Vector-Valued Control Variates

Zhuo Sun 1  Alessandro Barp 2 3  François-Xavier Briol 1 3

Abstract

Control variates are variance reduction tools for Monte Carlo estimators. They can provide significant variance reduction, but usually require a large number of samples, which can be prohibitive when sampling or evaluating the integrand is computationally expensive. Furthermore, there are many scenarios where we need to compute multiple related integrals simultaneously or sequentially, which can further exacerbate computational costs. In this paper, we propose vector-valued control variates, an extension of control variates which can be used to reduce the variance of multiple Monte Carlo estimators jointly. This allows for the transfer of information across integration tasks, and hence reduces the need for a large number of samples. We focus on control variates based on kernel interpolants and our novel construction is obtained through a generalised Stein identity and the development of novel matrix-valued Stein reproducing kernels. We demonstrate our methodology on a range of problems including multifidelity modelling, Bayesian inference for dynamical systems, and model evidence computation through thermodynamic integration.

1. Introduction

A significant computational challenge in statistics and machine learning is the approximation of intractable integrals. Examples include the computation of posterior moments, the model evidence (or marginal likelihood), Bayes factors, or integrating out latent variables. This challenge has lead to the development of a wide range of Monte Carlo (MC) methods; see (Green et al., 2015) for a review. Let $f : \mathbb{R}^d \to \mathbb{R}$ denote some integrand of interest, and $\Pi$ some distribution with Lebesgue density $\pi$ known up to an intractable normalisation constant. The integration task we consider can be expressed as estimating

$$
\Pi[f] := \int_{\mathbb{R}^d} f(x)\pi(x)dx
$$

using evaluations of the integrand at some points in the domain: $\{x_i, f(x_i)\}_{i=1}^n$. These evaluations are usually combined to create an estimate of $\Pi[f]$ of the form $\hat{\Pi}[f] = \frac{1}{n} \sum_{i=1}^n f(x_i)$. For example, when realisations are independent and identically distributed (IID), this corresponds to a MC estimator. In that case, assuming that $f$ is square-integrable with respect to $\Pi$ (i.e. $\Pi[f^2] < \infty$), we can use the central limit theorem (CLT) to show that such estimators converge to $\Pi[f]$ as $n \to \infty$, and this convergence is then controlled by the asymptotic variance of the integrand $f$. Analogous results can also be obtained for Markov chain Monte Carlo (MCMC) realisations (Jones, 2004), in which case case $\{x_i\}_{i=1}^n$ are realisations from a Markov Chain with invariant distribution $\Pi$, or for randomised quasi-Monte Carlo (Hickernell et al., 2005), in which case $\{x_i\}_{i=1}^n$ form some lattice or sequence filling some hypercube domain.

The main insight behind the concept of control variate (CV) is that it is instead often possible to use an estimator of $\Pi[f - g]$ for some $g : \mathbb{R}^d \to \mathbb{R}$. This is justified if $\Pi[g]$ is known in closed form, in which case we may use $\Pi^\text{CV}[f] := \Pi[f - g] + \Pi[g]$. Furthermore, if $g$ is chosen appropriately, the variance of the CLT for this new estimator will be much smaller than that of the original, and a smaller number of samples will be required to approximate $\Pi[f]$ at a given level of accuracy.

Suppose now that $n = (n_1, \ldots, n_T) \in \mathbb{N}^T$ ($T \in \mathbb{N}_+$) is a multi-index. In this paper, we will focus on cases where we have not just one integral, but a sequence of integrands $f_t : \mathbb{R}^d \to \mathbb{R}$ and distributions $\Pi_t$ for which we would like to use $\{\{x_{tj}, f_t(x_{tj})\}_{j=1}^{n_t}\}_{t=1}^T$ to estimate

$$
\Pi_t[f_t] := \int_{\mathbb{R}^d} f_t(x)\pi_t(x)dx \quad \text{for } t \in [T],
$$

where $[T] = \{1, \ldots, T\}$. This is a common situation in practice; for example, our paper considers the case of multifidelity modelling (Peherstorfer et al., 2018) where $f_1, \ldots, f_T$ may be a computationally expensive physical model $f$, and we might be interested in expectations of that model with respect to unknown parameters. Another example we will also study is when $\pi_1, \ldots, \pi_T$ are closely related posterior distributions, such as in the case of power posteriors (Friel & Pettitt, 2008).
Of course, the estimation of integrals in (1) could be tackled individually, and this is in fact the most common approach. However, the main insight from this paper is that if both the integrands and distributions are related across tasks, we can improve on this by sharing computation across these tasks. We propose to construct a CV to jointly reduce the variance of estimators for these integrals and hence obtain a more accurate approximation. We will call such a function a vector-valued control variate (vv-CV). In order to encode the relationship between integration tasks, we will propose a flexible class of CVs based on interpolation in reproducing kernel Hilbert space of vector-valued functions (vv-RKHS).

More precisely, we generalise existing constructions of Stein reproducing kernels to derive novel vv-RKHSs with the property that each output has mean zero.

We note that very few methods exist to tackle multiple integrals jointly. One exception is (Xi et al., 2018), which also proposes an algorithm based on vv-RKHSs. However, that work is limited to cases where the integral of the kernel is known in closed-form, which is rarely possible in practice. In contrast, our vv-CVs are applicable even when the kernel is unknown. Moreover, our method is non-parametric, whereas existing methods are parametric.

2. Background

We now briefly review existing constructions for Stein-based CVs for a single integration problem.

The first step consists of constructing a set of functions \( \mathcal{G} \) which all integrate to a known value against \( \Pi \). This can generally be challenging since \( \pi \) may not be computationally tractable, e.g., involving an unknown normalisation constant. Without loss of generality, we will discuss the construction of functions which integrate to zero, but notice that we can obtain functions with mean equal to any constant \( \beta \in \mathbb{R} \) by simply adding this constant \( \beta \) to a zero-mean function.

Zero-Mean Functions through Stein Operators

One way of constructing zero-mean functions is to use Stein’s method (Anastasiou et al., 2023). The main ingredients of Stein’s method are a function class and an operator acting on this class. More precisely, a Stein class of \( \mathcal{G} \) is a class of functions \( \mathcal{U} \) associated to an operator \( \mathcal{S} \), called Stein operator, such that a Stein identity holds: \( \Pi[\mathcal{S}[u]] = 0 \) \( \forall u \in \mathcal{U} \). An obvious choice for the class of zero-mean functions \( \mathcal{G} \) is to consider all functions of the form \( g = \mathcal{S}[u] \) for \( u \in \mathcal{U} \). To ensure such \( g \) has finite variance, we assume that all functions in \( \mathcal{G} \) are square-integrable with respect to \( \Pi \). This can be guaranteed under weak regularity conditions on \( \mathcal{U} \) and \( \mathcal{S} \); see Theorem 3.2. Note also that \( \mathcal{S} \) depends implicitly on \( \Pi \), but we only make this explicit in our notation (i.e., \( \mathcal{S}_\Pi \)) when it is helpful for clarity.

The most common choice of Stein operator is the Langevin Stein operator, which acts on differentiable vector-valued functions (vv-functions) \( u : \mathbb{R}^d \to \mathbb{R}^d \):

\[
\mathcal{L}[u](x) := \nabla_x \cdot u(x) + u(x) \cdot \nabla_x \log \pi(x). \tag{2}
\]

The advantage of \( \mathcal{L} \) is that it only requires knowledge of \( \Pi \) through evaluations of \( \nabla_x \log \pi \), which does not require the normalisation constant of \( \pi \). Indeed, let \( \pi = \pi/C \) for some unknown \( C \in \mathbb{R} \), then \( \nabla_x \log \pi = \nabla_x \log \tilde{\pi} \). For more general Stein operators, see (Anastasiou et al., 2023).

Parametric Spaces

\( \mathcal{G} \) is usually chosen to be a parametric space and we will hence write it \( \mathcal{G}_\Theta \), where \( \Theta \) denotes the space of parameter values. Most existing CVs can be obtained by taking \( g_\theta = \mathcal{S}[u_\theta] \) for some \( u_\theta \in \mathcal{U}_\Theta \) where \( \mathcal{U}_\Theta \) is another parametric class. However, note that there might not be a unique \( u_\theta \) leading to \( g_\theta \). For the remainder of the paper, \( \theta \) will hence be a parameter indexing \( g_\theta \) directly as opposed to an element of the Stein class. Examples of parametric CVs are the polynomial-based CVs of (Mira et al., 2013) (see also (Assaraf & Caffarel, 1999; Papamarkou et al., 2014; Oates et al., 2016)), in which case the Stein class is parametrised directly by coefficients of a polynomial. Using a space of neural networks has also been studied in (Wan et al., 2019; Si et al., 2021). This later choice can be advantageous due to the flexibility of this function class, but is much more challenging to implement because selecting a CV becomes a non-convex problem.

