higher dimensions.

One aim of this work is to develop derivative-based control variate methods which are inexpensive, effective and capable of handling higher dimensions than existing derivative-based methods. The novel methods that we develop are referred to as regularised ZV-CV and they are based on extending to higher order polynomials and considering two types of regularisation: penalisation methods for linear regression and what we refer to as $a$ priori regularisation. The penalised regression approach to ZV-CV is motivated by showing that $L_2$ penalised ZV-CV is equivalent to CF with a second-order differential operator and finite-dimensional polynomial kernel. Both regularisation methods have the potential to retain the unbiasedness property of the estimator and the empirical results in Section 5 suggest that significant variance reductions can be achieved with regularised ZV-CV. We have developed an R package, ZVCV, which implements standard ZV-CV as well as the regularised ZV-CV methods described in this paper. ZVCV is available at [https://github.com/LeahPrice/ZVCV](https://github.com/LeahPrice/ZVCV).

An important application area for ZV-CV and regularised ZV-CV is Bayesian inference, where Monte Carlo integration is commonly used. The use of ZV-CV and CF to improve posterior expectations based on samples from MCMC is well established (see e.g., Mira et al., 2013; Papamarkou et al., 2014; Oates et al., 2017b). ZV-CV and CF have also been applied to the power posterior [Friel and Pettitt, 2008] estimator of the normalising constant in an MCMC setting by Oates et al. (2016) and Oates et al. (2017b), where they refer to this method as controlled thermodynamic integration (CTI). We describe how regularised ZV-CV fits naturally into the context of sequential Monte Carlo samplers [Del Moral et al., 2006; Chopin, 2002]. In doing so, we provide a setting where adaptive methods can easily be applied to the CTI estimator. A novel reduced-variance normalising constant estimator using the standard SMC identity is also proposed.

An introduction to existing ZV-CV and CF methods is provided in Section 2. The main methodological contributions in terms of developing regularised ZV-CV methods can be found in Section 3. Section 4 covers existing applications to Bayesian inference and novel applications to the estimation of the normalising constant with SMC. Section 5 contains a simulation study comparing methods and
estimators. A final discussion of limitations and possible future work is given in Section 6.

2 Background

In this section, we recall previous work on control variate methods. The general framework for control variates [Ripley, 1987; Hammersley and Handscomb, 1964] is to determine an auxiliary function \( \hat{\varphi}(\theta) = \varphi(\theta) + h(\theta) \) such that \( \hat{\mathbb{E}}_p[\hat{\varphi}(\theta)] = \mathbb{E}_p[\varphi(\theta)] \) and \( \text{var}_p[\hat{\varphi}(\theta)] < \text{var}_p[\varphi(\theta)] \), where \( \text{var}_p \) denotes the variance with respect to \( p(\theta) \). Unbiasedness is satisfied by choosing a random variable \( h(\theta) \) that has zero expectation with respect to \( p(\theta) \). Estimator (1) for the expectation is replaced with the unbiased, reduced variance estimator,

\[
\hat{\mathbb{E}}_p[\varphi(\theta)] = \frac{1}{N} \sum_{i=1}^{N} [\varphi(\theta_i) + h(\theta_i)].
\]

2.1 Control Variates based on Stein’s Method

A control variate which has been considered in [Assaraf and Caffarel, 1999; Mira et al., 2013; Barp et al., 2018] is

\[
h(\theta) = \Delta g(\theta) + \nabla g(\theta) \cdot \nabla \log p(\theta),
\]

where \( \Delta \) represents the Laplacian operator, represented in coordinates as \( \sum_{j=1}^{d} \frac{\partial^2}{\partial \theta_j^2} \) on \( \mathbb{R}^d \), \( g : \Omega \rightarrow \mathbb{R} \) is a twice continuously differentiable function to be specified and \( \log p \) is assumed to be once continuously differentiable on \( \Omega \). This control variate can be motivated by interpreting it as a Stein operator acting on the function \( g(\theta) \) [Stein, 1972]. By definition a Stein operator \( \tau \) depending on \( p(\theta) \) satisfies \( \mathbb{E}_p[\tau g(\theta)] = 0 \) for all functions \( g(\theta) \) in a set called a Stein function class. Further details on this interpretation can be found in [Oates et al., 2017b]. An alternative derivation based on combining an operator \( \tau \) and a class of auxiliary functions \( g(\theta) \) using ideas from physics is described in [Assaraf and Caffarel, 1999] and [Mira et al., 2013].

Equation (3) uses \( \nabla \log p(\theta) \), which is often available, as well as a function \( g \). The function \( g \) for which \( \hat{\varphi}(\theta) \) is constant is generally intractable. In practice, a set of samples targeting \( p \) is used to estimate an approximating function, \( g \), which approximately makes \( \hat{\varphi}(\theta) \) constant.

Estimator (2) based on (3) has the desirable properties of unbiasedness and reduced variance, when compared to (1), under conditions which are described below. Additional theoretical properties of this estimator are described at length in [Oates et al., 2017a] and [Barp et al., 2018].

For given \( g \), unbiasedness, that is \( \mathbb{E}_p[h(\theta)] = 0 \), follows if \( \log p(\theta) \) has continuous first order derivatives, \( g(\theta) \) has continuous first and second order derivatives, and

\[
\int_{\delta\Omega} p(\theta) \nabla g(\theta) \cdot \mathbf{n}(\theta) S(d\theta) = 0,
\]

where \( \delta\Omega \) is the boundary of \( \Omega \), \( \mathbf{n}(\theta) \) is the unit vector orthogonal to \( \theta \) at the boundary \( \delta\Omega \) and \( S(d\theta) \) is the surface element at \( \theta \in \delta\Omega \). When \( \Omega = \mathbb{R}^d \) is unbounded, condition (4) becomes a tail condition which is satisfied if \( \int_{\Gamma_r} p(\theta) \nabla g(\theta) \cdot \mathbf{n}(\theta) S(d\theta) \rightarrow 0 \) as \( r \rightarrow \infty \) where \( \Gamma_r \in \mathbb{R}^d \) is a sphere centred at the origin with radius \( r \) and \( \mathbf{n} \) is the unit vector orthogonal to \( \theta \) at \( \Gamma_r \). This requirement is given in Equation 9 of [Mira et al., 2013] and Assumption 2 of [Oates et al., 2017b].

If \( g \) is to be estimated, then another requirement for unbiasedness is that estimation of \( g(\theta) \) and evaluation of (2) is not performed using the same samples, \( \{\theta_i\}_{i=1}^{N} \). In practice, the so-called “combined” estimator which uses the full set of \( N \) samples for both estimation of \( g(\theta) \) and evaluation of (2) can have lower mean square error (Oates et al., 2017b) than the unbiased so-called “split” estimator which separates the samples into two distinct subsets, one of which is used to select \( g \) and the other of which is used to evaluate the estimator in (2).

3
Variance reduction is effected through judicious choice of the function $g$. CF and ZV-CV are two methods in the literature which are based on different choices for $g$. CF [Oates et al., 2017b] Barp et al. [2018] is based on choosing $g$ from a Hilbert space. Mira et al. [2013] refer to a more general approach, of which (3) is a special case, as zero-variance control variates (ZV-CV) because theoretically one can obtain $V_p[\hat{\varphi}(\theta)] = 0$ through certain optimal choices of $h$ which are available in closed form only in simple examples. However, ZV-CV is generally used to refer to the choice of polynomial approximating functions as this is the specific choice made in Mira et al. [2013]. ZV-CV and CF are described in further detail below. Neural networks have also been considered for $g(\theta)$, in Zhu et al. [2018].

2.2 Control Functionals

The approach of Barp et al. [2018], a sequel to Oates et al. [2017b], proposed to select a functional $g \in \mathcal{H}$ where $\mathcal{H}$ is a user-specified Hilbert space of twice differentiable functionals on $\Omega$. The mechanism for selecting $g$ was to solve the optimisation problem

$$
(c, \hat{g}) \in \arg \inf_{c \in \mathbb{R}, g \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} [\varphi(\theta_i) - c + \Delta \theta g(\theta) + \nabla \theta g(\theta) \cdot \nabla \theta \log p(\theta)]^2 + \lambda \|g\|_{\mathcal{H}}^2
$$

where $\cdot \| \cdot_{\mathcal{H}}$ is the norm associated with the Hilbert space $\mathcal{H}$. The existence of a solution pair $(c, \hat{g}) \in \mathbb{R} \times \mathcal{H}$, together with an explicit algorithm for its computation, was obtained in that work under the assumption that the Hilbert space $\mathcal{H}$ admits a reproducing kernel (see Berlinet and Thomas-Agnan [2011] for background). This method leads to estimators with super-root-$N$ convergence under conditions described in Oates et al. [2017a] and Barp et al. [2018]. However, the cost associated with computation of $\hat{g}$ is $O(N^3)$, due to the need to invert a dense kernel matrix, and moreover this matrix is typically not well-conditioned. For applications that involve MCMC and SMC, typically $N$ will be at least $10^3$ and thus (in the absence of further approximations) the algorithm of Oates et al. [2017b]; Barp et al. [2018] can become impractical.

Recent extensions to (5) include the use of empirical variance minimisation (Belomestny et al. [2017]) since minimising a square error objective function may not be optimal.

Note that in Euclidean spaces, that is when $\theta \in \Omega \subseteq \mathbb{R}^d$, (3) can be replaced with $h(\theta) = \nabla \theta \cdot \hat{g}(\theta) + \hat{g}(\theta) \cdot \nabla \theta \log p(\theta)$ where $\hat{g}$ is a once differentiable and $\mathbb{R}^d$-valued function. The second order differential operator in (3) and (5) corresponds to the case where $\hat{g}$ is a gradient field; i.e. $\hat{g} = \nabla \theta g$ where $g$ is twice differentiable and scalar-valued. In this paper we focus on the second order differential operator to make comparisons between the ZV-CV and CF simpler.

2.3 Zero-Variance Control Variates

The specific choice of approximating function considered by Assaraf and Caffarel [1999] and Mira et al. [2013] is $g(\theta) = P(\theta)$ where $P(\theta)$ is a polynomial function in $\theta$. The polynomials $P(\theta)$ that we consider have total degree $Q \in \mathbb{Z}_{\geq 0}$, meaning that the maximum sum of exponents is $Q$ and the monomial basis is $\theta[1]^{\alpha_1} \cdots \theta[d]^{\alpha_d}$ where $\sum_{j=1}^{d} \alpha_j \leq Q$ and $\alpha \in \mathbb{Z}_{\geq 0}^d$.

Substituting $g(\theta) = P(\theta)$ into (3) gives $h(\theta) = \beta^\top x(\theta)$, where $\beta \in \mathbb{R}^d$ is the vector of polynomial coefficients and $x(\theta) \in \mathbb{R}^d$ is a vector of terms involving $\theta$ and $\nabla \theta \log p(\theta)$. The constant $J = \binom{d+Q}{d} - 1$ is the number of regression parameters, excluding the intercept, for a $Q$th order polynomial when the dimension of $\theta$ is $d$. The general form for $x$ is given in Appendix A.

The standard approach in the literature for choosing $\beta$ is to perform ordinary least squares (OLS)
\[(\hat{c}, \hat{\beta}) \in \arg \min_{c \in \mathbb{R}} \sum_{i=1}^{N} \left[ \varphi(\theta_i) - c + \beta^T x(\theta_i) \right]^2. \tag{6}\]

Unlike in CF, regularisation methods have not previously been used in connection with ZV-CV.

Super-root-$N$ convergence can be achieved with ZV-CV if and only if \(\varphi(\theta) = c + \Delta_\theta P(\theta) + \nabla_\theta P(\theta) \cdot \nabla_\theta \log p(\theta)\) for some fixed finite order polynomial \(P\) (Appendix 5 of [Oates et al. 2017b]). In general, however, ZV-CV is solving a misspecified regression problem as \(\varphi(\theta)\) is not typically a linear combination of the terms in \(x\). In this sense, using higher order polynomials in ZV-CV may not be as statistically efficient as using CF. Nevertheless, higher order polynomials are more flexible, so using them typically results in improved statistical efficiency over lower order polynomials. ZV-CV also has the benefit that it is less computationally demanding to perform than its non-parametric counterpart, CF. More specifically, ZV-CV has computational cost \(O(J^3 + N J^2)\) and CF has computational cost \(O(N^3)\), where often \(J \ll N\).

Given that the computational cost of ZV-CV scales poorly with the dimension \(d\) of \(\theta\), the degree of the polynomial should be chosen as a balance between potentially lower variance (higher degree polynomials) and lower cost (lower degree polynomials). It is standard practice to stop increasing the polynomial order once a reasonable level of variance reduction has been attained, due to the limitations associated with increasing the polynomial order in existing ZV-CV methods. [Mira et al. 2013] consider \(Q = 1\) to at most \(Q = 3\) and find that \(Q = 2\) is sufficient to achieve orders of magnitude variance reduction in most of their examples. [Papamarkou et al. 2014] consider \(Q \leq 2\), pointing out that “first and second degree polynomials suffice to attain considerable variance reduction.” Low polynomial orders are also typically used in applications, for example [Baker et al. 2017] use \(Q = 1\) and [Oates et al. 2010] use \(Q \leq 2\). [Oates et al. 2017b] compare CF with ZV-CV using \(Q = 2\) in most examples. Although [Oates et al. 2017b] considered using higher order polynomials in the supplementary materials, the comparison was focused on \(d = 1\), \(N \leq 100\) and on an integrand of \(\varphi(\theta) = \sin(\theta)\). We do a more thorough investigation of higher order polynomials in Section 5. In particular, we look at a wider range of \(N\), target distribution \(p\) and function \(\varphi(\theta)\). We also propose methods to improve the efficiency of higher order polynomials using fewer samples in Section 3.

### 2.4 Parameterisation

An additional consideration when performing either ZV-CV or CF is the parameterisation that is used. Any deterministic, invertible transformation of the random variables \(\psi = f(\theta)\) can be used so one can estimate
\[
\mathbb{E}_{p_\psi}[\varphi(\theta)] = \frac{1}{N} \sum_{i=1}^{N} \varphi(f^{-1}(\psi_i)) + \Delta_\psi g(\psi_i) + \nabla_\psi g(\psi_i) \cdot \nabla_\psi \log p_\psi(\psi_i) \tag{7}
\]
instead of \(\varphi(\theta)\), where \(p_\theta \equiv p\) is the probability density function for \(\theta\), \(p_\psi\) is the probability density function for \(\psi\) obtained through a change of measure and \(\{\psi_i\}_{i=1}^{N} \sim p_\psi\). For simplicity, the \(\theta\) parameterisation is used in notation throughout the paper. The best parametrisation to use for any given application is an open problem. If the original parameterisation does not satisfy boundary condition \(\varphi(\theta)\), one could consider a reparameterisation such that the boundary condition is satisfied.

### 3 Regularised Zero-Variance Control Variates

The aim of this section is to develop methods which are computationally less demanding than CF and offer improved statistical efficiency over standard ZV-CV. We describe two types of regularisation: regularisation through penalised regression and \textit{a priori} regularisation. The latter is primarily for
cases where not all derivatives of the log target are available or when $N \ll d$. Combinations of the two regularisation ideas are also possible. Methods to choose between control variates are described in Section 3.3.

3.1 Regularisation Through Penalised Regression

As mentioned earlier, the number of regression parameters in ZV-CV grows rapidly with the order $Q$ of the polynomial and with the dimension $d$ of $\theta$. Therefore, the polynomial order that could be considered is greatly limited by the number of samples required to ensure existence of a unique solution to the OLS problem, eliminating the potential reduction that could be achieved using higher order polynomials. In this section, we propose to use penalised regression techniques to help overcome this problem.

In most contexts, using penalised regression reduces variance at the cost of introducing bias. The use of penalisation does not automatically introduce bias in the context of ZV-CV. The key point here is that unbiasedness holds for any polynomial $P(\theta)$ under the regularity conditions described in Section 2.1, namely: $p(\theta)$ has continuous first order derivatives, the estimation of $P(\theta)$ and evaluation of $\theta$ are performed separately and the boundary condition in (4) is satisfied. This stems from the definition of a Stein operator. In standard ZV-CV, polynomial coefficients are chosen using OLS so that the variance of the estimator is minimised given a fixed $Q$. The only potential effect that choosing the coefficients differently can have on unbiasedness is through the boundary condition, which is an assumption that should, if possible, be investigated whether regularisation is used or not. There is no obvious reason why using regularisation would negatively impact this assumption.

3.1.1 $\mathcal{L}_2$ penalisation

The first type of penalisation that we consider is Tikhonov regularisation (Tikhonov et al., 2013), or ridge regression as it is known when applied in regression (Hoerl and Kennard, 1970). This involves using an $L_2$ ridge regression as it is known when applied in regression (Hoerl and Kennard, 1970). This involves

$$
(\hat{c}, \hat{\beta}_s) \in \arg\min_{c \in \mathbb{R}, \beta_s \in \mathbb{R}^J} \frac{1}{N} \sum_{i=1}^{N} \left[ \varphi_s(\theta_i) - c + \beta_s^T x_s(\theta_i) \right]^2 + \lambda_2 ||\beta_s||^2_2,
$$

where the subscript $s$ is in reference to the response and predictors being standardised by their sample mean and standard deviation. Specifically, using the notation $\bar{a} = \frac{\sum_{i=1}^{N} a_i}{N}$ and $\sigma_a = \sqrt{\frac{\sum_{i=1}^{N} (a_i - \bar{a})^2}{(N-1)}}$, we have that $\varphi_s(\theta_i) = (\varphi(\theta_i) - \bar{\varphi})/\sigma_{\varphi}$, $x_s[j](\theta_i) = (x[j](\theta_i) - \bar{x}[j])/\sigma_{x[j]}$, for $j = 1, \ldots, J$ and $\beta_s$ represents the coefficients on this standardised scale. The estimated coefficients on the originalescale are $\hat{\beta}[j] = \hat{\beta}_s[j] \frac{\sigma_{x[j]}}{\sigma_{\varphi}}$. Standardisation is used on the response for stability and on the predictors to put them on the same scale so they can be penalised consistently with a single penalty parameter.

Standard practice is to choose the penalty $\lambda_2 > 0$ by minimising the $k$-fold cross-validation error. Ridge regression mitigates overfitting and allows for estimation when the regression problem is ill-posed due to a small number of observations. Closed form solutions for $\hat{c}$ and $\hat{\beta}$ are available, leading to the same computational cost as OLS of $O(J^3 + NJ^3)$.

To motivate this particular form of penalisation, we now consider interpreting this method as a computationally efficient variant of CF. To facilitate a comparison with the approach of Barp et al. (2018), we consider a particular instance of (5) with a reproducing kernel Hilbert space $\mathcal{H}$ that is carefully selected to lead to an algorithm with lower computational cost. Namely, we select a polynomial kernel

$$
k(\theta, \theta') = \sum_{j=1}^{J} P_j(\theta) P_j(\theta')$$
where $P_j(\theta)$ denotes the $j$th of all $J$ monomial terms in $\theta$ up to order $Q$. For such a kernel, the Moore–Aronszajn theorem (Aronszajn 1950) ensures that a well-defined Hilbert space $\mathcal{H} = \text{span}\{P_j\}_{j=1}^J$ is reproduced and we have an explicit expression for the Hilbert norm

$$\left\| \sum_{j=1}^J \beta_j P_j \right\|_{\mathcal{H}} = \left( \sum_{j=1}^J \beta_j^2 \right)^{1/2}$$

which reveals the method of Barp et al. (2018) as an $L_2$-penalised regression method. As such, the optimisation problem in (8) is equivalent to the optimisation problem in (5) (without the standardisation of the response and predictors) and it can be solved as a least-squares problem with complexity $O(J^3 + NJ^2)$. The first main contribution of our work is to propose a more practical alternative to the method of Barp et al. (2018), which we recall has $O(N^3)$ computational cost, by using such a finite-dimensional polynomial kernel. Our results in this direction are empirical (only) and we explore the properties of this method for various values of $Q$ in Section 5.

Tikhonov regularisation has been applied implicitly in the context of CF but, to the best of our knowledge, this is the first time that general penalised regression methods have been proposed in the context of ZV-CV. Results in Section 5 demonstrate that the new estimators can offer substantial variance reduction in practice when the number of samples is small relative to the number of coefficients being estimated.

### 3.1.2 $L_1$-penalisation

The principal aim in the design of a control variate $h$ is to accurately predict the value that the function $\varphi$ takes at an input $\theta^*$ not included in the training dataset $\{(\theta_i, \varphi(\theta_i))\}_{i=1}^N$. It is well-understood that $L_1$-regularisation can outperform $L_2$-regularisation in the predictive context when the function $\varphi$ can be well-approximated by a relatively sparse linear combination of predictors. In our case, the unstandardised predictors are the functions in the set $\{1\} \cup \{\Delta_\theta P_j + \nabla_\theta P_j \cdot \nabla_\theta \log p\}_{j=1}^J$. Given that low-order polynomial approximation can often work well for integrands $\varphi$ of interest, it seems plausible that $L_1$-regularisation could offer an improvement over the $L_2$-regularisation used in Oates et al. (2017b); Barp et al. (2018). Investigating this question is the second main contribution of our work.

In the context of ZV-CV, $L_1$-penalisation can be interpreted as using the least absolute shrinkage and selection operator (LASSO, Tibshirani (1996)). LASSO introduces an $L_1$ penalty into the optimisation problem as follows:

$$\hat{c}, \hat{\beta} s) \in \arg\min_{c \in \mathbb{R}, \beta_s \in \mathbb{R}^d} \frac{1}{N} \sum_{i=1}^N \left[ \varphi_s(\theta_i) - c + \beta_s^\top x_s(\theta_i) \right]^2 + \lambda_1 \left\| \beta_s \right\|_1. \quad (9)$$

where $\left\| \beta_s \right\|_1 = \sum_j |\beta_s[j]|$ is the $L_1$ norm of $\beta_s$ and $\lambda_1 > 0$ is again typically chosen to minimise the $k$-fold cross-validation error. The effect of the penalty is that some coefficients are estimated to be exactly zero.

### 3.2 A priori Regularisation

As an alternative to penalised regression methods, in this section we consider restricting the function $g$ to vary only in a lower-dimensional subspace of the domain $\Omega \subseteq \mathbb{R}^d$. More specifically, a subset of parameters $S \subseteq \{1, \ldots, d\}$ is selected prior to estimation and the function $g$ is defined, in a slight abuse of notation, as $g(\theta) = P(\theta[S])$. The log target derivatives, $\nabla_\theta \log p(\theta)$, only appear in the control
variants through the dot product $\nabla_{\theta j}(\theta) \cdot \nabla_\theta \log p(\theta)$. Therefore if $j \notin S$ then the derivative $\nabla_{\theta[j]} \log p(\theta)$ is not required. We refer to this approach as a priori regularisation.

A priori regularisation makes ZV-CV feasible when some derivatives cannot be used, for example due to intractability, numerical instability, computational expense or storage constraints. An example of where some derivatives may be difficult to obtain is in Bayesian inference for ordinary differential equation (ODE) models. Evaluating $\nabla_\theta \log p(\theta)$ requires the sensitivities of the ODE to be computed, which involves augmenting the system of ODEs with additional equations. If some additional equations render the system stiff, then more costly implicit numerical solvers need to be used and in such cases it would be useful to avoid including sensitivities corresponding to the difficult elements of $\theta$. It may also be infeasible to store the full set of samples and derivatives, with the latter requiring roughly the same space as the former. Storing a subset of the parameters and derivatives for use in a priori regularisation may, however, be achievable. Another benefit of a priori ZV-CV is that it reduces the number of coefficients to estimate, making estimation feasible when $N \ll d$. Zhuo et al. (2018) consider similar ideas to a priori ZV-CV in the context of Stein variational gradient descent, where they use the conditional independence in $p(\theta)$ for probabilistic graphical models to separate high dimensional inference problems into a series of lower dimensional problems.

The concept of regularisation by selecting a subset of parameters is referred to as nonlinear approximation in approximation theory and applied mathematics (DeVore, 1998), and there is some theoretical evidence to suggest that this can outperform than linear approximation (e.g. penalised regression which is described in Section 3.1). Selecting a particular subset of monomials which are used in a polynomial interpolant is also the same idea as in sparse grid algorithms for numerical integration (Smolyak, 1963). These methods are known to work well in high dimensions.

The downside of using a priori ZV-CV is that the potential for variance reduction is reduced, except for under both conditions (a) $\theta[S]$ is independent of $\theta[S]$ according to $p(\theta)$, where $S = \{1, \ldots, d\} \setminus S$, and (b) $\varphi(\theta) = \varphi(\theta[S])$. Outside of this situation, restricting the polynomial to $g(\theta) = P(\theta[S])$ will give varying levels of reduction in performance depending on the subset that is selected. Intuitively, one may wish to choose the subset of variables so that $\theta[S]$ and/or $\nabla_{\theta[S]} \log p(\theta)$ have high correlations with $\varphi(\theta)$. In practice, this is easiest to do when there is a priori knowledge and therefore not all derivatives need to be calculated and stored. Given (b), it is suspected that this method will be more useful for individual parameter expectations than for expectations of functions of multiple parameters.

As with the penalised ZV-CV estimators from Section 3.1, the estimators using this approach are unbiased if the boundary condition in (4) is satisfied. This method is also applicable to CF, though nonlinear approximation may be more difficult in this non-parametric setting.

### 3.3 Automatic Selection of Control Variates

The performance of regularised ZV-CV depends upon the polynomial order, the penalisation type and on $S$. We demonstrate in Section 5 that the common practice of defaulting to $Q = 2$ with OLS is often sub-optimal and also that the optimal control variate depends on a variety of factors including $N$ and $p(\theta)$. It has previously been proposed to increase the number of control variates as the sample size increases (see e.g. Portier and Segers (2018) and the appendices of Oates et al. (2017b)). As described in Oates et al. (2017b), this approach can be motivated in the ZV-CV context by the Stone-Weierstrass theorem (Stone 1948) which states that polynomial functions can be used to uniformly approximate, to an arbitrary level of precision, continuous functions on closed intervals. However, in these existing works the mechanism whereby the complexity of the control variate was increased was not data-dependent.

To choose between control variates in this work, we use 5-fold cross-validation so that our selection is data-dependent. For each combination of penalisation type and $S$, we start with polynomial order $Q = 1$ and we continue to increase the polynomial order until the average cross-validation error is
larger for $Q + 1$ than for $Q$. The combination of regularisation method and polynomial order which gives the minimum cross-validation error is selected and we perform estimation using that method on the full set of samples. The cross-validation error that we use here is the sums of square residuals in the hold-out set, averaged across the five folds.

4 Applications to Bayesian Statistics

ZV-CV and CF can be applied in place of standard Monte Carlo integration, whenever $\nabla_\theta \log p(\theta)$ is available (or a subset of the derivatives, following the ideas in Section 3.2). A context where this is very common is Bayesian inference, and in this section we describe how both existing and proposed variance reduction methods can be applied.