Another example are kernel interpolants, which will be the main focus of our paper. This class is nonpara-
Vector-Valued Control Variates

metric, but it is often convenient to fix the dataset size and parametrise it. Let \( \mathcal{H}_k \) denote a reproducing kernel Hilbert space (RKHS) with kernel \( k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) (Berlinet & Thomas-Agnan, 2011), so that \( k \) is symmetric \((k(x, y) = k(y, x) \, \forall x, y \in \mathbb{R}^d)\) and positive semi-definite \((\forall m \in \mathbb{N}_+, \sum_{i,j=1}^m c_i c_j k(x_i, x_j) \geq 0 \, \forall c_1, \ldots, c_m \in \mathbb{R} \) and \( \forall x_1, \ldots, x_m \in \mathbb{R}^d \)). The kernel could be a squared-exponential kernel \( k(x, y) = \exp(-\|x-y\|^2/(2\ell^2)) \) with lengthscale \( \ell > 0 \), or a polynomial kernel \( k(x, y) = (x^\top y + c)^l \) where \( c \in \mathbb{R} \) and \( l \in \mathbb{N} \) is the degree of the polynomial. Oates et al. (2017) noticed that the image of \( \mathcal{L} = \mathcal{H}_k^d := \mathcal{H}_k \times \ldots \times \mathcal{H}_k \) under \( \mathcal{L} \) is a RKHS with kernel

\[
\begin{align*}
  k_0(x, y) := \nabla_x \cdot \nabla_y k(x, y) + \nabla_x \log \pi(x) \cdot \nabla_y k(x, y) \\
  + \nabla_y \log \pi(y) \cdot \nabla_x k(x, y) \\
  + (\nabla_x \log \pi(x) \cdot \nabla_y \log \pi(y)) k(x, y),
\end{align*}
\]

(3)

see also Thm 2.6 Barp et al. (2022b) for a more general result. Given \( m \) observations, it is known that the optimal interpolant in \( \mathcal{H}_{0, m} \) is of the form \( g_\theta(x) = \sum_{i=1}^m \theta_i k_0(x, x_i) \) where \( \theta_i \in \mathbb{R} \) for all \( i \in [m] \). This therefore provides a natural parametrisation for practical implementation. Oates et al. (2017) called this class of CVs control functionals (CF); see also (Briol et al., 2017; Oates et al., 2019; South et al., 2022a) for more details.

Selecting a CV In order to select a CV, we will pick the “best” element from \( g_\theta \), where “best” will refer to minimising MC variance:

\[
J(\theta) = \text{Var}_\Pi[f - g_\theta] := \Pi[(f - g_\theta - \Pi[f])^2],
\]

(4)

Following the framework of empirical risk minimisation, this can be approximated with \( \{x_j, f(x_j)\}_{j=1}^n \) as follows:

\[
J_m(\theta, \beta) := \frac{1}{m} \sum_{i,j=1}^m (f(x_i) - g_\theta(x_i) - \beta)^2 + \lambda \|g_\theta\|^2,
\]

where \( \beta \in \mathbb{R} \) is an additional parameter which tends to \( \Pi[f] \) as \( m \to \infty \) and \( \lambda \to 0 \). Here, \( \lambda \geq 0 \) is a regularisation parameter and \( \|g_\theta\| \) can be any suitable norm. For example, \( \|g_\theta\|_2 = \|\theta\|_2 \) or \( \|g_\theta\| = \|g_\theta\|_{\mathcal{H}_k} \) for some kernel \( k \). Assuming that \( \Theta \subseteq \mathbb{R}^d \), this objective can then be minimised by the solution to a linear system when \( \theta \to g_\theta \) is linear and \( \theta \to \|g_\theta\|^2 \) is quadratic. In more general cases, it can be minimised using stochastic optimisation (Si et al., 2021). In that case, we initialise \( \theta^{(0)} \) and \( \beta^{(0)} \), then iteratively take gradient steps with minibatches of size \( \hat{m} \ll m \).

There are two particular perspectives which motivate the objective in (4). Firstly, it can be interpreted as a least-squares objective for the function \( f - \Pi[f] \) (Leluc et al., 2021). Secondly, by noticing that for any square-integrable function \( h \) and MC estimator with \( n \) samples we have \( \text{Var}_\Pi[\hat{\Pi}_M[h]] = \text{Var}_\Pi[h]/n \), we can notice that \( J(\theta) \) fully determines the CLT variance of a MC estimator of \( \Pi[f - g_\theta] \), which makes it particularly well suited for these estimators. This latter viewpoint has also motivated alternative objectives based on the variance of the randomised quasi-Monte Carlo or MCMC CLT; see e.g. Hickernell et al. (2005); Oates & Girolami (2016); Dellaportas & Kontoyiannis (2012); Mijatovic & Vogrinc (2018). The MCMC case is briefly discussed in Appendix A.1, but the remainder of the paper will focus on the objective in (4) for simplicity.

The CV Estimator Recall that a CV estimator takes the form \( \hat{\Pi}^C[f] := \hat{\Pi}[f - g_\theta] + \Pi[g] \) for some CV \( g \). Once a function \( g_\theta \) has been selected through the procedure in the previous subsection, the only part missing is therefore an estimator for \( \Pi[f - g_\theta] \). We present two possible approaches below. A first option is to create an estimator based on the remainder of the data \( \{x_i, f(x_i)\}_{i=m+1}^{m+n} \):

\[
\hat{\Pi}[f - g_\theta] = \frac{1}{n} \sum_{i=m+1}^{m+n} (f(x_i) - g_\theta(x_i)).
\]

This estimator is unbiased whenever \( \hat{\Pi}[f - g_\theta] \) is unbiased. This is the case when using a MC estimator, but not when using a MCMC estimator. The question of how to select \( m \) is of practical importance for the quality of the estimator. When \( m \) is small, most of the function evaluations are used for the MC estimator, whereas when \( m \) is large, most of the evaluations are used to construct the CV.

Due to the difficulty of choosing \( m \), a second option is to use all of the data for selecting \( g_\theta \) (i.e. \( n = 0 \)). More precisely, denoting by \( (\hat{\theta}, \hat{\beta}) \) the minimiser of \( J_m(\theta, \beta) \), we could use \( \hat{\Pi}[f - g_\theta] = \hat{\beta} \). This estimator will be biased, but will also be more accurate than the first estimator if the least-squares problem can be solved at a fast rate than the MC CLT.

3. Methodology

We will now extend existing CVs to the case where multiple related integration problems are tackled jointly. This will be done through a multi-task learning approach (Micchelli & Pontil, 2005; Evgeniou et al., 2005), where each integral corresponds to a task and the relationship between tasks will be modelled explicitly. This will allow us to share information across integration tasks, and hence improve accuracy when the number of integrand evaluations is limited.

3.1. Vector-Valued Functions using Stein’s Method

For the remainder of this paper, we consider integrands corresponding to the outputs of a vector-valued function \( f : \mathbb{R}^d \to \mathbb{R}^T \) so that \( f(x) = (f_1(x), \ldots, f_T(x))^\top \). Our objective is to approximate \( \Pi[f] = (\Pi[f_1], \ldots, \Pi[f_T])^\top \), and we shall assume that \( f_1 \) is square-integrable with respect to \( \Pi_1 \forall t \in [T] \). Formally, \( \Pi \) is known as a vector probability distribution. To approximate \( \Pi[f] \), we will construct a class of zero-mean vv-functions through Stein’s method. This
can be done by considering a Stein class $\mathcal{U}$ whose image $\mathcal{G}$ under the Stein operator $S^\nu : \mathcal{U} \to \mathcal{G}$ is a class of $\mathbb{R}^T$-valued functions on $\mathbb{R}^d$. We will need a generalised form of Stein identity for vv-functions:

$$
\Pi_t[g_t] = \Pi_t[(S^\nu[u])_t] = 0, \quad \forall u \in \mathcal{U} \text{ and } \forall t \in [T].
$$

In other words, each output of the vv-function should integrate to zero against the corresponding probability distribution. Of course, the ordering of the sequence of integrands and distributions matters here, as we do not guarantee that $\Pi_t[g_{t'}] = 0$ for $t \neq t'$. The property above can be obtained by constructing an operator $S^\nu$ through a sequence of Stein operators $S^\nu_{1[t]}$ for $t \in [T]$ whose images are scalar-valued functions integrating to zero under $\Pi_t$. These can then be applied in an element-wise fashion as follows

$$
g = S^\nu[u] = (S^\nu_{1_1}[u_1], \ldots, S^\nu_{1_T}[u_T])^T. \quad (6)
$$

Once again, $\mathcal{G}$ can be parametrised and we will denote it $\mathcal{G}_\theta$. We can then use an objective based on the variances $f - g_0$ to select an optimal element:

$$
J^\nu(\theta) = \|\text{Var}_\Pi[f - g_0]\| = \|\Pi[(f - g_\theta - \Pi[f])^2]\|, \quad (7)
$$

where $g_\theta \in \mathcal{G}_\theta$. In the above $\text{Var}_\Pi$ should be thought of as applying $\text{Var}_{\Pi_t}$, the variance under $\Pi_t$, to the $t^{th}$ element of the vv-function. The norm could be any norm on $\mathbb{R}^T$, but we will usually make use of the 1-norm so as to interpret this objective as the sum of variances on each integrand. For this objective to make sense, we require $(g_\theta)$ to be squared-integrable with respect to $\Pi_t$, $\forall t \in [T]$. Similarly to the $T = 1$ case, we are focusing on a least-squares objective, which directly controls the variance of MC estimators, but this could be adapted to other estimators as previously discussed.

Let $m = (m_1, \ldots, m_T) \in \mathbb{N}_+^T$. Once again, the objective can be approximated via MC estimates based on the dataset $D = \{\{x_{t_1}, f_1(x_{t_1})\}^{m_1}_{j=1}, \ldots, \{x_{T}, f_T(x_{T})\}^{m_T}_{j=1}\}$ following the framework of empirical risk minimisation. For example, when the norm above is a 1-norm, the objective is simply the sum of individual variances:

$$
L^\nu_m(\theta, \beta) := J^\nu_m(\theta, \beta) + \lambda\|g_0\|^2 \quad (8)
$$

$$
= \sum_{t=1}^T \frac{1}{m_t}\sum_{j=1}^{m_t} (f_1(x_{t_1}) - (g_0(x_{t_1}))_t - \beta_t)^2 + \lambda\|g_0\|^2,
$$

where $\lambda \geq 0$ and $\beta = (\beta_1, \ldots, \beta_T) \in \mathbb{R}^T$. Once again, the second term is used to regularise $J^\nu_m$, but the norm acts on vv-functions. For $\mathcal{U}$, we could take a class of polynomials, kernels or neural networks, but will usually require flexible classes of vv-functions in order to encode relationships between tasks. Assuming that each $\Pi_t$ has a $C^{1,1}$ and strictly positive density $\pi_t$ with respect to the Lebesgue measure, we will also be able to use the Langevin Stein operators $\mathcal{L}_t$, which only require access to the score functions for each distribution $\Pi_1, \ldots, \Pi_T$. For this purpose, we now define $l : \mathbb{R}^d \to \mathbb{R}^{T \times d}$ to be the matrix-valued function with entries $l_{t_j}(x) = \partial^j \log \pi_t(x)$.