4.1 Bayesian Statistics

In Bayesian inference, the distribution of the parameters $\theta$ of a statistical model given observed data $y$, $p(\theta|y)$, is referred to as the posterior distribution. The posterior is related to the prior distribution, $\pi(\theta)$, and to the likelihood, $f(y|\theta)$, through Bayes’ rule:

$$p(\theta|y) = \frac{f(y|\theta)\pi(\theta)}{Z(y)}.$$  \hfill (10)

The quantities of interest in Bayesian statistics are posterior expectations, $E_{p_t}[\varphi(\theta)] = \int_{\theta} \varphi(\theta)p(\theta|y)d\theta$, and the normalising constant of the posterior, $Z(y) = \int_{\theta} f(y|\theta)\pi(\theta)d\theta$ or simply $Z$ for notational convenience (it is assumed that $Z > 0$). The normalising constant is also known as the marginal likelihood or the evidence and it is useful for model choice. Due to the $d$-dimensional integration involved in calculating $Z$, the posterior density is analytically intractable for all but simple examples. Monte Carlo integration is often used in estimating posterior functionals and $Z$.

A common method to obtain samples for Monte Carlo integration is Metropolis Hastings Markov chain Monte Carlo (MH-MCMC, Metropolis et al. (1953); Hastings (1970)). Given the current state of the Markov chain is $\theta$, a new state $\theta^*$ is proposed by sampling from a density $q(\theta^*|\theta)$ and accepted if

$$r < \frac{f(y|\theta^*)\pi(\theta^*)q(\theta^*|\theta)}{f(y|\theta)\pi(\theta)q(\theta|\theta^*)},$$

where $r \sim U[0,1]$, otherwise the current value $\theta$ is retained. Derivative based proposals for $q$ such as Metropolis adjusted Langevin Algorithm (MALA, Roberts and Stramer (2002); Girolami and Calderhead (2011)), Hamiltonian Monte Carlo (HMC, Duane et al. (1987); Girolami and Calderhead (2011)) and the no-u-turn sampler (NUTS, Hoffman and Gelman (2014)) have become increasingly common due to their ability to improve mixing, especially in high dimensional parameter spaces or where the parameters are highly correlated (Girolami and Calderhead, 2011). All of these methods use $\nabla_\theta \log p(\theta|y)$ to inform proposals, so ZV-CV does not require any additional derivative evaluations.

4.2 Control Variates in Bayesian Statistics

ZV-CV and CF have both been applied in the context of estimating posterior expectations, i.e. the distribution $p(\theta)$ from Section 2 is taken to be the posterior $p(\theta|y)$, for example by Mira et al. (2013); Papamarkou et al. (2014); Friel et al. (2016); Oates et al. (2017b); Baker et al. (2017). Oates et al. (2016) and Oates et al. (2017b) have also applied ZV-CV and CF, respectively, to the power posterior estimator for the evidence (Friel and Pettitt, 2008). The estimator,

$$\log Z = \int_0^1 E_{p_t}[\log f(y|\theta)]dt,$$  \hfill (11)
is based on thermodynamic integration (TI, Gelman and Meng (1998); Ogata (1989)) and it gives the log evidence as an integral with respect to the inverse temperature \( t \), where \( p_t = f(y|\theta)^t p(\theta)/Z_t \). For points in a discrete set \( \{ t_j \}_{j=0}^T \) of inverse temperatures where \( 0 = t_0 < \ldots < t_T = 1 \), this integral is estimated using quadrature methods. The second order quadrature method of Friel et al. (2014) estimates \((11)\) using

\[
\log Z = \frac{T}{2} \sum_{j=0}^{T-1} \left( \mathbb{E}_{p_t}[\log f(y|\theta)] + \mathbb{E}_{p_{t+1}}[\log f(y|\theta)] \right) - \frac{(t_{j+1} - t_j)^2}{12} \left( \mathbb{V}_{p_{t+1}}[\log f(y|\theta)] - \mathbb{V}_{p_t}[\log f(y|\theta)] \right). \tag{12}
\]

A simpler, first order quadrature approximation which is equivalent to the first sum in \((12)\) was described in Friel and Pettitt (2008).

It is straightforward to apply ZV-CV to \((12)\) by noticing that the estimator is simply a sum of expectations where

\[
\mathbb{V}_{p_t}[\log f(y|\theta)] = \mathbb{E}_{p_t} \left[ (\log f(y|\theta) - \mathbb{E}_{p_t}[\log f(y|\theta)])^2 \right].
\]

Oates et al. (2016) refer to the use of ZV-CV for this purpose as controlled TI (CTI) and they implement CTI in an MCMC framework. In the MCMC context, the inverse temperatures are fixed prior to the runs, making it difficult to balance low quadrature bias from using a large number of inverse temperatures with low computational effort from using a small number of inverse temperatures. Furthermore, sampling from the target distributions \( p_t \) for \( j = 1, \ldots, T \) requires tuning which is often done manually in MCMC. One contribution of this work is to use the CTI estimator in the SMC framework which allows for online choice of the inverse temperature schedule and online tuning of the MCMC proposal. Another contribution, which is described in Appendix B, is a method for adjusting inverse temperatures after the MCMC or SMC runs have completed. We note that \((11)\) has been used in the SMC framework by Zhou et al. (2012), but CTI has not previously been used in SMC.

4.3 Sequential Monte Carlo and Control Variates

SMC samplers are naturally adaptive and parallelisable alternatives to standard MCMC for sampling from the posterior of static Bayesian models (Del Moral et al. 2006). A set of \( N \) weighted samples, \( \{W_j^i, \theta_j^i\}_{i=1}^N \), are moved through a sequence of distributions, \( p_t(\theta|y) \), for \( j = 0, \ldots, T \). The distributions \( p_t \), henceforth \( p_j \) for brevity, are properly normalised and \( \eta_j \) represents the unnormalised distributions, i.e. \( p_j \propto \eta_j \) for \( j = 0, \ldots, T \). The samples, or particles, are moved through these distributions using importance sampling, resampling and move steps.

The importance sampling step reweights particles \( \{W_j^i, \theta_j^i\}_{i=1}^N \) from \( p_{j-1} \) to target \( p_j \) using

\[
w_j^i = W_{j-1}^i \frac{\eta_j(\theta_j^i)}{\eta_{j-1}(\theta_{j-1}^i)},
\]

for \( i = 1, \ldots, N \), where \( w_j^i \) is the unnormalised weight for particle \( \theta_j^i = \theta_{j-1}^i \) and \( W_j^0 = 1/N \) if perfect samples are drawn from the initial distribution \( p_0 \). The normalised weights are \( W_j^i = w_j^i / \sum_{i=1}^N w_j^i \). Resampling, most commonly multinomial resampling, is used to remove particles with negligible weights and replicate particles with high weights. After resampling, the weights are set to \( 1/N \). Finally a move step, most commonly in the form of several iterations of a \( p_j \)-invariant MCMC kernel, is used to diversify the particles. Derivative based proposals have recently been used for the MCMC kernel in SMC (Sim et al. 2012), which means that ZV-CV can easily be performed on expectations with respect to \( p_j \) for \( j = 1, \ldots, T \).
It is straightforward to adapt SMC algorithms online. Recent work has proposed adapting the MCMC kernel parameters online using the population of particles. For example, Fearnhead and Taylor (2013) and Salomone et al. (2018) propose adaptation methods for generic MCMC kernels. Buchholz et al. (2018) propose methods for performing the notoriously challenging tuning of HMC kernel parameters in SMC. It is also possible to adaptively choose whether to perform the resampling and move steps based on some measure of the weight degeneracy (Del Moral et al., 2012). In this context, the weights are updated when resampling and move steps are not performed but the particle values remain the same. The particles do not have equal weights at every iteration so ZV-CV requires weighted means and weighted linear regression to estimate expectations with respect to \( p_j \).

An added benefit of SMC samplers over alternatives like standard MCMC is that an estimate of the normalising constant is produced as a by-product in SMC. The standard SMC evidence estimator, \( \hat{Z} = \prod_{j=1}^{T} \sum_{i=1}^{N} w_i^j \), is unbiased when adaptive methods are not used. We propose the use of ZV-CV on each of the expectations in (13) to obtain a lower variance estimator, i.e. we take \( \rho(\theta) \) in Section 2 to be the power posterior \( p_j(\theta | y) \). Although ZV-CV may not change the individual expectations due to its unbiasedness property, it is not clear whether the product of these estimators, \( Z \), remains unbiased under ZV-CV. Nevertheless, we find in practice that the SMC estimator with ZV-CV has lower mean square error than the SMC estimator without control variates.

Commonly used sequences for \( p_j \) in the literature are data annealing and likelihood annealing. In data annealing SMC (Chopin, 2002), the data are introduced sequentially so the targets are \( p_j(\theta | y_{1:j}) \) where \( y_{1:j} \) denotes the first \( j \) data points and \( p_0(\theta) \equiv \pi(\theta) \). Likelihood annealing smoothly introduces the effect of the likelihood to help explore complex targets (Neal, 2001) through the sequence \( p_j(\theta | y) = f(y | \theta)^{t_j} \pi(\theta) / Z_j \), the same sequence that is used in TI. Unlike in the MCMC setting, where \( t_j \) for \( j = 0, \ldots, T \) needs to be fixed for TI, the inverse temperatures in SMC can easily be adapted online, for example using the methods described in Jasra et al. (2011) and detailed in Appendix B.

ZV-CV can be used in evidence estimation and in estimating posterior expectations for both data annealing and likelihood annealing SMC. The most straightforward way to estimate posterior expectations in SMC is to use the particles \( \{ W_j^i, \theta_j^i \}_{i=1}^N \) from the final target \( p_T \) in Monte Carlo integration. The estimator for the \( j \)-th marginal posterior mean is \( \bar{\theta}[j] = \sum_{i=1}^{N} W_j^i \theta_j^i / \sum_{i=1}^{N} W_j^i \), where \( \theta[j] \) denotes the \( j \)-th marginal. A method to reuse all past particles in posterior expectations is discussed in Section 6 as a potential avenue for future research. ZV-CV has not been applied before in the streaming data context so this application to data annealing SMC may be useful. However, we choose to focus on likelihood annealing SMC because comparisons help to reveal whether the SMC evidence estimator, \( \hat{Z} = \prod_{j=1}^{T} \sum_{i=1}^{N} W_j^i f(y_j | \theta_j^i)^{t_j} / \sum_{i=1}^{N} W_j^i \), is more amenable to a control variate treatment.

5 Empirical Assessment

In this section, we perform an empirical comparison of the following methods using examples of varying complexity:

- **vanilla**: Monte Carlo integration without control variates.
- **ZVQ**: ZV-CV with OLS and order \( Q \) polynomial.
• $l$-$ZV_Q$: ZV-CV with LASSO and order $Q$ polynomial.
• $r$-$ZV_Q$: ZV-CV with ridge regression and order $Q$ polynomial.
• $\text{sub}_k$: This prefix indicates \textit{a priori} ZV-CV with a subset of size $k$.
• $\text{crossval}$: Control variate selection using 5-fold cross-validation. This method chooses between all of the above for posterior expectations and between vanilla, $ZV_Q$, $l$-$ZV_Q$ and $r$-$ZV_Q$ for evidence estimation.

The main purposes of these comparisons are to investigate the performance of higher order polynomials, the utility of penalised regression and the ability to achieve variance reduction using a subset of derivatives. A variety of sample sizes, integrands $\phi(\theta)$ and target distributions $p$ are used for fair comparisons.

Estimators are compared on the basis of variance reduction and bias, where bias is measured by comparing to a gold standard of estimation which is carefully chosen for each example. The main quantity of interest reported in this section is $\text{MSE}_p[\text{vanilla}] / \text{MSE}_p[\cdot]$, the mean square error (MSE) of the vanilla Monte Carlo estimator estimated from 100 independent SMC runs divided by the estimated MSE for the method in question. This quantity is referred to as efficiency because it reports the number of times more efficient the estimator under consideration is than vanilla Monte Carlo for a fixed $N$. Values above one are preferred. ZV-CV with higher order polynomials and penalised regression require more computing time than vanilla Monte Carlo integration or ZV-CV with OLS. However, we do not take this into account in our comparisons because there are many tools available to perform linear regression efficiently, such as the glmnet R package (Friedman et al., 2010) which is used here (with 10-fold cross-validation as the default to select $\lambda$). Furthermore, it is unlikely that the cost of a linear regression would be prohibitive in comparison to the cost of increasing the number of samples in Monte Carlo integration for most realistic problems.

As described in Section 4.3, another novelty of this work is in applying ZV-CV within SMC. The SMC and the CTI evidence estimators are compared to make recommendations on which one practitioners should use when derivatives are available. Another benefit of using two evidence estimators along with estimating marginal posterior expectations is that ZV-CV can be compared on a variety of functions $\phi(\theta)$. The function $\phi(\theta)$ for posterior expectations may be intuitively more amenable to \textit{a priori} ZV-CV than complex functions of $\theta$. The two evidence estimators both involve expectations of non-linear transformations to $f(y|\theta)$. The integrand is on the logarithmic scale for the CTI estimator, so CTI may improve more with ZV-CV than the SMC estimator.

To avoid confounding the effects of ZV-CV with the effects of kernel parameter and inverse temperature choice, we do a single adaptive SMC run for each example. The inverse temperatures and kernel parameters from this run are then used in 100 independent SMC runs for each value of $N$. Doing fixed runs in this way also means that the vanilla estimate of the SMC normalising constant is unbiased so it is possible to investigate bias from the combined ZV-CV estimator. Inverse temperatures are adjusted post-hoc using the method described in Appendix B to reduce quadrature bias for the CTI estimator. The full set of inverse temperatures are used for both the CTI and SMC estimators. Additional inverse temperatures without resample and move steps do not improve the vanilla SMC evidence estimator, but we find that they can lead to substantial reductions in the ZV-CV SMC evidence estimator. Specific implementation details regarding the adaptive SMC runs are given in Appendix C. To improve stability, the ZV-CV regression for the SMC evidence estimator is performed using the integrand divided by its maximum value and the results are adjusted to correct for this.

Three examples of dimensions $d = 1$, $d = 11$ and $d = 9$ are described in detail in this section. All results are based on combined estimators as opposed to split estimators, so all pairs $(\theta_i, \phi(\theta_i))_{i=1}^N$ are used to build $\hat{\phi}$ and also to estimate $E_p[\hat{\phi}(\theta)]$. The results for a $d = 61$ dimensional logistic regression example are also given in Appendix F. The benefits of \textit{a priori} regularisation are especially obvious.
In this example due to the non-trivial storage requirements. Boundary condition for unbiasedness of ZV-CV estimators is satisfied using the specified parameterisations for all examples considered in this paper. This can be verified through the sufficient condition that the tails of \( p \) decay faster than polynomially and \( \Omega = \mathbb{R}^d \) (Appendix B of Oates et al. (2016)).

5.1 Van der Pol

This example based on the Van der Pol oscillatory differential equations (Van der Pol, 1926) demonstrates the potential to improve the performance of ZV-CV by using higher order polynomials. Oates et al. (2017b) applied \( ZV_2 \) and CF to reduce the variance of the power posterior log evidence estimator and found that \( ZV_2 \) offered only modest improvements. By illustrating the improvements with \( Q > 2 \), we motivate the use of higher order polynomials. Regularisation is not required in this one-dimensional example.

In the Van der Pol oscillatory differential equations, position \( x(t) \) is governed by the second order differential equation

\[
\frac{d^2x}{dt^2} - \theta(1 - x^2) \frac{dx}{dt} + x = 0,
\]

which can also be written as a system of first order differential equations,

\[
\begin{align*}
\frac{dx_1}{dt} & = x_2 \\
\frac{dx_2}{dt} & = \theta(1 - x_1^2)x_2 - x_1,
\end{align*}
\]

where \( x_1 = x \) and \( x_2 = dx/dt \). The parameter \( \theta \) represents the non-linearity of the system and the damping strength. We use the same data as Oates et al. (2017b) which is based on \( \theta = 1 \), initial position \( x_1 = 0 \), initial velocity \( x_2 = 2 \) and noisy observations \( y_t \sim \mathcal{N}(x_1(t), 0.1^2) \) recorded at times \( t = 0, 1, \ldots, 10 \). The prior is \( \log(\theta) \sim \mathcal{N}(0, 0.25^2) \). Derivatives are obtained by augmenting the system of differential equations with sensitivity equations (see e.g. Appendix 7 of Oates et al. (2017b)).

Oates et al. (2017b) found that second order polynomials resulted in mediocre performance for evidence estimation in this example. Oates et al. (2017b) used population MCMC with within-temperature and between-temperature proposals to obtain samples from the power posteriors. The sampling algorithm used here is SMC, which is simpler and easier to adapt. Their MCMC proposals and use of CF are both based on \( \theta \) in its original scale. Given that the prior is such that \( \theta > 0 \), we have performed a log transform so that the MCMC proposals and ZV-CV are both based on \( \psi = \log \theta \). Expectations are calculated using (7), for example posterior expectations can be expressed as \( E_\psi[e^\psi] \).

The gold standard evidence estimate for this example is based on numerical integration. For the posterior mean, the gold standard of \( \hat{\theta} \) is based on the mean of 100 estimates using split \( ZV_9 \) at \( N = 1000 \).

5.1.1 Posterior Expectations

With this simple integrand, ZV-CV is able to perform extremely well. It is apparent from Figure 1 that larger \( Q \) is preferable for this problem, with the selected polynomial order from cross-validation increasing with \( N \).

5.1.2 Evidence Estimation

Figures 2a and 2b show the efficiency, \( \text{MSE}_{\text{p[vanilla]}} / \text{MSE}_{\text{p[·]}} \), of the two evidence estimators for different \( N \). It is clear from these figures that higher order polynomials can offer substantial improvements in efficiency given a sufficient number of samples.

\[\text{This evidence estimate differs from the estimates in Oates et al. (2017b). The code available at http://warwick.ac.uk/control_functionals is missing a square root in the normal probability density function which appears in the likelihood function.}\]
Figure 1: Van der Pol example: (a) Efficiency for $\widehat{E}_p[\theta]$ and (b) the polynomial orders selected using cross-validation for different $N$.

The cross-validation method results in estimators with similar MSE to fixed polynomial orders of $Q = 2$ or $Q = 3$. Although the chosen control variates lead to efficiency improvements of one to three orders of magnitude over the vanilla estimator, the improvements are not as substantial as for the optimal fixed $Q \in \{1, 2, \ldots, 9\}$. The cross-validation method is stopping at a sub-optimal $Q$, potentially because there is little to no improvement from one (sub-optimal) polynomial order to the next (sub-optimal) polynomial order for many of the expectations involved here. This hypothesis is supported by the polynomial order selection results in Appendix C. One potential solution in practice may be to force the cross-validation to compare up to at least some fixed polynomial order.

At $N = 10$, the evidence estimates for the CTI estimator appear to be approximately unbiased despite the use of the combined estimator (Figure 2c). The estimators also have low variance with the exception of the polynomial with $Q = 9$, for which there are not enough samples for a reasonable fit. The SMC combined estimator suffers from more bias (Figure 2d), but this bias disappears when the samples are split to facilitate independent estimation of $g(\theta)$ and evaluation of (2) (results not shown).

The two evidence estimators have a similar MSE prior to ZV-CV and can both be improved with ZV-CV, but the improvements over the vanilla Monte Carlo estimator are greater for the CTI estimator.

5.2 Recapture

Standard ZV-CV with higher order polynomials is less feasible in this 11-dimensional example. Polynomials with $Q = 3$ and $Q = 4$ require 364 and 1365 regression coefficients, respectively, compared to only 12 and 78 for $Q = 1$ and $Q = 2$, respectively. Results suggest that reduced variance estimators can be obtained with the use of higher order polynomials and regularisation.

Marzolin (1988) collected data on the capture and recapture of the bird species Cinclus cinclus, also known as the European Dipper, over six years. Like Brooks et al. (2000), Nott et al. (2018) and South et al. (2018), we use a Bayesian approach to estimate the parameters of a Cormack-Jolly-Seber model (Lebreton et al., 1992) for the capture and recapture of this species. The parameters of the Cormack-Jolly-Seber model used here are the probability of survival from year $i$ to $i + 1$, $\phi_i$, and the probability of being captured in year $k$, $p_k$, where $i = 1, \ldots, 6$ and $k = 2, \ldots, 7$. Denote the number of birds released in year $i$ as $D_i$ and the number of animals caught in year $k$ out of the number released
in year $i$ as $y_{ik}$. It is simple to show that the number released in year $i$ that are never caught is $d_i = D_i - \sum_{k=i+1}^{7} y_{ik}$ and the probability of a bird being released in year $i$ and never being caught is $\chi_i = 1 - \sum_{k=i+1}^{7} \phi_i p_k \prod_{m=i+1}^{k-1} \phi_m (1-p_m)$. The likelihood is given by

$$f(y|\theta) \propto \prod_{i=1}^{6} \phi_i^{d_i} \prod_{k=i+1}^{7} \phi_i p_k \prod_{m=i+1}^{k-1} \phi_m (1-p_m)^{y_{ik}},$$

where $\theta = (\phi_1, \ldots, \phi_5, p_2, \ldots, p_6, \phi_7 p_7)$. Following South et al. (2018), the parameters $\phi_6$ and $p_7$ are combined due to a parameter identifiability issue.

The prior is $\theta[j] \sim U(0, 1)$ for $j = 1, \ldots, 11$. To satisfy boundary condition (4) and to improve the efficiency of MCMC proposals, all parameters are transformed to the real line using $\psi[j] = \log(\theta[j]/(1-\theta[j]))$ so the prior density for $\psi[j]$ is $e^{\psi[j]}/(1+e^{\psi[j]})^2$, for $j = 1, \ldots, 11$.

The gold standard of evidence estimation for this example is the mean evidence estimate for $l$-ZV.
at $N = 5000$. The posterior expectation gold standard is the average posterior mean for $ZV_4$ at $N = 5000$.

### 5.2.1 Posterior Expectations

The average efficiency across parameters is shown in Figure 3, excluding a priori regularisation results for simplicity. More detailed results showing the efficiency for each individual parameter, including with a priori ZV-CV, are available in Appendix D. Higher order polynomials become more efficient as $N$ increases and the use of penalised regression means that higher order polynomials can be considered for smaller $N$. LASSO regression is preferable over ridge regression for this example.

Using a priori ZV-CV with $S = j$, where $j$ is the index of the current parameter of interest, is approximately 10 times more efficient than using vanilla Monte Carlo integration on average for this example.

Cross-validation generally gives similar results to the best performing fixed method. The selected control variates for the 1100 expectations at $N = 50$ and $N = 1000$ can be seen in Table 1.

![Figure 3: Recapture example: efficiency averaged over 11 parameters.](image)

**Table 1**: Recapture example: control variate selection for marginal posterior expectations using cross-validation. Each value of $N$ has a total of 1100 expectations, that is 100 independent runs are used to estimate each marginal posterior expectation.

|     |     |     |     |
|-----|-----|-----|-----|
| a) $N = 50$ | sub1-ZV | ZV | l-ZV | r-ZV |
| 1   | 0   | 80 | 405 | 53  |
| 2   | 1   | 0  | 436 | 10  |
| 3   | 0   | 0  | 109 | 0   |
| 4   | 0   | 0  | 1   | 0   |
| 5   | 5   | 0  | 0   | 0   |
| b) $N = 1000$ | Q | ZV | l-ZV | r-ZV |
| 2   | 0   | 5  | 0   |
| 3   | 680 | 200| 3   |
| 4   | 0   | 112| 0   |
| 5   | 0   | 75 | 0   |
| 6   | 0   | 22 | 0   |
| 7   | 0   | 2  | 0   |
| 8   | 0   | 1  | 0   |
5.2.2 Evidence Estimation

Regularised ZV-CV gives improved efficiency over ZV-CV for the range of $N$ that are considered here, as seen in Figure 4. Automatic control variate selection leads to estimators which have similar efficiency to the highest performing fixed polynomial order. This is true across both evidence estimators, although the two estimators have similar initial MSE and the CTI estimator benefits more from ZV-CV. The selected control variates for $N = 50$ and $N = 1000$ can be found in Appendix D.

![Figure 4: Recapture example: (a) efficiency for the CTI estimator and (b) efficiency for the SMC estimator.](image)

5.3 ODE

Potential limitations of ZV-CV and regularised ZV-CV are illustrated through this challenging example with non-linear posterior dependencies. For the most part, the performance with low sample sizes is poor and the performance with larger sample sizes is modest compared to the examples in Section 5.1 and Appendix D.

Geyer (1991) describe the following system of coupled ordinary differential equations (ODEs) for modelling biochemical pathways,

$$
\begin{align*}
\frac{dS}{dt} &= -k_1 S \\
\frac{dD}{dt} &= k_1 S \\
\frac{dR}{dt} &= -\frac{V_1 R S}{K_m_1 + R} + \frac{V_2 R_{pp}}{K_m_2 + R_{pp}} \\
\frac{dR_{pp}}{dt} &= \frac{V_1 R S}{K_m_1 + R} - \frac{V_2 R_{pp}}{K_m_2 + R_{pp}}.
\end{align*}
$$

This example has been considered from a Bayesian context in Girolami (2008), South et al. (2018) and Salomone et al. (2018). Following South et al. (2018), observations $y(t)$ of $R_{pp}(t)$ are observed with noise such that $y(t) \sim N(R_{pp}(t), 0.02^2)$ for $t = 0, 3, \ldots, 57$. The nine parameters of interest are $\theta = (k_1, V_1, K_{m_1}, K_{m_2}, V_2, S_0, D_0, R_0, R_{pp})$, the last four being the initial values of $S$, $D$, $R$ and $R_{pp}$. We use the same simulated data as South et al. (2018) which is based on $\theta = (0.05, 0.20, 0.1, 0.1, 0.1, 0.1, 0.00, 0, 1.00, 0)$ and we use the priors from Girolami (2008),

$$
\begin{align*}
k_1, V_1, K_{m_1}, V_2, K_{m_2} &\sim \mathcal{G}(1,1) \\
S_0, R_0 &\sim \mathcal{G}(5, 0.2)
\end{align*}
$$
where $G(a, b)$ represents the Gamma distribution with shape parameter $a$, scale parameter $b$ and mean $ab$. The log-transformed parameters, $\psi = \log \theta$, are used for MCMC proposals and for ZV-CV through (7).

As explained in South et al. (2018), this example has non-linear posterior dependencies (see Appendix G of South et al. (2018) for an illustrative figure) and is challenging partially because of numerous practical and structural identifiability issues in the model. It is also interesting to note that no information is obtained about $D_0$ by observing $R_{pp}$, so $D_0$ is practically non-identifiable. $D_0$ is therefore independent of other parameters and of the data, so the posterior marginal for $D_0$ is simply its prior, $G(1, 0.1)$. This helps to explain the extremely good performance of ZV-CV and subset regularised ZV-CV in estimating its posterior mean. The parameter $R_{pp}$ is well identified based on the data and is therefore conditionally independent of other parameters given the data, making it another parameter which is potentially easier to estimate.