### 3.2. Kernel-based Vector-Valued CVs

The main choice of Stein class $\mathcal{U}$ studied in this paper is vv-RKHSs ($\text{Carmeli et al., 2006; 2010; Álvarez et al., 2012}$). This choice is particularly convenient as it allows us to build on the rich literature in statistical learning theory which considers kernels encoding relationships between tasks. A main contribution of this section will be the design of novel Stein reproducing kernels specifically for numerical integration, a task not commonly tackled in statistical learning theory.

A vv-RKHS $\mathcal{H}_K$ is a Hilbert space of functions mapping from $\mathbb{R}^d$ to $\mathbb{R}^T$ with an associated matrix-valued reproducing kernel (mv-kernel) $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{T \times T}$ which is symmetric ($K(x, y) = K(y, x)$ $\forall x, y \in \mathbb{R}^d$) and positive semi-definite ($\forall m \in \mathbb{N}_+, \sum_{t=1}^m c_t K(x_t, x_t) c_t \geq 0$ for all $c_1, \ldots, c_m \in \mathbb{R}^T$ and $x_1, \ldots, x_m \in \mathbb{R}^d$). Any vv-RKHS satisfies a reproducing property, so that $\forall f \in \mathcal{H}_K$, $f(x)^T = \langle f, K(\cdot, x) \rangle_{\mathcal{H}_K}$ and $K(\cdot, x) \in \mathcal{H}_K \forall x \in \mathbb{R}^d$ and $\forall c \in \mathbb{R}^T$. The reproducing kernels discussed in Section 2 are a special case which can be recovered when $T = 1$. We say that $K$ is $C^{1,1}(\mathbb{R}^d \times \mathbb{R}^d)$ provided that $\partial^\alpha_0 \partial^\beta_y K(x, y)$ is continuous for all multi-indices $\alpha = (\alpha_1, \ldots, \alpha_d)$ with $\alpha_1 + \cdots + \alpha_d \leq r$, and that $K$ is bounded with bounded derivatives if there exists $C \geq 0$ for which $\|\partial^\alpha_0 \partial^\beta_y K(x, y)\|_F \leq C$ for all $x, y \in \mathbb{R}^d$ and multi-indices $\alpha$ with $\alpha_1 + \cdots + \alpha_d \leq 1$.

To construct vv-CVs, a natural approach is to construct a mv-kernel $K_0$ using another mv-kernel $K$ and an operator $S^\nu$. Then, assuming we have access to such a $K_0$ and to data $D$, a natural generalisation of the scalar valued case is:

$$
g_\theta(x) = \sum_{t=1}^T \sum_{j=1}^{m_t} K_0(x, x_{t_j}) \theta_{t_j}, \quad (9)
$$

where $\theta_{t_j} \in \mathbb{R}^T$, for all $t \in [T], j \in [m_t]$. The remainder of this section will hence focus on how to obtain $K_0$. Our construction is based on the CFs of ($\text{Outes et al., 2017; 2019}$), which use a scalar-valued kernel $k_0$ obtained through a tensor product structure $\mathcal{U} = \mathcal{H}_K^d$. The initial motivation for introducing vv-functions in this setting was that $\mathcal{C}$ requires inputs which are vv-functions which can be thought of as introducing a dummy dimension for convenience, and is in no way related to the multitask setting in this paper. We now illustrate the natural extension of $k_0$ to a mv-kernel.

**Theorem 3.1.** Consider $\mathcal{H}_K$ which is a vv-RKHS $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{T \times T}$, and suppose that $K \in C^{1,1}(\mathbb{R}^d \times \mathbb{R}^d)$. Furthermore, assume $u = (u_1, \ldots, u_T) \in \mathcal{H}_K$, let $S^\nu[u] = (\mathcal{L}_1[u_1], \ldots, \mathcal{L}_T[u_T])^T$. Then, the image of $\mathcal{H}_K^d = \mathcal{H}_K \times \cdots \times \mathcal{H}_K$ under $S^\nu$ is a vv-RKHS with kernel $K_0 : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{T \times T}$ with:

$$
(K_0(x, y))_{t'} = \sum_{t=1}^T \partial^\alpha_0 \partial^\beta_y K(x, y)_{t,t'} + l_{t'}(x) \partial^\alpha_0 \partial^\beta_y K(x, y)_{t,t'} + l_{t'}(x) l_{t'}(y) K(x, y)_{t,t'},
$$

where
The proof is in Appendix B.1. Notice that $(K_{0}(x, y))_{t,t'}$ depends only on the score function of $\Pi_t$ and $\Pi_{t'}$, and so we (once again) do not require knowledge of normalisation constants. However, in order to evaluate $K_{0}(x, y)$ for some $x, y \in \mathbb{R}^d$, we will require pointwise evaluation of $\nabla_x \log \pi_t(x)$ and $\nabla_y \log \pi_{t'}(y)$ for all $t \in [T]$. Finally, another interesting point is that $(K_{0}(x, y))_{t,t'}$ is a scalar-valued kernel when $t = t'$, but this is not the case for $t \neq t'$ since it is not symmetric in that case.

To use elements of this RKHS as vv-CVs, we will require that the least-squares objective in (7) is well-defined. This can be guaranteed when the elements of the RKHS are square-integrable, and the theorem below, proved in Appendix B.2, provides sufficient conditions for this to hold.

**Theorem 3.2.** Suppose that $K$ is bounded with bounded derivatives, and $\Pi_t[|\nabla_x \log \pi_t|^2] < \infty$ for all $t \in [T]$. Then, for any $g \in \mathcal{H}_{K,o}$, $g_t$ is square-integrable with respect to $\Pi_t$ for all $t \in [T]$.

Now the mv-kernel in Theorem 3.1 takes a very general form as it has minimal requirements on $K$ or $\Pi_1, \ldots, \Pi_T$. This is as convenient as it can be applied in a wide range of settings, but this generality comes at the cost of computational complexity. We will now study several special cases which will often be sufficient for applications.

**Special Case I: Separable kernel $K$** For simplicity, the literature on multi-task learning often focuses on the case of separable kernels. We say a mv-kernel $K$ is separable if it can be written as $K(x, y) = Bk(x, y)$, where $k$ is a scalar valued kernel and $B \in \mathbb{S}^T$. The advantage of this formulation is that it decouples the model for individual outputs (as given by $k$) from the model of their relationship, as given by the components of the matrix $B$, which can be thought of as a covariance matrix for tasks. As we will see in Section 4, this can be particularly advantageous for selecting the hyperparameters of vv-CVs. Using such a kernel $K$, the kernel $K_0$ in Theorem 3.1 becomes:

$$(K_{0}(x, y))_{t,t'} = B_{t,t'} \sum_{r=1}^{d} \partial_x^r \partial_y^r k(x, y) + l_{t,r}(y) \partial_x^r k(x, y) + l_{t,r}(x) \partial_y^r k(x, y),$$

for $\forall t, t' \in [T]$. This expression is interesting because it reduces the choice of $K$ to the choice of a matrix $B$ and a kernel $k$, and this matrix $B$ has a natural interpretation in that $B_{t,t'}$ denotes the covariance between $f_t$ and $f_{t'}$. See Appendix E.1 for illustrations of such $K_0$.

**Special Case II: Separable kernel $K$ with one target distribution** A further simplification of the kernel is possible when $K$ is separable and all distributions are the same: $\Pi_1 = \cdots = \Pi_T \equiv \Pi$. In this case $K_{0}$ itself becomes a separable kernel of the form: $(K_{0}(x, y))_{t,t'} = B_{t,t'} k_{0}(x, y)$ for all $t, t' \in [T]$, where $k_{0}$ is given in (3). The scalar case can then be recovered by taking $T = 1$ and $B = 1$.

**Selecting a Base Kernel and Alternative Constructions**

The base kernel $K$ needs to be chosen by the user. As for the scalar case, we expect that the performance of our approach will depend on whether the smoothness of $K_{0}$ closely matches the smoothness of the integrand $f$, and the smoothness of $K$ should therefore be chosen accordingly. We also suggest choosing the hyperparameters of $K$ through either cross validation or through maximisation of the log-marginal likelihood of a zero-mean multi-output Gaussian process with kernel $K_{0}$; see Appendix D.2 for details. Furthermore, see Appendix C for alternative constructions, including vv-CVs derived from the second-order matrix-valued Stein kernels and vv-CVs based on other parametric spaces such as polynomials and neural networks.

**4. Selecting a Vector-Valued CV**

We will now derive both a closed-form expression for the optimal parameters of these kernel-based vv-CVs and a stochastic optimisation scheme to approximate it.

**Closed-form Solutions** We start with a theorem which provides a result akin to the RKHS representer theorem, but which focuses specifically on the function which minimises the objective in (8). This theorem shows that there exists a unique parameter minimising the variance objective.

**Theorem 4.1.** Let $\mathcal{D} = \{\{x_{1j}, f_1(x_{1j})\}_{j=1}^{m_1}, \ldots, \{x_{Tj}, f_T(x_{Tj})\}_{j=1}^{m_T}\}$. The function which minimises the objective in (8) where $\|g\| := \|g\|_{\mathcal{H}_{K,o}}$ and $\beta \in \mathbb{R}^T$ is of the form:

$$g_0(x) = \sum_{t=1}^{T} \sum_{j=1}^{m_t} \beta_{t,j} K_0(x, x_{tj}), \beta_{t,j} \in \mathbb{R}^T$$

with optimal parameter $\theta^*$ given by the solution of this convex linear system of equations:

$$\sum_{t} \sum_{j'} \left( \sum_{i} \frac{1}{m_t} \sum_{j} K_0(x_{tj''}, x_{tj}), K_0(x_{tj}, x_{tj''}), \right) \theta_{t,j'}^* = \sum_{i} \frac{1}{m_t} \sum_{j} K_0(x_{tj''}, x_{tj}), \left( f_t(x_{tj}) - \beta_t \right),$$

for all $t, j'' \in [m_T]$.

Furthermore, if $K_{0}$ is strictly positive definite and the points $x_{tj}$ are distinct, then the system is strictly convex and $\theta^*$ is unique.

See Appendix B.3 for the proof. Theorem 4.1 assumes that $\beta$ is known and fixed, which may not be the case in practice. However, given a fixed $g_0$ the objective (8) is a quadratic in $\beta$ with the optimal value $\beta_* = \frac{1}{m_t} \sum_{j=1}^{m_t} f_t(x_{tj}) - (g_0(x_{tj})).$ This naturally leads to the use of block coordinate descent
We now use Algorithm 1 (Kingma & Ba, 2015), a first-order method with estimates and can be straightforwardly minimised through stochastic optimisation algorithms is assumed to only scale with the cost of stochastic estimates of the gradient of $J^\nu$.

### Algorithm 1 Block-coordinate descent for vv-CVs with unknown task relationship

**Input:** $D, \tilde{m}, L, \lambda, \beta^{(0)}, \theta^{(0)}$ and $B^{(0)}$

for iteration $l = 1$ to $L$ do

Select a mini-batch $D_m$ of size $m = (\tilde{m}_1, \ldots, \tilde{m}_T)^\top$

$(\theta^{(l)}, \beta^{(l)}) \leftarrow \text{UPDATE}_{\theta, \beta}(\theta^{(l-1)}, \beta^{(l-1)}, B^{(l-1)}, D_m)$

$B^{(l)} \leftarrow \text{UPDATE}_B(\theta^{(l)}, \beta^{(l)}, B^{(l-1)}; D_m)$

end for

**Return:** $\theta^{(L)}, \beta^{(L)}$ and $B^{(L)}$

approaches which iterate between optimising $\beta$ and $\theta$. This could be either directly implemented using the closed-form solutions, or through the use of numerical optimisers such as the stochastic optimisation approaches we will now present. The next paragraph highlights how this can be implemented for special cases I and II. We remark that the use of stochastic optimisation tools will be essential in most applications due to the size of the linear systems leading exact solutions to being intractable in practice.

**Unknown Task Relationship** We now extend our approach to account for simultaneously estimating $\beta$, $\theta$, but also the matrix $B$. In this setting, we will use the same objective as in (8), but penalised by the norm of $B$:

$$L_{mL}^\nu(\theta, \beta, B) = J_{mL}^\nu(\theta, \beta, B) + \lambda \|g_\theta\|^2 + \|B\|^2,$$  

We now use $J_{mL}^\nu(\theta, \beta, B)$ to denote $J_{mL}^\nu(\theta, B)$ in order to emphasise the dependence on $B$. A second regularisation parameter is unnecessary as this would be equivalent to rescaling $k$. The objective in (10) is a natural extension to (8) and can be straightforwardly minimised through stochastic optimisation; see Algorithm 1. To ensure $B$ is strictly positive definite, we can take $B = LL^\top$, where $L$ is a lower triangular matrix with diagonal elements forced to be greater than zero via an exponential transformation. The pseudo-code in Algorithm 1 presents this abstractly as a function UPDATE. This is because different choices of vv-CVs might benefit from different updates. For example, pre-conditioners for the gradients could be used when easily available, or when these can be estimated from data. In Section 5, we will exclusively be using the Adam optimiser (Kingma & Ba, 2015), a first-order method with estimates of lower-order moments. Additionally, we study the convex case when $B$ is known and only $\beta$ and $\theta$ are required to be estimated in Appendix A.2.

**Computational Complexity** Although vv-CVs can be beneficial from an accuracy viewpoint, they also incur a significant computational cost. Whether they should be used will therefore depend on the computational budget available. In particular, when evaluations of $f$ or $\nabla \log \pi$ are expensive, the higher cost of using vv-CVs may be negligible. Table 1 provides the computational complexity of all approaches considered in the paper. We emphasise the impact of $T$, the number of tasks. In the case of existing kernel-based CVs, the dependence is $O(T)$. In contrast, the computational cost of vv-CVs is between $O(T^4)$ and $O(T^6)$. Table 1 also highlights the difference in computational complexity between obtaining closed form solutions of $\theta$ and $\beta$ by solving the linear system of equations in Theorem 4.1, and using the stochastic-optimisation approaches in Appendix A.2 and Section 4. Here, the difference is mainly in terms of powers of $T$, $m_t$ and $\tilde{m}_t$. As we can see the exact solutions usually come with an $O(m_t^3)$ cost, whereas the stochastic optimisation approach is associated with a $O(m_t \tilde{m}_t L)$ cost. In this case, whenever $\tilde{m}_t L$ is small relative to $m_t$, this will lead to computational gains.

In all applications considered, both $m_t$ and $T$ were small so the overall cost is controlled. However, this computational complexity can be further significantly reduced in special cases. When using a kernel corresponding to a finite-dimensional RKHS (e.g., a polynomial kernel), the scaling becomes linear in $m_t$, but is $O(q^3)$ instead of $O(m_t^3)$, where $q \ll m_t$ is the dimensionality of the RKHS. Alternatively, for certain choices of point sets and kernels, it is possible to reduce the computational complexity to $O(m_t \log m_t)$ instead of $O(m_t^3)$ by using scalable kernel methods such as fast Fourier features or inducing points. When the integrands are evaluated at the same set of points and the separable kernel is used, the computational cost in $T$ also becomes $O(T^2)$ instead of $O(T^6)$, once again significantly reducing the computational complexity.

### 5. Experimental Results

We now illustrate our method on a range of problems including multi-fidelity models, computation of the model evidence for dynamical systems through thermodynamic integration and Bayesian inference for the abundance of preys using a Lotka-Volterra system. See Appendix E for additional experiments including illustrations of matrix-valued Stein kernels $K_0$ in Appendix E.1 and a synthetic example when the Stein kernel matches the smoothness of integrands in Appendix E.2. Since we are interested in gains obtained from the CVs, we fix $n = 0$ which means we are using all the data to construct vv-CVs. The code to reproduce the re-
Figure 1. Numerical integration of univariate discontinuous multi-fidelity model. Upper: fitted CVs for both functions. Lower Left: performance of CVs based on a squared-exponential kernel for the high-fidelity function as a number of epochs of the optimisation algorithm. The lines provide the mean over 100 repetitions of the experiment, whereas the shaded areas provide one standard deviation above and below the mean. Lower Right: same experiment for a polynomial kernel for the high-fidelity function.

5.1. Multifidelity Modelling in the Physical Sciences

Many problems in the engineering and physical sciences can be tackled with multiple models of a single system of interest. These models are often associated with varying computational costs and levels of accuracy, and their combination to solve a task is usually called multi-fidelity modelling; see (Pecherstorfer et al., 2018) for a review. We will consider a high-fidelity model \( f_H \) and a low-fidelity model \( f_L \), and will attempt to estimate the integral of \( f_H \) with our vv-CVs and using function evaluations from both the high- and low-fidelity models. For clarity, we will now denote the function \( f = (f_L, f_H) \) and the vector-probability distribution \( \Pi = (\Pi_L, \Pi_H) \). We note that this is a special case of the problem considered in our paper since we use evaluations of multiple functions but are only interested in \( \Pi_H [f_H] \) (whereas \( \Pi_L [f_L] \) is not of interest).

Univariate Step Function The first example considered is a toy problem from the multi-fidelity literature (Xi et al., 2018). The low-fidelity function is \( f_L(x) = 2 \) if \( x \geq 0 \) and \(-1\) otherwise. The high-fidelity function is \( f_H(x) = 1 \) if \( x \geq 0 \) and \(0\) otherwise. In this example, \( K_0 \) is smoother than \( f_1 \) and \( f_2 \), which are both discontinuous. The integral is over the real line and taken against \( \Pi = \mathcal{N}(0,1) \), and we fix the sample sizes to \( m_1, m_H = (40, 40) \).

Results with a squared-exponential and 1st order polynomial kernel \( k \) can be found in Figure 1. The upper plots clearly show that the approximations are not of very high-quality, but the lower plots show that all CVs can still lead to an order of two gain in accuracy over MC methods. We also observe that vv-CVs can lead to further gains over existing CVs by leveraging evaluations of \( f_L \). For both kernels, we provide three different versions of the vv-CVs with separable structure to highlight the impact of the matrix \( B \). The first two cases use Algorithm 2 with a fix value of \( B \). In the first instance, \( B_{11} = B_{22} = 0.1, B_{12} = B_{21} = 0.01 \), whereas in the second instance \( B_{11} = B_{22} = 0.5, B_{12} = B_{21} = 0.01 \). The third case is based on estimating \( B \) through Algorithm 1. Clearly, \( B \) can have a significant impact on the performance of the vv-CV, and estimating a good value from data can provide further gains. The choice of \( k \) is also significant: all CVs based on the squared-exponential kernel significantly outperform the CVs based on a 1st order polynomial kernel. It is also found that even when the model is mis-specified, the proposed method still perform better than standard scalar-valued CVs.