The gold standard of posterior expectation and evidence estimation is the mean from 100 fixed SMC runs with $N = 10000$, except for the posterior mean for $D_0$ for which we use the true value of 0.1. When using the SMC evidence estimator, it is possible to obtain a negative estimate for the evidence and this happened in some runs with low $N$ for this example. To avoid this issue, we repeat the coefficient estimation with a fixed intercept of $c = \frac{1}{N} \sum_{i=1}^{N} \varphi(\theta_i)$ when the evidence estimate is negative.

### 5.3.1 Posterior Expectations

Tables containing the efficiencies for individual posterior expectations are given in Appendix E. Given the complex target distribution and strong dependencies between parameters, it is not possible to achieve improvements on vanilla Monte Carlo integration using $N < 100$ for most parameters. The worst performing marginal expectation improves on vanilla Monte Carlo integration by at factor of at most 3.8 at $N = 1000$.

There is generally no difference in efficiency between vanilla Monte Carlo integration and a priori ZV-CV, with the exceptions of $D_0$ and $R_{pp}$. Even for a sample size as small as $N = 10$, using ZV-CV either with a full polynomial in $\psi$ or with a polynomial only in $\log D_0$ gives a posterior mean for $D_0$ that is correct to 15 significant figures. Using a polynomial in $\log R_{pp}$ gives an estimate of $R_{pp}$ which is 1.7 times more efficient than vanilla Monte Carlo integration at $N = 1000$.

### 5.3.2 Evidence Estimation

The vanilla Monte Carlo estimators of the evidence have very high variance in this example. From Figure 5 it can be seen that the distribution of SMC evidence estimates using vanilla Monte Carlo is positively skewed. The estimator underestimates with a high probability and overestimates by a large amount with small probability. The behaviour of the CTI estimator is similar.

Figure 5b illustrates the performance of ZV-CV for $N = 1000$ compared to vanilla Monte Carlo integration with the gold standard of $N = 10000$. ZV-CV significantly reduces the variance, but it introduces a negative bias. As suspected, the MSE is reduced by using ZV-CV but the amount by which it is reduced is not stable across $N$ (Tables 2 and 3) owing to the introduction of bias. Further research may be required to investigate the performance of ZV-CV when the vanilla estimator is highly positively skewed.

Despite the challenges in this example, automatic control variate selection performs reasonably well.
Figure 5: ODE example: (a) Vanilla Monte Carlo SMC evidence estimates for increasing $N$ and (b) SMC evidence estimates for $N = 1000$, with results for $N = 10000$ vanilla Monte Carlo shown for comparison.

Table 2: ODE example: efficiency of the CTI evidence estimates for a range of $N$. Ridge regression performs either similarly or worse than LASSO and has therefore been excluded from this table. The * indicates that cross-validation efficiency values for $N = 100$, $N = 500$ and $N = 1000$ are based on 98, 99 and 97 runs, respectively. The remaining 6 runs reached a polynomial order which required too much RAM.

| $N$  | $ZV_1$ | $l-ZV_1$ | $ZV_2$ | $l-ZV_2$ | $ZV_3$ | $l-ZV_3$ | $ZV_4$ | $l-ZV_4$ | crossval |
|------|--------|----------|--------|----------|--------|----------|--------|----------|----------|
| 50   | 29     | 2.2      | 33     | 30       | 59     | 29       |
| 100  | 28     | 5.0      | 210    | 50       | 3.5    | 1.7      | 240*   |
| 500  | 6.0    | 5.7      | 8.4    | 7.0      | 7.3    | 6.6      | 8.1*   |
| 1000 | 7.3    | 7.0      | 10     | 9.9      | 9.3    | 8.7      | 7.3    | 9.6*     |

Table 3: ODE example: efficiency of the SMC evidence estimates for a range of $N$. Ridge regression performs either similarly or worse than LASSO and has therefore been excluded from this table.

| $N$  | $ZV_1$ | $l-ZV_1$ | $ZV_2$ | $l-ZV_2$ | $ZV_3$ | $l-ZV_3$ | $ZV_4$ | $l-ZV_4$ | crossval |
|------|--------|----------|--------|----------|--------|----------|--------|----------|----------|
| 50   | 5.6    | 3.4      | 9.2    | 9.3      | 9.1    | 5.4      |
| 100  | 33     | 7.1      | 240    | 28       | 1.7    | 3.0      | 29     |
| 500  | 5.5    | 5.3      | 7.8    | 8.2      | 6.9    | 7.1      | 6.2    | 7.3      |
| 1000 | 6.9    | 6.6      | 9.1    | 9.0      | 8.6    | 8.1      | 4.7    | 6.8      | 8.1      |

6 Discussion

In this paper, we introduced two types of regularised ZV-CV: regularisation through penalised regression and regularisation by selecting a subset of parameters to include in the polynomial. Higher order polynomials have the potential to outperform the commonly used polynomial with $Q = 2$ as $N$ increases, and our penalised ZV-CV ensures that the resulting functional approximation problem remains well-defined. For the examples considered here, we found that LASSO generally resulted in better performance than ridge regression. A priori ZV-CV led to significant improvements over vanilla Monte Carlo for posterior expectations in some examples. We believe that a priori ZV-CV could be a
useful tool when not all derivatives are available, when a very small number of samples are available or when information about the relationships between the integrand and parameters is known (for example when $p(\theta)$ has a directed acyclic graph factorisation).

Some other potentially useful regularisation methods for the situation where $N < \binom{d+Q}{d}$ are elastic net (Zou and Hastie (2005)) and partial least squares (PLS, Wold (1975)). Elastic net is a compromise between LASSO and ridge regression which uses two tuning parameters. PLS is based on choosing the $k < \binom{d+Q}{d} - 1$ independent linear combinations of covariates that explain the maximum variance in the response, where $k$ is chosen through cross-validation. It would be of interest in future research to compare our LASSO and ridge regression ZV-CV methods with these alternatives and also with existing CF methods.

Finding the optimal parameterisation for a given application is a challenging open problem. Choosing the parameterisation is a trade-off between making $p_\phi$ simpler and making $\phi(f^-1(\phi))$ simpler. Another potential benefit of reparameterising for ZV-CV is that there is the potential to enforce more sparsity in the predictors for improved performance in $\ell_1$ penalisation.

Derivatives are available in closed form or can be unbiasedly estimated for a large class of problems. ZV-CV has been applied in big data settings in the context of post-processing after stochastic gradient MCMC (Baker et al., 2017) and for models with intractable likelihoods (Friel et al., 2016). Regularised ZV-CV also applies in these settings. Regularised ZV-CV could also be used in exact approximate settings where a particle filtering estimate of the likelihood is used (see for example Dahlin et al. (2015) and Nemeth et al. (2016)). An interesting avenue for future research may be to consider automatic differentiation. However, derivative-based methods are most appealing when the derivative of the log target can be obtained with little additional cost relative to the likelihood itself.

The examples considered in this work are based on estimating posterior expectations and the normalising constant of a Bayesian model using likelihood annealing SMC. Given that the CTI estimator appears to be more amenable to a control variates treatment, we propose its use over the SMC estimator when practitioners wish to make the best use of derivatives for evidence estimation. However, when the prior is highly diffuse, the SMC estimator may be preferable since the CTI estimator can suffer from high variance as a consequence of extreme values in the initial draws. In future research, it may be interesting to consider recycling samples from previous likelihood annealing targets in SMC for posterior expectations and evidence estimation. This recycling would extend the work of Briol et al. (2017) for improving tail coverage with the split estimator and could also improve the performance of higher order polynomials due to higher degrees of freedom.

We have proposed a cross-validation method to select control variates in Section 5 based on increasing the polynomial order until the average cross-validation error decreases. This method is easy to implement and may potentially lead to super-root-$N$ convergence. However, a lower than optimal $Q$ may be selected if the difference between some polynomial orders is small. Increasing amounts of memory in storing the regression design matrix are also required as the polynomial order becomes large. In practice, one could impose a minimum polynomial order to prevent early stopping and/or a maximum polynomial order to reduce memory requirements and computational effort. Given that the optimal control variate may not be the same for all $T$ expectations in the SMC and CTI evidence estimators, efficient choice of the optimal control variates is an important problem. Ultimately, more research is required to determine efficient methods to choose between control variates but our preliminary findings support a role for regularisation-based extensions of ZV-CV.

7 Acknowledgements

The authors would like to thank Nial Friel for the suggestion to reduce the variance of the SMC evidence estimator using ZV-CV and for comments on an earlier draft. LFS and CD are associated with the ARC Centre of Excellence for Mathematical & Statistical Frontiers (ACEMS). CD was supported by an
LFS would like to thank Matthew Sutton for useful discussions about penalised regression methods. LFS was supported by an Australian Research Training Program Stipend and by ACEMS. CJO was supported by the Lloyd’s Register Foundation programme on data centric engineering at the Alan Turing Institute, UK. Computational resources used in this work were provided by the HPC and Research Support Group, Queensland University of Technology, Brisbane, Australia.

8 References

Aronszajn, N. (1950). Theory of reproducing kernels. *Transactions of the American Mathematical Society*, 68(3):337–404.

Assaraf, R. and Caffarel, M. (1999). Zero-variance principle for Monte Carlo algorithms. *Physical Review Letters*, 83(23):4682–4685.

Baker, J., Fearnhead, P., Fox, E. B., and Nemeth, C. (2017). Control variates for stochastic gradient MCMC. https://arxiv.org/pdf/1706.05439.pdf.

Barp, A., Oates, C. J., Porcu, E., and Girolami, M. (2018). A Riemannian-Stein kernel method. arXiv:1810.03946.

Belomestny, D., Iosipoi, L., and Zhivotovskiy, N. (2017). Variance reduction via empirical variance minimization: convergence and complexity. arXiv:1712.04667.

Berlinet, A. and Thomas-Agnan, C. (2011). *Reproducing kernel Hilbert spaces in probability and statistics*. Springer Science & Business Media.

Briol, F.-X., Oates, C. J., Cockayne, J., Chen, W. Y., and Girolami, M. (2017). On the sampling problem for kernel quadrature. arXiv:1706.03369.

Brooks, S. P., Catchpole, E. A., and Morgan, B. J. T. (2000). Bayesian animal survival estimation. *Statistical Science*, 15(4):357–376.

Buchholz, A., Chopin, N., and Jacob, P. E. (2018). Adaptive tuning of Hamiltonian Monte Carlo within sequential Monte Carlo. arXiv:1808.07730.

Chopin, N. (2002). A sequential particle filter method for static models. *Biometrika*, 89(3):539–552.

Chopin, N. (2017). Leave Pima Indians alone: binary regression as a benchmark for Bayesian computation. *Statistical Science*, 32(1):64–87.

Dahlin, J., Lindsten, F., and Schon, T. B. (2015). Particle Metropolis-Hastings using gradient and Hessian information. *Statistics and Computing*, 25:81–92.

Del Moral, P., Doucet, A., and Jasra, A. (2006). Sequential Monte Carlo samplers. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68:411–436.

Del Moral, P., Doucet, A., and Jasra, A. (2012). On adaptive resampling strategies for sequential Monte Carlo methods. *Bernoulli*, 18(1):252–278.

DeVore, R. A. (1998). Nonlinear approximation. *Acta numerica*, 7:51–150.

Dheeru, D. and Karra Taniskidou, E. (2017). UCI machine learning repository.

Duane, S., Kennedy, A. D., Pendleton, B. J., and Roweth, D. (1987). Hybrid Monte Carlo. *Physical Letters B*, 195(2).
Fearnhead, P. and Taylor, B. M. (2013). An adaptive sequential Monte Carlo sampler. *Bayesian Analysis*, 8(2):411–438.

Friedman, J., Hastie, T., and Tibshirani, R. (2010). Regularization paths for generalized linear models via coordinate descent. *Journal of Statistical Software*, 33(1):1–22.

Friel, N., Hurn, M., and Wyse, J. (2014). Improving power posterior estimation of statistical evidence. *Statistics and Computing*, 24(5):709–723.

Friel, N., Mira, A., and Oates, C. J. (2016). Exploiting multi-core architectures for reduced-variance estimation with intractable likelihoods. *Bayesian Analysis*, 11(1):215–245.

Friel, N. and Pettitt, A. N. (2008). Marginal likelihood estimation via power posteriors. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 70(3):589–607.

Gelman, A., Jakulin, A., Pittau, M. G., and Su, Y.-S. (2008). A weakly informative default prior distribution for logistic and other regression models. *The Annals of Applied Statistics*, 2(4):1360–1383.

Gelman, A. and Meng, X.-L. (1998). Simulating normalising constants: from importance sampling to bridge sampling to path sampling. *Statistical Science*, 13(2):163–185.

Geyer, C. (1991). Parallel tempering. *Computing Science and Statistics: Proceedings of the 23rd Symposium on Computing Science and S*, American Statistical Association, page 156.

Girolami, M. (2008). Bayesian inference for differential equations. *Theoretical Computer Science*, 408:4–16.

Girolami, M. and Calderhead, B. (2011). Riemann manifold Langevin and Hamiltonian Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 73(2):123–214.

Glasserman, P. (2003). *Monte Carlo methods in financial engineering*, chapter 4, pages 185–279. Springer Science & Business Media.

Gorman, R. P. and Sejnowski, T. J. (1988). Analysis of hidden units in a layered network trained to classify sonar targets. *Neural networks*, 1(1):75–89.

Hammersley, J. M. and Handscomb, D. C. (1964). *Monte Carlo Methods*. Chapman & Hall.