Modelling of Waterflow through a Borehole A more complex example often used to assess multifidelity methods is the following model of water flow passing through a borehole (Xiong et al., 2013; Kandasamy et al., 2016; Park et al., 2017). Both \( f_L \) and \( f_H \) have \( d = 8 \) inputs representing a range of parameters influencing the geometry and hydraulic conductivity of the borehole, as well as transmissivity of the aquifer. Prior distributions have been elicited from scientists over input parameters to account for uncertainties about their exact value. See Appendix E.4 for the details of each input and the multi-fidelity models. One quantity of interest here is the expected water flow under these distributions, and we hence have \( \Pi_L = \Pi_H \).

| \( m \) | vv-CV-EST. B | vv-CV-FIX. B | CF | MC |
|---|---|---|---|---|
| 10 | 3.72 (0.27) | 1.94 (0.15) | 2.24 (0.16) | 6.42 (0.44) |
| 20 | 1.29 (0.10) | 1.35 (0.10) | 1.96 (0.10) | 4.31 (0.31) |
| 50 | 1.04 (0.06) | 1.77 (0.12) | 1.76 (0.07) | 2.63 (0.17) |
| 100 | 1.07 (0.06) | 1.65 (0.14) | 1.71 (0.05) | 1.83 (0.15) |
| 150 | 0.85 (0.05) | 1.30 (0.09) | 1.67 (0.04) | 1.42 (0.10) |

Results of our simulation study are presented in Table 2. We compare a standard MC estimator with a kernel-based
CV fitted with a closed form solution (denoted CF) and two kernel-based vv-CVs corresponding to special case II in Section 3. The first with $B_{11} = B_{22} = 5 \times 10^{-4}$ and $B_{12} = B_{21} = 5 \times 10^{-5}$, and the second with $B$ estimated using Algorithm 1. The kernel used is a tensor product of squared-exponential kernels with a separate lengthscale for each dimension. Clearly, vv-CVs significantly outperform MC in the large majority of cases, and estimating $B$ can lead to significant gains over using a fixed $B$. The worst performance for vv-CVs with estimated $B$ is when values of $m$ are the lowest. This is because $m$ is not large enough to learn a good $B$. See Appendix E.4 for further details.

5.2. Model Evidence for Dynamical Systems

We now consider Bayesian inference for non-linear differential equations such as dynamical systems, which can be particularly challenging due to the need to compute the model evidence. This is usually a computationally expensive task since sampling from the posterior repeatedly requires the use of a numerical solver for differential equations which needs to be used at a fine resolution.

![Illustration of the van der Poll oscillator model](image)

**Figure 2. Model evidence computation through thermodynamic integration. Left:** Illustration of the van der Poll oscillator model (black line) and corresponding observations (red dots). **Center:** Estimates of the model evidence as a function of the number of posterior samples for kernel-based CVs. The box-plots were created by repeating the experiment 20 times and the black line gives an estimate of the truth obtained from (Oates et al., 2017) (25.58). **Right:** Same experiment but with kernel-based vv-CVs.

In (Calderhead & Girolami, 2009), the authors propose to use thermodynamic integration (TI) (Friel & Pettitt, 2008) to tackle this problem, and (Oates et al., 2016; 2017) later showed that CVs can lead to significant gains in accuracy in this context. TI introduces a path from the prior $p(x)$ to the posterior $p(x|y)$, where $y$ and $x$ represent the observations and the unknown parameters respectively. This is accomplished by the power posterior $p(x|y, t) \propto p(y|x)^t p(x)$, where $t \in [0, 1]$ is called the inverse temperature. When $t = 0$, $p(x|y, t) = p(x)$, whereas when $t = 1$, $p(x|y, t) = p(x|y)$. The standard TI formula for the model evidence has a simple form which can be approximated using second-order quadrature over a discretised temperature ladder $0 = t_1 \leq \cdots \leq t_w = 1$ (Friel et al., 2014). It takes the following form

$$
\log p(y) = \int_0^1 \left[ \int_X \log p(y|x)p(x|y, t) \, dx \right] \, dt \\
\approx \sum_{i=1}^w \left[ \frac{t_{i+1} - t_i}{2} \left( \mu_i + \mu_{i+1} \right) - \frac{(t_{i+1} - t_i)^2}{12} \right] (w_i - 1),
$$

where $\mu_i$ is the mean and $v_i$ the variance of the integrand $f(x) := \log p(y|x)$ with respect to $\pi_i(x) := p(x|y, t_i)$. To estimate $\{\mu_i, v_i\}_{i=1}^w$, we need to sample from all power posteriors on the ladder, then use a MCMC estimator which can be enhanced through CVs. This gives $T = 2w$ integrals which are related: $w$ integrals to compute means and $w$ integrals to compute variances, each against different power posteriors. As we will see, this structure will allow vv-CVs to provide significant gains in accuracy.

Our experiments will focus on the van der Poll oscillator, which is an oscillator $u : \mathbb{R}_+ \times X \rightarrow \mathbb{R}$ (where $x \in \mathbb{R}$) given by the solution of $d^2 u/ds^2 - x(1-u^2)du/ds + u = 0$, where $s$ represents the time index. For this experiment, we will follow the exact setup of (Oates et al., 2017) and transform the equation into a system of first order equations:

$$
du/ds = u_2, \\
du_2/ds = x(1-u_2^2)u_2 - u_1,
$$

which can be tackled with ODE solvers. Our data will consist of noisy observation of $u_1$ (the first component of that system) given by $y(s) = N(u_1(s); x, \sigma^2)$ with $\sigma = 0.1$ at each point $s \in \{0, 1, \ldots, 10\}$; see the left-most plot of Figure 2 for an illustration. We will take a ladder of size $w = 31$ with $t_i = ((i-1)/30)^5$ for $i \in \{1, \ldots, 31\}$. This gives a total of $T = 62$ integrals will need to be computed simultaneously, which is likely to be too computationally expensive for vv-CVs in their full generality. As a result, we chose $B$ to be a block diagonal matrix which puts integrands in groups of 4 means or 4 variances (except one group of 3 for mean and variance). To sample from the power-posteriors, we use population MC with the manifold Metropolis-adjusted Langevin algorithm (Girolami & Calderhead, 2011). Due to the high computational cost of using ODE solvers, our number of samples will be limited to less than 100 per integrand and this number will be the same for each integration task.

Our results are presented in Figure 2. The kernel parameters were taken to be identical to those in (Oates et al., 2017). As observed in the centre plot, kernel-based CVs provide relatively accurate estimates of the model evidence. As the sample size increases, we notice less variability in these estimates, but the central 50% of the runs are contained in an interval which excludes the true value. In comparison, the right-most plot shows that kernel-based vv-CVs can provide significant further reduction in variance. The distribution of estimates is also much more concentrated and centered around the true value.

5.3. Bayesian Inference of Lotka-Volterra System

We now consider another model: the Lotka-Volterra system (Lotka, 1925; Volterra, 1926; Lotka, 1927) of ordinary dif-
Vector-Valued Control Variates

Table 3. Posterior Expected Abundance of Preys. The numbers provided give the sum of the mean absolute integration error for 10 repetition of each task. To provide the absolute error, the true values of the associated expectations are estimated by MCMC estimators with $8 \times 10^5$ posterior samples.

| $T$ | $m$ | vv-CV-Ext. B | vv-CV-Fix. B | CF | MCMC |
|-----|-----|--------------|--------------|----|------|
| 2   | 500 | 0.462        | 0.404        | 0.666 | 0.368 |
| 5   | 500 | 0.393        | 0.319        | 0.521 | 0.587 |
| 10  | 500 | **0.938**    | 1.031        | 2.540 | 2.663 |

The proposed solution, vector-valued control variates, was shown to lead to significant variance reduction for problems in multi-fidelity modelling and Bayesian computation. Our approach is, to the best of our knowledge, the first algorithm able to perform multi-task learning for numerical integration by using only evaluation of the score functions of the corresponding target distributions. It is also the first algorithm which can simultaneously learn the relationship between integrands and provide estimates of the corresponding integrals without the requirement of a tractable kernel mean as in (Xi et al., 2018).

On an algorithmic level, further work will be needed to make the method more computationally practical and efficient. One particular line of research which could be considered is how special cases of our matrix-valued Stein kernels in Theorem 3.1 can be selected to reduce the computational cost whilst still producing a rich class of vv-CVs. Since a preprint version of this paper appeared online, it has been shown that approaches based on meta-learning could be competitive for very large $T$; see Sun et al. (2023).

On a theoretical level, we could also look at the question of when transferring information across tasks will lead to sufficient gains in accuracy to warrant the additional computational cost. In addition, it could be of interest to understand the negative transfer problems which can arise when the integrands are not in RKHS $\mathcal{H}_{K_{\alpha}}$ or when the sample size is too small to estimate $B$ well.

Acknowledgements

The authors would like to thank Chris J. Oates for helpful discussions and for sharing some of his code for the thermo-dynamic integration example. ZS was supported under the EPSRC grant [EP/N510129/1]. AB was supported by the Department of Engineering at the University of Cambridge, and this material is based upon work supported by, or in part by, the U.S. Army Research Laboratory and the U. S. Army Research Office, and by the U.K. Ministry of Defence and under the EPSRC grant [EP/R018413/2]. FXB was supported by the Lloyd’s Register Foundation Programme on Data-Centric Engineering and The Alan Turing Institute under the EPSRC grant [EP/N510129/1], and through an Amazon Research Award on “Transfer Learning for Numerical Integration in Expensive Machine Learning Systems”.

References

Álvarez, M. A., Rosasco, L., and Lawrence, N. D. Kernels for vector-valued functions: A review. Foundations and Trends in Machine Learning, 4(3):195–266, 2012.

Anastasiou, A., Barp, A., Briol, F.-X., Ebner, B., Gaunt, R. E., Ghaderinezhad, F., Gorham, J., Gretton, A., Ley,
Vector-Valued Control Variates

C., Liu, Q., Mackey, L., Oates, C. J., Reinert, G., and Swan, Y. Stein’s method meets Statistics: A review of some recent developments. *Statistical Science*, 38(1): 120–139, 2023.

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

Barp, A., Takao, S., Betancourt, M., Arnaudon, A., and Girolami, M. A unifying and canonical description of measure-preserving diffusions. *arXiv preprint arXiv:2105.02845*, 2021.

Barp, A., Oates, C. J., Porcu, E., and Girolami, M. A riemann–stein kernel method. *Bernoulli*, 28(4): 2181–2208, 2022a.

Berliner, A. and Thomas-Agnan, C. *Reproducing Kernel Hilbert Spaces in Probability and Statistics*. Springer Science & Business Media, 2011.

Bottou, L., Curtis, F. E., and Nocedal, J. Optimization methods for large-scale machine learning. *SIAM Review*, 60(2): 223–311, 2018. ISSN 00361445. doi: 10.1137/16M1080173.

Briol, F.-X., Oates, C. J., Cockayne, J., Chen, W. Y., and Girolami, M. On the sampling problem for kernel quadrature. In *Proceedings of the International Conference on Machine Learning*, pp. 586–595, 2017.

Calderhead, B. and Girolami, M. Estimating Bayes factors via thermodynamic integration and population MCMC. *Computational Statistics and Data Analysis*, 53(12): 4028–4045, 2009.

Carmeli, C., De Vito, E., and Toigo, A. Vector valued reproducing kernel Hilbert spaces of integrable functions and Mercer theorem. *Analysis and Applications*, 4(4): 377–408, 2006.

Carmeli, C., De Vito, E., Toigo, A., and Umanita, V. Vector valued reproducing kernel Hilbert spaces and universality. *Analysis and Applications*, 8(1): 19–61, 2010.

Carpenter, B., Gelman, A., Hoffman, M. D., Lee, D., Goodrich, B., Betancourt, M., Brubaker, M., Guo, J., Li, P., and Riddell, A. Stan: A probabilistic programming language. *Journal of statistical software*, 76(1), 2017.

Ciliberto, C., Mroueh, Y., Poggio, T., and Rosasco, L. Convex learning of multiple tasks and their structure. In *International Conference on Machine Learning*, pp. 1548–1557, 2015.

Dellaportas, P. and Kontoyiannis, I. Control variates for estimation based on reversible Markov chain Monte Carlo samplers. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 74(1): 133–161, 2012.

Dinuzzo, F., Ong, C. S., Gehler, P. V., and Pillonetto, G. Learning output kernels with block coordinate descent. In *International Conference on Machine Learning*, 2011.

Evgeniou, T., Micchelli, C. A., and Pontil, M. Learning multiple tasks with kernel methods. *Journal of Machine Learning Research*, 6: 615–637, 2005.

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

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

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

Green, P., Latuszyski, K., Pereyra, M., and Robert, C. Bayesian computation: a summary of the current state, and samples backwards and forwards. *Statistics and Computing*, 25: 835–862, 2015.

Hewitt, C. G. *The conservation of the wild life of Canada*. New York: C. Scribner, 1921.

Hickernell, F. J., Lemieux, C., and Owen, A. B. Control variates for quasi-Monte Carlo. *Statistical Science*, 20(1): 1–31, 2005.

Jones, G. L. On the Markov chain central limit theorem. *Probability Surveys*, 1: 299–320, 2004.

Kandasamy, K., Dasarathy, G., Oliva, J., Schneider, J., and Poczos, B. Gaussian process optimisation with multifidelity evaluations. In *Neural Information Processing Systems*, pp. 992–1000, 2016.

Kingma, D. P. and Ba, J. L. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2015.

Leluc, R., Portier, F., and Segers, J. Control variate selection for monte carlo integration. *Statistics and Computing*, 31(4): 1–27, 2021.

Lotka, A. J. *Elements of physical biology*. Williams & Wilkins, 1925.
Lotka, A. J. Fluctuations in the abundance of a species considered mathematically. *Nature*, 119(2983):12–12, 1927.

Micchelli, C. A. and Pontil, M. On learning vector-valued functions. *Neural Computation*, 17(1):177–204, 2005.

Mijatovic, A. and Voegrinc, J. On the Poisson equation for Metropolis-Hastings chains. *Bernoulli*, 24(3):2401–2428, 2018. ISSN 13507265.

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

Oates, C. J. and Girolami, M. Control functionals for quasi-Monte Carlo integration. In *Proceedings of the International Conference on Artificial Intelligence and Statistics*, volume 51, pp. 56–65, 2016.

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

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

Oates, C. J., Cockayne, J., Briol, F.-X., Girolami, M., et al. Convergence rates for a class of estimators based on Stein’s method. *Bernoulli*, 25(2):1141–1159, 2019.

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

Park, C., Haftka, R. T., and Kim, N. H. Remarks on multifidelity surrogates. *Structural and Multidisciplinary Optimization*, 55(3):1029–1050, 2017.

Peherstorfer, B., Willcox, K., and Gunzburger, M. Survey of multifidelity methods in uncertainty propagation, inference, and optimization. *SIAM Review*, 60(3):550–591, 2018.

Si, S., Oates, C. J., Duncan, A. B., Carin, L., and Briol, F.-X. Scalable control variates for Monte Carlo methods via stochastic optimization. *Proceedings of the 14th Conference on Monte Carlo and Quasi-Monte Carlo Methods*. arXiv:2006.07487, 2021.

South, L. F., Karvonen, T., Nemeth, C., Girolami, M., and Oates, C. J. Semi-exact control functionals from Sard’s method. *Biometrika*, 109(2):351–367, 2022a.

South, L. F., Riabiz, M., Teymur, O., and Oates, C. J. Post-Processing of MCMC. *Annual Review of Statistics and Its Application*, 2022b.

Steinwart, I. and Christmann, A. *Support vector machines*. Springer Science & Business Media, 2008.

Sun, Z., Oates, C. J., and Briol, F.-X. Meta-learning control variates: Variance reduction with limited data. *arXiv:2303.04756, to appear at UAI*, 2023.

Volterra, V. *Variazioni e fluttuazioni del numero d’individui in specie animali conviventi*. Società anonima tipografica” Leonardo da Vinci”, 1926.

Wan, R., Zhong, M., Xiong, H., and Zhu, Z. Neural control variates for variance reduction. *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pp. 533–547, 2019.

Xi, X., Briol, F.-X., and Girolami, M. Bayesian quadrature for multiple related integrals. In *International Conference on Machine Learning*, pp. 5373–5382, 2018.

Xiong, S., Qian, P. Z. G., and Wu, C. F. J. Sequential design and analysis of high-accuracy and low-accuracy computer codes. *Technometrics*, 55(1):37–46, 2013.
Appendix

We now complement the main text with additional details. Firstly, we provide additional methodology in Appendix A, including alternative objectives based on the variance of MCMC, stochastic optimisation algorithm for vv-CVs when the task relationship $B$ is known (under special case I and II) and the calculation of the computational complexity that is presented in Table 1. Secondly, in Appendix B, we provide the proofs of all the theoretical results in the main text. Then, in Appendix C, we present alternative constructions of vv-CVs. These constructions include a more general form of kernel-based vv-CVs as well as some polynomial-based CVs. Finally, in Appendix D and Appendix E, we provide additional details on our implementation of vv-CVs and provide additional numerical experiments.

A. Additional Methodology

In this first appendix, we will present additional methodology for Section 3. We briefly discuss an alternative objective based on the variance of the MCMC case in Appendix A.1. The selection of vv-CVs under special case I and II when $B$ is known and the corresponding algorithm is presented in Appendix A.2.

A.1. Alternative Objectives based on the Variance of MCMC

We present an alternative objective based on the variance of MCMC here, which is given by the following remark.

**Remark 1.** Given $\{X_i\}_{i=1}^{\infty}$ an ergodic Markov chain with invariant distribution $\Pi$, the variance of the MCMC CLT is proportional to

$$J(\theta) + 2 \sum_{i=1}^{\infty} \text{Cov}_\Pi[f(X_1) - g_0(X_1), f(X_i) - g_0(X_i)]$$

where the second term accounts for the correlation in the Markov chain. Given some realisation of the Markov chain $\{x_j\}_{j=1}^m$ and the corresponding evaluations $\{f(x_j)\}_{j=1}^m$, this can be approximated as:

$$J_m(\theta, \beta) + 2 \sum_{s=1}^{m-1} \frac{1}{m} \sum_{i=1}^{m-s} (f(x_i) - g_0(x_i) - \hat{\Pi}^{MC}[f - g_0]) \big(f(x_{i+s} - g_0(x_{i+s}) - \hat{\Pi}^{MC}[f - g_0])\big).$$

A.2. Stochastic Optimisation with a Known Task Relationship

In this section, we discuss the selection of vv-CVs under special case I and II when $B$ is known and give the corresponding algorithm in Algorithm 2.