Hastie, R., Tibshirani, R., and Wainwright, M. (2015). *Statistical Learning with Sparsity: The Lasso and Generalizations*. CRC Press.

Hastings, W. K. (1970). Monte Carlo sampling methods using Markov chain and their applications. *Biometrika*, 57(1):97–109.

Hoerl, A. E. and Kennard, R. W. (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1):55–67.

Hoffman, M. D. and Gelman, A. (2014). The no-u-turn sampler: adaptively setting path lengths in Hamiltonian Monte Carlo. *Journal of Machine Learning Research*, 15(1):1593–1623.

Jasra, A., Stephens, D. A., Doucet, A., and Tsagaris, T. (2011). Inference for Lévy-driven stochastic volatility models via adaptive sequential Monte Carlo. *Scandinavian Journal of Statistics*, 38(1):1–22.

Lebreton, J. D., Burnham, K. P., Clobert, J., and Anderson, D. R. (1992). Modeling survival and testing biological hypotheses using marked animals: a unified approach with case studies. *Ecological Monographs*, 61(1):67–118.
Marzolin, G. (1988). Polygynie du cîncle plongeur (cinclus cinclus) dans le côtes de Loraine. *Oiseau et la Revue Francaise d'Ornithologie*, 58(4):277–286.

Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E. (1953). Equations of state calculations by fast computing machines. *Journal of Chemical Physics*, 12(6):1087–1092.

Mira, A., Solgi, R., and Imparato, D. (2013). Zero variance Markov chain Monte Carlo for Bayesian estimators. *Statistics and Computing*, 23(5):653–662.

Neal, R. M. (2001). Annealed importance sampling. *Statistics and Computing*, 11:125–139.

Nemeth, C., Fearnhead, P., and Mihaylova, L. (2016). Particle approximations of the score and observed information matrix for parameter estimation in state-space models with linear computational cost. *Journal of Computational and Graphical Statistics*, 25(4):1138–1157.

Nott, D. J., Drovandi, C. C., Mengersen, K., and Evans, M. (2018). Approximation of Bayesian predictive p-values with regression ABC. *Bayesian Analysis*, 13(1):59–83.

Oates, C. J., Cockayne, J., Briol, F. X., and Girolami, M. (2017a). Convergence rates for a class of estimators based on Stein’s method. *To appear in Bernoulli*.

Oates, C. J., Girolami, M., and Chopin, N. (2017b). Control functionals for Monte Carlo integration. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 79(3):695–718.

Oates, C. J., Papamarkou, T., and Girolami, M. (2016). The controlled thermodynamic integral for Bayesian model evidence evaluation. *Journal of the American Statistical Association*, 111(514):634–645.

Ogata, Y. (1989). A Monte Carlo method for high dimensional integration. *Numerical Mathematics*, 55(2):137–157.

Papamarkou, T., Mira, A., and Girolami, M. (2014). Zero variance differential geometric Markov chain Monte Carlo algorithms. *Bayesian Analysis*, 9(1):97–128.

Pasarica, C. and Gelman, A. (2010). Adaptively scaling the Metropolis Hastings algorithm using expected squared jumped distance. *Statistica Sinica*, 20(1):343–364.

Portier, F. and Segers, J. (2018). Monte Carlo integration with a growing number of control variates. *arXiv:1801.01797*.

Ripley, B. (1987). *Stochastic Simulation*. John Wiley & Sons.

Roberts, G. O. and Stramer, O. (2002). Langevin diffusions and Metropolis-Hastings algorithms. *Methodology and Computing in Applied Probability*, 4(4):337–357.

Salomone, R., South, L. F., Drovandi, C. C., and Kroese, D. P. (2018). Unbiased and consistent nested sampling via sequential Monte Carlo. *arXiv:1805.03924*.

Sim, A., Filippi, S., and Stumpf, M. P. H. (2012). Information geometry and sequential Monte Carlo samplers. *arXiv:1212.0764*.

Smolyak, S. A. (1963). Quadrature and interpolation formulas for tensor products of certain classes of functions. In *Doklady Akademii Nauk*, volume 148, pages 1042–1045. Russian Academy of Sciences.

South, L. F., Pettitt, A. N., and Drovandi, C. C. (2018). Sequential Monte Carlo samplers with independent MCMC proposals. *To appear in Bayesian Analysis*.
Stein (1972). A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. In Cam, M. L., Neyman, J., and Scott, E. L., editors, Proc. 6th Berkeley Symp. Mathematical Statistics and Probability, volume 2, pages 583–602. Berkeley: University of California Press.

Stone, M. H. (1948). The generalized Weierstrass approximation theorem. Mathematics Magazine, 21(5):237–254.

Tibshirani, R. (1996). Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 58(1):267–288.

Tikhonov, A. N., Goncharsky, A., Stepanov, V. V., and Yagola, A. G. (2013). Numerical methods for the solution of ill-posed problems. Springer Science & Business Media.

Van der Pol, B. (1926). On relaxation-oscillations. The London, Edinburgh and Dublin Philosophical Magazine and Journal of Science, 2(11):978–992.

Wold, H. (1975). Soft modeling by latent variables; the non-linear iterative partial least squares approach. In Gani, J., editor, Perspectives in Probability and Statistics, Papers in Honour of M. S. Bartlett, volume 12, pages 117–142, London. Academic Press.

Zhou, Y., Johansen, A. M., and Aston, J. A. D. (2012). Bayesian model comparison via path-sampling sequential Monte Carlo. In IEEE Statistical Signal Processing Workshop (SSP), pages 245–248.

Zhou, Y., Johansen, A. M., and Aston, J. A. D. (2015). Towards automatic model comparison: An adaptive sequential Monte Carlo approach. Journal of Computational and Graphical Statistics, 25(3):701–726.

Zhu, Z., Wan, R., and Zhong, M. (2018). Neural control variates for variance reduction. arXiv:1806.00159.

Zhuo, J., Liu, C., Shi, J., Zhu, J., Chen, N., and Zhang, B. (2018). Message passing Stein variational gradient descent. In Dy, J. and Krause, A., editors, Proceedings of the 35th International Conference on Machine Learning, pages 6018–6027. PMLR.

Zou, H. and Hastie, T. (2005). Regularization and variable selection via the elastic net. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 67(2):301–320.
Appendices

A Covariates in the ZV-CV Regression

As described in Section 2.3, ZV-CV uses control variates of the form $\beta^\top x(\theta)$ where $\beta \in \mathbb{R}^J$ and $J = (d+Q) - 1$. This appendix gives the general form for $x(\theta)$ for a polynomial of order $Q$.

The $j$th element of $x(\theta)$ is:

$$x[j] = \sum_{k=1}^{d} \max[0, A_{j,k}] \theta[k] A_{j,k}^{-1} \nabla_{\theta[k]} \log p(\theta) \prod_{z=1, z \neq k}^{d} \theta[z] A_{j,z}^{A_{j,z} - 1} + \max[0, A_{j,k}(A_{j,k} - 1)] \theta[k] A_{j,k}^{-2} \prod_{z=1, z \neq k}^{d} \theta[z] A_{j,z},$$

where $j = 1, \ldots, J$. The matrix $A \in \mathbb{Z}_{\geq 0}^{J \times d}$ has $J$ rows where each row corresponds to a unique vector $A_{j, \cdot}$ such that $1 \leq \sum_{k=1}^{d} A_{j,k} \leq Q$. In other words, $A$ contains all permutations of powers to $\theta[1], \ldots, \theta[d]$ that lead to a sum of exponents between 1 and $Q$.

It is straightforward to verify that $x = \nabla_{\theta} \log p(\theta) \in \mathbb{R}^d$ for the first order polynomial $P(\theta) = c + \sum_{k=1}^{d} \beta[k] \theta[k]$.

B Post-hoc Temperature Choice

Using an insufficient number of inverse temperatures can lead to significant bias in the power posterior log evidence estimator. However, it is difficult to know a priori how many inverse temperatures will be required to achieve reasonably small bias. This appendix briefly describes some existing methods for choosing the inverse temperature schedule before describing our post-hoc approach. The proposed method is useful for both CTI and SMC evidence estimation.

The simplest approach for choosing the inverse temperatures is to use a fixed schedule, for example $t_j = (j/T)^5$ for $j = 0, \ldots, T$ [Friel and Pettitt, 2008]. If this schedule is conservative in that $T$ is very high, then some costly resampling and move steps can be avoided by performing these steps only when an approximation to the effective sample size (ESS) becomes low. The ESS is the number of independent samples from the target that would be required to achieve the same variance of the estimator and the ESS at inverse temperature $t_j$ is approximated in SMC by $1 / \sum_{i=1}^{N} (W^i_j)^2$.

[Hyv"{a}rinen et al., 2011] describe a method for adaptively choosing the inverse temperature schedule with the goal of minimising the discretisation error in the power posterior log evidence estimator. Their method is used to calibrate the inverse temperatures prior to implementing the full sampler and it may be useful when evidence estimation is the primary focus.

In the SMC context, the most popular method for adaptively choosing the inverse temperatures is based on fixing the approximated ESS at $\rho N$ using the bisection method, where $0 < \rho < N$ [Jasra et al., 2011]. This approach maintains a fixed discrepancy between $p_{j-1}$ and $p_j$ for $j = 1, \ldots, T$ when resampling and move steps are performed at each iteration. [Zhou et al., 2015] use the conditional ESS (CESS),

$$\text{CESS}_{t_j} = \frac{N \left( \sum_{i=1}^{N} W_{j-1}^i \frac{\eta_j(\theta_{j-1}^i)}{\eta_{j-1}(\theta_{j-1}^i)} \right)^2}{\sum_{i=1}^{N} W_{j-1}^i \left( \frac{\eta_j(\theta_{j-1}^i)}{\eta_{j-1}(\theta_{j-1}^i)} \right)^2},$$

where $W_{j-1}^i$ is the weight of the $i$th particle at iteration $j-1$.
instead of the ESS when resampling is not performed at every inverse temperature, because this a more accurate measure of the discrepancy between $p_{j-1}$ and $p_j$ when $p_{j-1}$ is approximated with a weighted sample.

Using the approaches above, it is difficult to be confident that the quadrature bias will be sufficiently low without being overly conservative. Performing ZV-CV on the power posterior log evidence estimator requires $T$ regressions to be performed, that is one at each inverse temperature regardless of whether resample and move steps were performed. A conservative choice of inverse temperature schedule increases the post-processing time in ZV-CV.

We propose a post-hoc method to adjust the inverse temperatures when the original choice is either not conservative enough or too conservative. To start with, any approach can be used to provide $T$ distinct sets of particles and inverse temperatures,

\[
\{\{\theta^i_j\}_{i=1}^N, \tilde{t}_j\}_{j=0}^T.
\]  

(14)

Inverse temperatures at which the particles are not moved (for example due to adaptive resampling methods in SMC) are not included in these $T$ inverse temperatures. If (14) is too conservative or not conservative enough, then a new set of inverse temperatures $\{\tilde{t}_j\}_{j=0}^T$ is selected as follows.

Given an inverse temperature $\tilde{t}_j$ (starting at $\tilde{t}_0 = 0$), the bisection method is used to select $\tilde{t}_j$ such that $\text{CESS}_{\tilde{t}_j} = \tilde{\rho}N$. This process continues until an inverse temperature of $\tilde{t}_\tilde{\rho} = 1$ satisfies $\text{CESS}_{\tilde{t}_\tilde{\rho}} \geq \tilde{\rho}N$. Each of the inverse temperatures must be assigned a relevant particle population and this is done by selecting population $\{\theta_k^i\}_{i=1}^N$ such that $t_k \leq \tilde{t}_j$. The new population is

\[
\{\{\theta^i_{\text{argmax}_k(t_k \geq \tilde{t}_j)}\}_{i=1}^N, \tilde{t}_j\}_{j=0}^T.
\]  

(15)

Put simply, the method involves choosing inverse temperatures post-hoc so that the CESS is fixed at $\tilde{\rho}N$ where $0 < \tilde{\rho} < N$. The inverse temperatures $\{t_j\}_{j=0}^T$ need not appear in $\{\tilde{t}_j\}_{j=0}^T$, but they may for some choices of initial inverse temperatures and $\tilde{\rho}$.

C Van der Pol Example

Table 4 shows the selected polynomial order for each of the expectations in the SMC evidence estimator across 100 independent runs. Where two large numbers in a column are separated by a zero, it may be a sign that there is only a small improvement (or a decrease in efficiency) from one polynomial order to the next. Each of the 26 expectations is based on a different weighted particle set, some with higher ESS than others. The differences in ESS along with the different integrand in each expectation both contribute to the difference in optimal polynomial orders across the 26 expectations.

D Recapture Example

Tables 5-15 show the efficiency, $\text{MSE}_{\text{p[vanilla]}}/\text{MSE}_{\text{p[LASSO]}}$, for each posterior expectation. Results with ridge regression are consistently either similar or much worse than results with LASSO, with the worst results for ridge regression being when $N$ is small relative to the number of regression parameters. Ridge regression has therefore been excluded from these tables for brevity.

Figure 6 shows the control variates which were selected in cross-validation for evidence estimation based on $N = 50$ and $N = 1000$. 

26
Table 4: Van der Pol example: The chosen polynomial order counts using cross-validation for each of the 26 expectations in the SMC evidence estimator. Results are based on \( N = 1000 \)

| Q | ZV_1 | l-ZV_1 | ZV_2 | l-ZV_2 | ZV_3 | l-ZV_3 | ZV_4 | l-ZV_4 | sub_1-ZV_1 | sub_1-ZV_2 | crossval |
|---|------|--------|------|--------|------|--------|------|--------|------------|------------|----------|
| 0 | 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 0          | 0        |
| 1 | 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 0          | 0        |
| 2 | 5    | 30     | 71   | 100    | 9    | 53     | 94   | 99     | 60         | 17         | 25       |
| 3 | 1    | 1      | 0    | 4      | 1    | 0      | 0    | 0      | 0          | 2          | 0        |
| 4 | 8    | 0      | 0    | 1      | 0    | 0      | 1    | 3      | 11         | 21         | 37       |
| 5 | 53   | 12     | 32   | 14     | 0    | 52     | 27   | 3      | 0          | 10         | 7        |
| 6 | 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 0          | 0        |
| 7 | 13   | 26     | 11   | 0      | 22   | 8      | 0    | 0      | 0          | 0          | 0        |
| 8 | 7    | 3      | 0    | 3      | 4    | 0      | 0    | 6      | 8          | 19         | 16       |
| 9 | 1    | 3      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 2          | 2        |
| 10| 5    | 2      | 3    | 0      | 1    | 0      | 0    | 0      | 0          | 0          | 0        |
| 11| 0    | 0      | 1    | 0      | 3    | 6      | 3    | 0      | 0          | 1          | 4        |
| 12| 2    | 1      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 0          | 0        |
| 13| 3    | 1      | 0    | 0      | 0    | 0      | 0    | 0      | 2          | 0          | 2        |
| 14| 0    | 0      | 0    | 3      | 1    | 0      | 0    | 0      | 0          | 1          | 0        |
| 15| 2    | 0      | 0    | 0      | 1    | 0      | 0    | 0      | 0          | 0          | 1        |
| 16| 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 1          | 2        |
| 17| 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 1          | 2        |
| 18| 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 1          | 1        |
| 19| 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 1          | 0        |
| 20| 0    | 0      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 1          | 2        |
| 21| 0    | 1      | 0    | 0      | 0    | 0      | 0    | 0      | 0          | 1          | 0        |

Table 5: Recapture example: marginal 1

| N  | ZV_1 | l-ZV_1 | ZV_2 | l-ZV_2 | ZV_3 | l-ZV_3 | ZV_4 | l-ZV_4 | sub_1-ZV_1 | sub_1-ZV_2 | crossval |
|----|------|--------|------|--------|------|--------|------|--------|------------|------------|----------|
| 50 | 3.7  | 4.1    | 12   | 11     | 2.4  | 3.2    | 4.1  | 11     |            |            |          |
| 100| 4.7  | 4.7    | 4.6  | 15     | 33   | 13     | 2.9  | 3.4    | 18         |            |          |
| 500| 5.1  | 5.0    | 16   | 19     | 15   | 36     | 39   | 2.8    | 3.6        | 28         |          |
| 1000| 3.7 | 3.7    | 17   | 18     | 26   | 35     | 38   | 3.0    | 4.7        | 22         |          |

Table 6: Recapture example: marginal 2

| N  | ZV_1 | l-ZV_1 | ZV_2 | l-ZV_2 | ZV_3 | l-ZV_3 | ZV_4 | l-ZV_4 | sub_1-ZV_1 | sub_1-ZV_2 | crossval |
|----|------|--------|------|--------|------|--------|------|--------|------------|------------|----------|
| 50 | 24   | 22     | 22   | 13     | 5.6  | 8.3    | 7.6  | 16     |            |            |          |
| 100| 12   | 12     | 20   | 49     | 29   | 17     | 4.8  | 5.0    | 44         |            |          |
| 500| 25   | 24     | 70   | 79     | 110  | 140    | 84   | 7.5    | 7.7        | 130        |          |
| 1000| 19  | 19     | 71   | 76     | 150  | 160    | 130  | 6.1    | 6.1        | 150        |          |

Table 7: Recapture example: marginal 3

| N  | ZV_1 | l-ZV_1 | ZV_2 | l-ZV_2 | ZV_3 | l-ZV_3 | ZV_4 | l-ZV_4 | sub_1-ZV_1 | sub_1-ZV_2 | crossval |
|----|------|--------|------|--------|------|--------|------|--------|------------|------------|----------|
| 50 | 47   | 51     | 40   | 30     | 22   | 11     | 10   | 45     |            |            |          |
| 100| 48   | 50     | 110  | 180    | 93   | 68     | 9.9  | 10     | 170        |            |          |
| 500| 60   | 61     | 370  | 360    | 990  | 380    | 300  | 13     | 13         | 650        |          |
| 1000| 70  | 70     | 320  | 330    | 1,700| 790    | 820  | 9.8    | 9.8        | 1,700      |          |
| N  | ZV1 | l-ZV1 | ZV2 | l-ZV2 | ZV3 | l-ZV3 | ZV4 | l-ZV4 | sub1-ZV1 | sub1-ZV2 | crossval |
|----|-----|-------|-----|-------|-----|-------|-----|-------|----------|----------|----------|
| 50 | 43  | 43    | 31  | 32    | 19  | 9.0   | 8.5 | 39    | 39       | 39       |          |
| 100| 35  | 35    | 62  | 150   | 99  | 63    | 9.0 | 8.7   | 140      |          | 140      |
| 500| 42  | 42    | 190 | 840   | 450 | 290   | 7.0 | 7.3   | 580      |          |          |
| 1000|41  | 41    | 260 | 1,400 | 700 | 820   | 6.8 | 7.0   | 1,400    |          |          |

Table 8: Recapture example: marginal 4

| N  | ZV1 | l-ZV1 | ZV2 | l-ZV2 | ZV3 | l-ZV3 | ZV4 | l-ZV4 | sub1-ZV1 | sub1-ZV2 | crossval |
|----|-----|-------|-----|-------|-----|-------|-----|-------|----------|----------|----------|
| 50 | 46  | 50    | 32  | 28    | 21  | 8.7   | 8.0 | 39    | 39       | 39       |          |
| 100| 46  | 48    | 38  | 93    | 75  | 54    | 6.1 | 6.3   | 77       |          | 77       |
| 500| 60  | 59    | 290 | 330   | 470 | 250   | 8.8 | 8.9   | 500      |          |          |
| 1000|48  | 48    | 310 | 1,700 | 960 | 810   | 8.8 | 8.7   | 1,600    |          |          |

Table 9: Recapture example: marginal 5

| N  | ZV1 | l-ZV1 | ZV2 | l-ZV2 | ZV3 | l-ZV3 | ZV4 | l-ZV4 | sub1-ZV1 | sub1-ZV2 | crossval |
|----|-----|-------|-----|-------|-----|-------|-----|-------|----------|----------|----------|
| 50 | 5.0 | 5.3   | 19  | 19    | 2.9 | 3.2   | 3.4 | 13    |          |          | 13       |
| 100| 8.3 | 8.1   | 9.1 | 34    | 74  | 45    | 4.0 | 4.1   | 60       |          |          |
| 500| 7.9 | 7.6   | 29  | 35    | 65  | 65    | 3.7 | 4.0   | 58       |          | 58       |
| 1000|4.9 | 4.9   | 24  | 26    | 53  | 53    | 2.9 | 3.1   | 58       |          |          |

Table 10: Recapture example: marginal 6

| N  | ZV1 | l-ZV1 | ZV2 | l-ZV2 | ZV3 | l-ZV3 | ZV4 | l-ZV4 | sub1-ZV1 | sub1-ZV2 | crossval |
|----|-----|-------|-----|-------|-----|-------|-----|-------|----------|----------|----------|
| 50 | 13  | 13    | 17  | 12    | 6.5 | 3.6   | 4.4 | 9.5   |          |          |          |
| 100| 12  | 12    | 23  | 70    | 35  | 26    | 6.3 | 6.8   | 70       |          | 70       |
| 500| 15  | 15    | 72  | 200   | 340 | 190   | 4.3 | 4.5   | 360      |          |          |
| 1000|25  | 24    | 140 | 150   | 960 | 950   | 7.8 | 8.3   | 870      |          |          |

Table 11: Recapture example: marginal 7

| N  | ZV1 | l-ZV1 | ZV2 | l-ZV2 | ZV3 | l-ZV3 | ZV4 | l-ZV4 | sub1-ZV1 | sub1-ZV2 | crossval |
|----|-----|-------|-----|-------|-----|-------|-----|-------|----------|----------|----------|
| 50 | 22  | 25    | 27  | 24    | 23  | 7.6   | 7.6 | 27    |          |          |          |
| 100| 31  | 34    | 93  | 200   | 95  | 64    | 13  | 13    | 190      |          | 190      |
| 500| 36  | 38    | 410 | 450   | 200 | 470   | 12  | 13    | 860      |          | 860      |
| 1000|62  | 61    | 480 | 490   | 3,700| 1,700| 1,500| 16    | 3,700    |          |          |

Table 12: Recapture example: marginal 8

### E ODE Example

Tables 16-24 show the efficiency, $\text{MSE}_{\bar{\hat{p}}}^\text{vanilla}/\text{MSE}_{\hat{p}}^\text{vanilla}$, for each posterior expectation.
| N | ZV₁ | l-ZV₁ | ZV₂ | l-ZV₂ | ZV₃ | l-ZV₃ | ZV₄ | l-ZV₄ | sub₁-ZV₁ | sub₁-ZV₂ | crossval |
|---|-----|------|-----|------|-----|------|-----|------|---------|---------|----------|
| 50 | 29  | 30   | 31  | 25   | 17  | 7.5  | 7.4 | 29   |         |         |          |
| 100| 22  | 22   | 43  | 140  | 95  | 59   | 7.3 | 7.7  | 140     |         |          |
| 500| 37  | 36   | 190 | 220  | 990 | 490  | 330 | 8.4  | 8.3     | 600     |          |
| 1000|37  | 36   | 250 | 270  | 1,700| 940  | 1,200| 9.6  | 9.9     | 1,800   |          |

Table 13: Recapture example: marginal 9

| N | ZV₁ | l-ZV₁ | ZV₂ | l-ZV₂ | ZV₃ | l-ZV₃ | ZV₄ | l-ZV₄ | sub₁-ZV₁ | sub₁-ZV₂ | crossval |
|---|-----|------|-----|------|-----|------|-----|------|---------|---------|----------|
| 50 | 31  | 32   | 24  | 22   | 20  | 8.2  | 8.4 | 28   |         |         |          |
| 100| 37  | 39   | 47  | 120  | 78  | 48   | 9.1 | 8.9  | 120     |         |          |
| 500| 27  | 26   | 190 | 210  | 680 | 280  | 180 | 7.0  | 7.4     | 330     |          |
| 1000|25 | 25   | 200 | 200  | 1,200| 680  | 590 | 7.0  | 7.2     | 1,400   |          |

Table 14: Recapture example: marginal 10

| N | ZV₁ | l-ZV₁ | ZV₂ | l-ZV₂ | ZV₃ | l-ZV₃ | ZV₄ | l-ZV₄ | m₁-ZV₁ | m₁-ZV₂ | crossval |
|---|-----|------|-----|------|-----|------|-----|------|--------|--------|----------|
| 50 | 210 | 230  | 170 | 140  | 120 | 28   | 28  | 210  |        |        |          |
| 100| 400 | 430  | 440 | 1,100| 910 | 680  | 48  | 48   | 1,000  |        |          |
| 500| 260 | 250  | 1,600| 1,700| 4,400| 1,800| 970 | 33   | 2,400  |        |          |
| 1000|230 | 230  | 1,500| 1,500| 8,100| 2,600| 1,900| 36   | 8,100  |        |          |

Table 15: Recapture example: marginal 11

| N | ZV₁ | l-ZV₁ | r-ZV₁ | ZV₂ | l-ZV₂ | r-ZV₂ | ZV₃ | l-ZV₃ | r-ZV₃ | ZV₄ | l-ZV₄ | r-ZV₄ | sub₁-ZV₁ | crossval |
|---|-----|------|------|-----|------|------|-----|------|------|-----|------|------|----------|----------|
| 50 | 0.55| 0.63 | 0.62 | 0.93| 0.93 | 0.72 | 0.79| 0.70 | 0.77 | 1.0 | 0.76 |      |          |          |
| 100| 0.80| 0.85 | 0.84 | 2.0 | 2.3  | 1.7  | 0.92| 0.76 | 0.94 | 0.86| 1.0  | 1.7   |          |          |
| 500| 0.97| 0.97 | 0.97 | 8.7 | 5.3  | 6.0  | 3.6 | 7.6  | 5.3  | 7.2 | 4.3  | 1.0   | 6.2     |          |
| 1000|0.92| 0.95 | 0.94 | 5.7 | 5.0  | 5.9  | 4.5 | 5.3  | 4.4  | 0.97| 4.5  | 3.5   | 1.0     | 4.3     |

Table 16: ODE example: marginal 1

| N | ZV₁ | l-ZV₁ | r-ZV₁ | ZV₂ | l-ZV₂ | r-ZV₂ | ZV₃ | l-ZV₃ | r-ZV₃ | ZV₄ | l-ZV₄ | r-ZV₄ | sub₁-ZV₁ | crossval |
|---|-----|------|------|-----|------|------|-----|------|------|-----|------|------|----------|----------|
| 50 | 0.56| 0.98 | 1.2  | 0.34| 0.34 | 0.66 | 0.70| 0.78 | 0.79 | 1.0 | 0.79 | 1.0   | 0.55     |          |
| 100| 1.7 | 1.9  | 2.0  | 2.0 | 0.80 | 0.86 | 0.90| 0.77 | 1.0  | 0.92| 1.0  | 1.0   | 1.9     |          |
| 500| 1.7 | 1.7  | 4.1  | 1.4 | 2.9  | 7.4  | 2.3 | 3.3  | 1.7  | 1.7 | 1.0  | 7.2   |          |          |
| 1000|1.1 | 1.4  | 1.8  | 1.1 | 1.9  | 3.8  | 1.4 | 2.4  | 1.7  | 1.6 | 1.6  | 1.0   | 3.8     |          |