In this case, we will assume that $B \in S_1^T$ is known. The proposed algorithm is a stochastic optimisation algorithm which we run for $L$ time steps; pseudo-code is provided in Algorithm 2. We propose to initialise the algorithm at $\theta^{(0)} = (0, \ldots, 0) \in \mathbb{R}^p$, since this is equivalent to having $g_0(x) = 0$ (i.e. having no CV) for both the kernel- and polynomial-based vv-CVs. We also suggest initialising the parameter $\beta \in \mathbb{R}^T$ with any estimate of $\Pi[f]$. This is a natural initialisation since we expect $\beta_t$ to equal $\Pi[f]_t$ for all $t \in [T]$ when $m_1, \ldots, m_T \to \infty$. For example, when the data consists of IID realisations from $\Pi_1, \ldots, \Pi_T$, a natural initialisation point is $\beta^{(0)} = (\hat{\Pi}^{MC}_T[f_1], \ldots, \hat{\Pi}^{MC}_T[f_T])^T$.

For each iteration, we take mini-batches of size $\tilde{m} \in \mathbb{N}^T$ where $|\tilde{m}| \leq |m|$. Note here that $\tilde{m} = (\tilde{m}_1, \ldots, \tilde{m}_T)^T$ is a multi-index giving the size of the mini-batch for each of the $T$ datasets. This formulation allows for the use of different datasets across integrands, but also different mini-batch sizes for each task (which may be useful if the datasets are of different size for each integrand). An epoch consists of having gone through all data points for all $T$ tasks, and we randomly shuffle the indices for mini-batches after each epoch. As default, we propose to take $\tilde{m}_t \propto m_t/\left(\sum_{t=1}^{T} m_t\right)$ for all $t \in [T]$. This choice guarantees that the number of samples for each integrand in the mini-batches is proportional to the proportion of samples for that integrand in the full dataset.

Once a mini-batch has been selected, we update our current estimate of the parameters $\theta$ and $\beta$ using steps based on the gradient of our loss function: $\nabla_{(\theta, \beta)} L^{\text{MC}}_m(\theta, \beta)$. The pseudo-code in Algorithm 2 presents this abstractly as a function $\text{Update}_{\theta, \beta}(\theta, \beta, B, D)$, which takes in the current estimates of the parameters, the value of $B$ and the dataset (or minibatch) used for the update; this is because different choices of vv-CVs might benefit from different updates. For example, preconditioners for the gradients could be used when readily available, or when these can be estimated from data. In Section 5, we will exclusively be using the Adam optimiser (Kingma & Ba, 2015), a first order method with estimates of lower-order moments.
Algorithm 2 Stochastic optimisation for vv-CVs with known task relationship

Input: $D$, $\tilde{m}$, $L$, $\lambda$, $\beta(0)$ and $\theta(0)$.

for iterations $l$ from 1 to $L$
do
Select a mini-batch $D_{\tilde{m}}$ of size $\tilde{m}$
$(\theta^{(l)}, \beta^{(l)}) \leftarrow \text{UPDATE}_{\theta, \beta}(\theta^{(l-1)}, \beta^{(l-1)}; B; D_{\tilde{m}})$
end for

Return: $\theta^{(L)}$, $\beta^{(L)}$

For the penalisation term, it would be natural to take the RKHS norm $\|g_{\theta}\| = \|g_{\theta}\|_{H_{K}}$ since this would lead to the objective used in Theorem 4.1. However, this can be impractical from a computational viewpoint since this norm depends on kernel evaluations for all of the training points. For this reason, we follow the recommendation of (Si et al., 2021) and use instead the Euclidean norm: $\|g_{\theta}\| = \|\theta\|_2$. This still leads to a convex objective since the objective remains quadratic in $\theta$.

Algorithm 2 is a natural approach to minimising our objective since our kernel-based vv-CVs are linear in $\theta$ and $L_{\text{vv}}$ is convex in $(\theta, \beta)$. Many stochastic optimisation methods, such as stochastic gradient descent, will hence converge to a global minimum under regularity conditions (Bottou et al., 2018). However, note that Algorithm 2 naturally applies to other vv-CVs whether linear or not.

### A.3. Calculation of Computational Complexity

In this section, we derive the computational complexity reported in Table 1. Suppose we have $m_t$ samples for each of $T$ tasks and similarly for all $\tilde{m}_t$ with $t \in [T]$.

**Computational cost of CV:**

- **Exact solution**: For each task, we need to compute $k_0(\cdot, \cdot)$ for all pairs, which results in a cost of $O(dm_t^2)$ per task. To compute the exact solution of kernel-based control variates, it takes $O(m_t^3)$ per task. So, in total, the computational cost of the exact solution of CV is $O((dm_t^2 + m_t^3)T)$.

- **Stochastic optimisation**: To use stochastic optimisation, suppose we use $L$ epochs. At each iteration of one epoch, we need to compute $k_0(\cdot, \cdot)$ for $\tilde{m}_t m_t$ pairs, which costs $O(d\tilde{m}_t m_t)$. We need to do this for all $L$ iterations. This results in $O(d\tilde{m}_t m_t L)$ per task. Hence, in total, the computational cost of stochastic optimisation of CV is $O(d\tilde{m}_t m_t LT)$ for all $T$ tasks.

**Computational cost of vv-CV:**

- **Exact solution**: There are $m_t T$ samples (i.e. $m_t^2T^2$ pairs) in total and we are using mv-Stein kernels. Thus, the computational cost of computing $K_0(\cdot, \cdot)$ is $O(d(m_tT)^2T^2) = O(dm_t^2T^4)$. To compute the exact solution of vv-CV, we can re-arrange the Gram tensor of all samples into a matrix of size $m_tT^2 \times m_tT^2$. Hence, the computational cost of computing the exact solution of vv-CV is $O((m_tT^2)^3) = O(m_t^3T^6)$. Thus, in total, the computational cost of computing the exact solution of vv-CV is $O(dm_t^2T^4 + m_t^3T^6)$.

- **Stochastic optimisation**: At each iteration, one mini-batch of the stochastic optimisation of vv-CV has $\tilde{m}_t T$ samples. We need to compute $K_0(\cdot, \cdot)$ for these samples with all $m_t T$ samples. This leads to a cost of $O(d\tilde{m}_t T m_t T d T^2) = O(d\tilde{m}_t m_t T d T^2)$ per iteration. Note that we need to do this for all $L$ iterations. So, in total, the computational cost of stochastic optimisation of vv-CV is $O(d\tilde{m}_t m_t L T^4)$.

### B. Proofs of the Main Theoretical Results

In this second appendix, we recall the proofs of the theoretical results in the main text. The derivation of the mv-kernel $K_0$ from Theorem 3.1 can be found in Appendix B.1. The proof that kernel-based vv-CVs are square-integrable (Theorem 3.2) is in Appendix B.2. Finally, the proof of the existence of the optimal parameters as the solution to a linear system (Theorem 4.1) is given in Appendix B.3.
B.1. Proof of Theorem 3.1

Proof. We will show \( K_0 \) is a kernel and derive its matrix components by constructing an appropriate feature map. The first order Stein operator maps matrix-valued functions \( u = (u_1, u_2, \ldots, u_T) : \mathbb{R}^d \to \mathbb{R}^{d \times T} \) to the \( \text{vv} \)-function \( S^{\text{vv}}[u] : \mathbb{R}^d \to \mathbb{R}^T \) given by

\[
S^{\text{vv}}[u](x) = (\mathcal{L}_{H}[u_1], \ldots, \mathcal{L}_{H}[u_T])^T
\]

where \( \mathcal{L}_{H}[u_t](x) = \nabla_x \cdot u_t(x) + \nabla_x \log \pi_t(x) \cdot u_t(x) \quad \forall t \in [T]. \)

Since \( K \in C^{1,1}(\mathbb{R}^d \times \mathbb{R}^d) \), we can use Corollary 4.36 of (Steinwart & Christmann, 2008) to conclude that \( \mathcal{H}_K \) is a vector-valued RKHS of continuously differentiable functions from \( \mathbb{R}^d \) to \( \mathbb{R}^T \), hence the tensor product \( \mathcal{H}_K^{\text{tr}} \) consists of suitable functions \( u \in \mathcal{H}_K^{\text{tr}} \), with components \( u^i = (u_1^i, \ldots, u_T^i) \in \mathcal{H}_K \) for \( i \in [d] \). Now since the RKHS consists of differentiable functions, we have by Lemma C.8 in Barp et al. (2022b):

\[
\langle \partial_x^i K(x, x)e_t, u^i \rangle_{\mathcal{H}_K} = e_t \cdot \partial_x u^i(x) = \partial_x u^i_t(x) = \partial_x u^i_t(x) \quad \forall t \in [T]
\]

where \( e_t \in \mathbb{R}^T \) is a vector of zeros with value 1 in the \( t \)th component. Then, writing \( K_{\text{tr}}^i \equiv K(:, x)e_t \),

\[
S^{\text{vv}}[u](x) = \sum_{t=1}^T \sum_{r=1}^d (\partial_x^r u^i_t(x) + \partial_x^r u^i_t(x) \pi_t(x)) e_t
\]

\[
= \sum_{t=1}^T \sum_{r=1}^d \langle \partial_x^r K^i_t, u^i \rangle_{\mathcal{H}_K} e_t
\]

\[
= \sum_{t=1}^T \sum_{r=1}^d (\partial_x^r K^i_t + l_{tr}(x) K^i_t, u^i)_{\mathcal{H}_K} e_t,
\]

where \( l_{tr}(x) = \partial_x^r \pi(x), \) and \( \partial_x^r K^i_t \) and \( l_{tr}(x) \) denote respectively the tuples \((\partial_x^1 K^i_t, \ldots, \partial_x^d K^i_t) \) and \((l_{1, tr}(x), \ldots, l_{d, tr}(x)) \) in \( \mathbb{R}^d \).