Table 17: ODE example: marginal 2

| N | ZV₁ | l-ZV₁ | r-ZV₁ | ZV₂ | l-ZV₂ | r-ZV₂ | ZV₃ | l-ZV₃ | r-ZV₃ | ZV₄ | l-ZV₄ | r-ZV₄ | sub₁-ZV₁ | crossval |
|---|-----|------|------|-----|------|------|-----|------|------|-----|------|------|----------|----------|
| 50 | 0.60| 0.70 | 0.75 | 0.30| 0.35 | 0.90 | 0.68| 1.2  | 0.44 | 1.0 | 0.29 |      |          |          |
| 100| 1.1 | 1.1  | 1.1  | 1.1 | 1.5  | 1.3  | 1.3 | 1.1  | 1.4 | 1.2 | 1.0  | 1.2   |          |          |
| 500| 1.4 | 1.3  | 4.6  | 1.7 | 2.4  | 19   | 3.7 | 4.0  | 2.7 | 2.2 | 1.0  | 5.6   |          |          |
| 1000|1.3 | 1.2  | 1.2  | 1.3 | 1.3  | 5.1  | 2.1 | 2.3  | 2.7 | 2.1 | 1.5  | 1.0   | 4.3     |          |

Table 18: ODE example: marginal 3
Figure 6: Recapture example: The selected control variates based on cross-validation for (a) The $E$ terms in CTI [12] with $N = 50$, (b) The $V$ terms in CTI [12] with $N = 50$, (c) The $E$ terms in (13) with $N = 50$, (d)-(f) the same for $N = 1000$.

| $N$ | $ZV_1$ | $l-ZV_1$ | $r-ZV_1$ | $ZV_2$ | $l-ZV_2$ | $r-ZV_2$ | $ZV_3$ | $l-ZV_3$ | $r-ZV_3$ | $ZV_4$ | $l-ZV_4$ | $r-ZV_4$ | sub1-$ZV_1$ | crossval |
|-----|--------|----------|----------|--------|----------|----------|--------|----------|----------|--------|----------|----------|----------|----------|
| 50  | 0.51   | 0.60     | 0.58     | 0.35   | 0.34     | 0.37     | 0.41   | 0.34     | 0.51     | 1.0    | 0.39     |          |          |          |
| 100 | 0.91   | 0.89     | 0.88     | 1.7    | 1.5      | 0.99     | 1.9    | 1.3      | 1.2      | 1.0    | 1.0      | 1.7      |          |          |
| 500 | 1.2    | 1.2      | 1.2      | 5.1    | 4.8      | 4.7      | 3.0    | 7.8      | 7.0      | 5.9    | 5.7      | 1.0      | 5.7      |          |
| 1000| 1.2    | 1.2      | 1.2      | 5.4    | 5.4      | 6.0      | 4.2    | 11       | 11       | 9.0    | 7.8      | 1.0      | 5.5      |          |

Table 19: ODE example: marginal 4

**F Sonar Example**

Using all derivative information to perform ZV-CV with higher order polynomials may simply be unrealistic for some examples, due to storage constraints or to the number of regression parameters.
Table 20: ODE example: marginal 5

| N  | ZV₁ | l-ZV₁ | r-ZV₁ | ZV₂ | l-ZV₂ | r-ZV₂ | ZV₃ | l-ZV₃ | r-ZV₃ | ZV₄ | l-ZV₄ | r-ZV₄ | sub₁-ZV₁ | crossval |
|----|-----|-------|-------|-----|-------|-------|-----|-------|-------|-----|-------|-------|-----------|-----------|
| 50  | 0.62 | 0.69  | 0.69  | 0.96 | 0.98  | 0.85  | 0.86 | 0.86  | 0.88  | 1.0  | 0.80  |
| 100 | 0.85 | 0.86  | 0.85  | 1.8  | 1.7   | 1.0   | 0.88 | 0.90  | 1.0   | 1.4  |
| 500 | 0.99 | 0.99  | 0.99  | 6.9  | 3.8   | 6.2   | 6.1  | 7.9   | 6.7   | 7.4  | 1.0   | 7.3   |
| 1000| 0.98 | 1.0   | 0.99  | 6.6  | 5.4   | 7.0   | 7.3  | 9.9   | 8.9   | 2.0  | 11    | 9.1   | 1.0       | 8.0       |

Table 21: ODE example: marginal 6

| N  | ZV₁ | l-ZV₁ | r-ZV₁ | ZV₂ | l-ZV₂ | r-ZV₂ | ZV₃ | l-ZV₃ | r-ZV₃ | ZV₄ | l-ZV₄ | r-ZV₄ | sub₁-ZV₁ | crossval |
|----|-----|-------|-------|-----|-------|-------|-----|-------|-------|-----|-------|-------|-----------|-----------|
| 50  | 39  | 1.8   | 2.1   | 0.62 | 0.70  | 0.71  | 0.53 | 0.84  | 0.91  | 1.0  | 39    |
| 100 | 55  | 5.3   | 7.9   | 59   | 1.7   | 1.9   | 0.85 | 0.73  | 0.88  | 0.87 | 1.0   | 64    |
| 500 | 63  | 8.9   | 14    | 69   | 5.3   | 23    | 55   | 9.9   | 3.5   | 2.6  | 1.0   | 54    |
| 1000| 52  | 3.9   | 6.4   | 44   | 19    | 32    | 3.7  | 8.7   | 35    | 3.4  | 3.0   | 1.0   | 32       |

Table 22: ODE example: marginal 7. Results are scaled down by a factor of $10^{-29}$. That is, the smallest and largest improvements are $1.0 \times 10^{-29}$ and $8.6 \times 10^{31}$, respectively. Ridge regression is excluded from this table because its performance is far worse than LASSO (by a factor of at least $10^{22}$ for all $Q$ and $N$).

Table 23: ODE example: marginal 8

| N  | ZV₁ | l-ZV₁ | r-ZV₁ | ZV₂ | l-ZV₂ | r-ZV₂ | ZV₃ | l-ZV₃ | r-ZV₃ | ZV₄ | l-ZV₄ | r-ZV₄ | sub₁-ZV₁ | crossval |
|----|-----|-------|-------|-----|-------|-------|-----|-------|-------|-----|-------|-------|-----------|-----------|
| 50  | 80  | 97    | 120   | 78  | 860   | 210   | 98  |
| 100 | 6.3 | 6.2   | 4.2   | 6.1 | 6.7   | 7.2   | 7.3 | 7.1   |
| 500 | 15  | 5.9   | 17    | 13  | 3.0   | 13    | 18  | 17    | 16   |
| 1000| 14  | 5.5   | 15    | 9.2 | 8.6   | 11    | 1.0 | 14    | 14   |

Table 24: ODE example: marginal 9

required. The 61-dimensional example below falls into this class of problems. A polynomial with $Q = 2$ for this example requires a restrictive 1953 regression parameters while $Q = 3$ and $Q = 4$ polynomials require an unrealistic number of samples with 41,664 and 677,040 regression parameters, respectively.

The purpose of this example is to demonstrate the potential to achieve variance reduction with a subset of derivatives, with a focus on posterior expectation.

This binary regression problem is based on discriminating between sonar signals bouncing off a metal cylinder versus sonar signals bouncing off a roughly cylindrical rock. The 60 covariates represent the total energy within a given frequency band over a fixed period of time, with increasing aspect angle from covariate 1 to covariate 60. Observations $y_i$ for $i = 1, \ldots, 208$ are coded as 0 for rock and 1 for...
metal. The corresponding log likelihood is

$$ \log f(y, X|\theta) = \sum_{i=1}^{208} \left( y_i X_i, \theta - \log(1 + e^{X_i, \theta}) \right) $$

(16)

where $X \in \mathbb{R}^{208 \times 61}$ is the matrix of covariates starting with a column of 1’s for the intercept, $y \in \mathbb{R}^{208}$ is the vector of indicators for the response and $\theta \in \mathbb{R}^{61}$ is the vector of coefficients. Using (16) with \{0, 1\} encoding of the response is equivalent to using $\log f(y, X|\theta) = -\sum_{i=1}^{208} \log(1 + e^{-y_i X_i, \theta})$ with \{-1, 1\} encoding (see e.g. Hastie et al. (2015)). Following Chopin (2017), we standardise the predictors (columns 2-61 of $X$) to have standard deviation 0.5 and we use $N(0, 5^2)$ priors. The intercept has a $N(0, 20^2)$ prior. This prior specification is chosen over the Cauchy priors of Gelman et al. (2008) so that the expectations exist and boundary condition (7) is satisfied. The data used here is from the UCI machine learning repository (Dheeru and Karra Taniskidou, 2017) and was originally collected by Gorman and Sejnowski (1988).

This example is more challenging than most standard logistic regression problems due to the the high number of covariates and high correlations between covariates (Chopin, 2017). The aspect angle is increasing from covariate 1 to covariate 60, so it is reasonable to assume that coefficients of nearby covariates will be correlated. This gives useful information in choosing the subset of parameters for a priori ZV-CV. We perform ZV-CV with subsets of 1 or 5 parameters in estimating marginal posterior expectations. The polynomials with a subset of five parameters are based on the four closest angles, for example when estimating the posterior expectation of $\theta[30]$, the polynomial is a function of a subset of the five parameters $S = \{28, 29, 30, 31, 32\}$. The gold standard of posterior expectation in this example is the average posterior expectation across 100 independent SMC runs using $N = 10000$ and ZV-CV with $Q = 2$.

Due to memory constraints, a maximum polynomial order of $Q = 2$ was used when working with $N \leq 100$. This prevents the highly variable cross-validation error from a small sample size leading to a $Q$ which produces a matrix $\mathbb{R}^{N \times (61+Q)}$ that is too large to handle.

Table 25 shows the mean efficiency for posterior expectations. For small $N$, one can obtain better results using a subset of parameters than with l-ZV, whereas for large $N$ polynomials with $Q = 2$ become more efficient. Out of the 6100 expectations for $N = 50$, 86.2% of the control variates selected based on cross-validation use the subset of five parameters, 7.5% use the full 61 parameters with penalised regression methods, 6.1% use the subset of one parameter and 0.2% use no control variates at all. At $N = 5000$, 99.6% of selected control variates are l-ZV and the remaining 0.4% are ZV.

Table 25: Sonar example: efficiency for marginal expectations, averaged over results for all 61 parameters. Results for individual parameters are similar. Blank values indicate that the number of samples is not sufficient for this order polynomial and bold values indicate the most efficient control variate for a fixed $N$.

| $N$ | ZV | l-ZV | r-ZV | ZV | l-ZV | r-ZV | sub1-ZV | sub5-ZV | crossval |
|-----|----|------|------|----|------|------|---------|---------|----------|
| 50  | 1.4| 1.0  | 1.0  | 1.0| 1.2  | 1.9  | 1.7     |
| 100 | 4.4| 4.8  | 4.5  | 1.2| 1.1  | 1.2  | 2.1     | 4.6     |
| 500 | 13 | 13   | 13   | 3.3| 2.3  | 1.2  | 2.1     | 13      |
| 5000| 14 | 14   | 14   | 46 | 43   | 45   | 1.2     | 2.2     | 43       |

32
The adaptive SMC methods used to select the tuning parameters and inverse temperatures are described in Salomone et al. (2018) and Jasra et al. (2011), respectively. The post-hoc method for adapting the inverse temperatures is described in Appendix B.

Table 26 gives all tuning parameter specifications. The number of particles in the adaptive SMC run is \( N \). Inverse temperatures in the adaptive SMC run are chosen to maintain an ESS of \( \rho N \) and they are adjusted post-hoc to maintain a CESS of \( \tilde{\rho} N \). The MCMC moves targeting \( p_j \) use MALA proposals of the form

\[
q(\theta^*|\theta_i^j) = \mathcal{N}(\theta^*; \theta_i^j + \frac{h_j^2}{2} \hat{\Sigma}_j \nabla_{\theta} \log p_j(\theta|y), h_j^2 \hat{\Sigma}_j),
\]

where \( \hat{\Sigma}_j \) is the empirical covariance and \( h_j \) is a tuning parameter. We specify a set of 20 values which are log-uniform on the range of \( h_{\text{min}} \) to \( h_{\text{max}} \) and, following Salomone et al. (2018), we select the value which maximises the highest median estimated expected square jumping distance (ESJD, Pasarica and Gelman (2010)). Finally, we choose the number of MCMC repeats so that a given percentage of particles have a total absolute jumping distance greater than the mean Mahalanobis distance between particles before resampling (Salomone et al., 2018).

Table 26: Details of the adaptive SMC and post-hoc method tuning parameters for each example.

| example    | \( N \) | \( h_{\text{min}} \) | \( h_{\text{max}} \) | \( \rho \) | \( \tilde{\rho} \) | \% > median |
|------------|---------|-----------------------|-----------------------|----------|----------------|-------------|
| Van Der Pol | 1000    | 0.01                  | 2                     | 0.9      | 0.99           | 0.5         |
| Recapture   | 10000   | 0.01                  | 1                     | 0.5      | 0.9            | 0.5         |
| Sonar      | 10000   | 0.01                  | 1                     | 0.5      | 0.9            | 0.5         |
| ODE        | 1000    | 0.01                  | 1                     | 0.5      | 0.9            | 0.5         |