We have thus obtained a feature map, i.e., a map \( \gamma : \mathbb{R}^d \to \mathcal{B}(\mathcal{H}_K^{\text{tr}}, \mathbb{R}^T) \), where \( \mathcal{B}(\mathcal{H}_K^{\text{tr}}, \mathbb{R}^T) \) denotes the space of bounded linear maps from \( \mathcal{H}_K^{\text{tr}} \) to \( \mathbb{R}^T \), via the relation

\[
\gamma(u)[x] = S^{\text{vv}}[u](x),
\]

with adjoint \( \gamma(x)^* = \sum_{t=1}^T (\partial_x^r K^i_t + l_{tr}(x) K^i_t)e_t \). Recall the adjoint map \( \gamma(y)^* \in \mathcal{B}(\mathbb{R}^T, \mathcal{H}_K^{\text{tr}}) \) to \( \gamma(y) \), is defined for any \( a \in \mathbb{R}^T, u \in \mathcal{H}_K^{\text{tr}} \) by the relation

\[
\langle \gamma(y)^*[a], u \rangle_{\mathcal{H}_K^{\text{tr}}} = \gamma(y)[u] : a.
\]

In particular, by Proposition 1 of Carmeli et al. (2010) we have that

\[
K_0(x, y) = \gamma(x) \circ \gamma(y)^* \in \mathbb{R}^{T \times T}
\]

will then be the kernel associated to the “feature operator” (that is, a surjective partial isometry whose image is \( \mathcal{H}_{K_0} \)) \( S^{\text{vv}} : \mathcal{H}_K^{\text{tr}} \to \mathcal{H}_{K_0} \). Subbing in the expressions for the feature map and its adjoint derived above, and using the equalities

\[
\langle \partial_x^r K(:, x)e_t, \partial_y^s K(:, y)e_{t'} \rangle_{\mathcal{H}_K} = e_t \cdot \partial_x^r \partial_y^s K(x, y)e_{t'} = (\partial_x^r \partial_y^s K(x, y))_{tt'} \quad \forall t, t' \in [T]
\]

and

\[
\langle \partial_x^a K(:, x)e_t, \partial_y^s K(:, y)e_{t'} \rangle_{\mathcal{H}_K} = (\partial_x^a \partial_y^s K(x, y))_{tt'} \quad \forall t, t' \in [T],
\]

which hold for any differentiable matrix-valued kernel (Barp et al., 2022b), we obtain the following expression for the components of \( K_0 \)

\[
(K_0(x, y))_{tt'} = \sum_{r=1}^d \left( \partial_x^r \partial_y^r K(x, y) \right)_{tt'} + l_{tr}(y) (\partial_y^r K(x, y))_{tt'} + l_{tr}(x) (\partial_x^r K(x, y))_{tt'}.
\]

In particular for separable kernels (i.e. \( K(x, y) = Bk(x, y) \)) we have

\[
(K_0(x, y))_{tt'} = B_{tt'} \sum_{r=1}^d \partial_x^r \partial_y^r k(x, y) + l_{tr}(y) \partial_y^r k(x, y) + l_{tr}(x) \partial_x^r k(x, y) + l_{tr}(x) l_{tr}(y) k(x, y).
\]

\[\square\]
B.2. Proof of Theorem 3.2

Proof. Recall that if a scalar kernel $k$ satisfies $\int_R k(x, x) d \mu(x) < \infty$, then its RKHS consists of square $\mu$-integrable functions (for any finite measure $\mu$) (Steinwart & Christmann, 2008, Theorem 4.26).

If $g \in \mathcal{H}_K$, then $g_\epsilon$ belongs to the RKHS with scalar-valued kernel (this follows from (Carmeli et al., 2010, Prop. 1), using as feature operator the dot product with respect to $\epsilon_t$, where $\epsilon_t$ is defined in Appendix B.1)

$$(K_0(x, y))_{tt} = \sum_{r=1}^d (\partial_x^r \partial_y^r K(x, y))_{tt} + l_{tr}(y) \partial_y^r(K(x, y))_{tt} + l_{tr}(x) \partial_x^r(k(x, y))_{tt} \quad \forall t \in [T].$$

In particular since $K$ is bounded with bounded derivatives, and

$$\Pi_t \|l_{tr}\| + \Pi_t \|l_{tr}\|^2 \leq \sqrt{\Pi_t \|l_{tr}\|^2} + \Pi_t \|l_{tr}\|^2 \quad \forall t \in [T], r \in [d]$$

then $\int_R (K_0(x, y))_{tt} d \Pi_t(x) < \infty$ if $\|\nabla_x \log \pi_t(x)\|_2$ is square integrable with respect to $\Pi_t$, and the result follows.

B.3. Proof of Theorem 4.1

Proof. We want to find

$$\arg \min_{g \in \mathcal{H}_K} L_m^\gamma(g, \beta)$$

where

$$L_m^\gamma(g, \beta) := \sum_{t=1}^T \frac{1}{m_t} \sum_{j=1}^{m_t} (f_t(x_{tj}) - g_t(x_{tj}) - \beta_t)^2 + \lambda \|g\|_{\mathcal{H}_K}^2.$$

Note that the objective is the same as that in (8), with the only difference being that the first input is now a function as opposed to the parameter value parameterising this function. We will abuse notation by using the same mathematical expression for both objectives.

By Ciliberto et al. (2015, Section 2.1), any solution of the minimization problem has the form $\hat{g}(\cdot) = \sum_{t'=1}^T \sum_{j'=1}^{m_{t'}} K_0(\cdot, x_{t'j'}) \theta_{t'j'}$. Subbing this solution into $L_m^\gamma(g, \beta)$ yields

$$L_m^\gamma(\hat{g}, \beta) = \sum_{t=1}^T \frac{1}{m_t} \sum_{j=1}^{m_t} (f_t(x_{tj}) - (\sum_{t'=1}^T \sum_{j'=1}^{m_{t'}} K_0(x_{tj}, x_{t'j'}) \theta_{t'j'} - \beta_t)^2 + \lambda \|\theta\|_{\mathcal{H}_K}^2$$

where $y_{tj} \equiv f_t(x_{tj}) - \beta_t$. The problem thus becomes a minimization problem over the coefficients $\theta$,

$$\arg \min_{\theta \in \mathbb{R}^{|\Theta|}} \lambda \sum_{t',t''=1}^T \sum_{j_1=1}^{m_{t'}} \sum_{j_2=1}^{m_{t''}} \theta_{t'j'}^T K_0(x_{t'j'}, x_{t''j''}) \theta_{t''j''} + 2 \sum_{t'=1}^T \frac{1}{m_t} \sum_{j=1}^{m_t} y_{tj}^2$$

Since the quadratic terms are positive definite, the resulting objective is a convex function of $\theta$, thus, by differentiating it, we obtain that the solution $\theta$ is the solution to

$$\sum_{t'=1}^T \sum_{j'=1}^{m_{t'}} \left( \sum_{t=1}^T \frac{1}{m_t} \sum_{j=1}^{m_t} K_0(x_{t'j'}, x_{tj}) + \lambda K_0(x_{t'j'}, x_{tj}) \right) \theta_{t'j'} = \sum_{t} \frac{1}{m_t} \sum_{j=1}^{m_t} K_0(x_{t'j'}, x_{tj}) (f_t(x_{tj}) - \beta_t), \quad \forall t'' \in [T], j'' \in [m_{T'}].$$

Finally, generalising the scalar case, we say that a matrix-valued reproducing kernel $K_0$ is strictly positive definite if for any finite set of $\gamma_s \in \mathbb{R}^T$ and distinct points $y_s \in \mathbb{R}^d$ we have $\sum_s \gamma_s K_0(y_s, y_t) = 0$ implies each $\gamma_s$ is zero –
this means that the mean embedding of $K_0$ is injective (or characteristic) over the set of linear functionals of the form $\delta^g_y : f \mapsto \sum_t f_t(y)\gamma_t$. It follows that the map $\mathbb{R}^{D_x} \times \mathbb{R}^T \to \mathbb{R}^{D_x} \times \mathbb{R}^T$, where $D_x = \{ x_1, \ldots, x_{T-m} \}$, defined as

$$
\theta \mapsto \left( \sum_{t=1}^{T-m} \sum_{j=1}^{m_i} K_0(x_{ij}, \theta_{tj}) \ldots, \sum_{t=1}^{T-m} \sum_{j=1}^{m_i} K_0(x_{T-m}, \theta_{tj}) \right)
$$

is injective between vector spaces of the same dimension, and thus invertible by the rank theorem. Hence, since by above the quadratic term is positive definite, the linear system may be inverted to find $\theta^*$.

## C. Alternative Constructions

In this third appendix, we will now provide alternative constructions to those presented in the main text. First, in Appendix C.1, we present kernel-based vv-CVs derived from the second order Langevin Stein operator. Then, in Appendix C.2 and Appendix C.3 we point out how these constructions can lead to polynomial-based vv-CVs.

### C.1. Kernel-based vv-CVs from Second-Order Langevin Stein Operators

The **Langevin Stein operator** can also be adapted to apply to the derivative of twice differentiable scalar-valued functions $u : \mathbb{R}^d \to \mathbb{R}$, in which case it is called the **second-order Langevin Stein operator**:

$$
\mathcal{L}'[u](x) := \Delta_x u(x) + \nabla_x u(x) \cdot \nabla_x \log \pi(x),
$$

where $\Delta_x = \nabla_x \cdot \nabla_x$.

In this section we will consider the second-order Langevin Stein operator which acts on scalar-valued functions. The following theorem provides a characterisation of the class of vv-functions obtained when applying this operator to functions in a vv-RKHS.

**Theorem C.1.** Consider $\mathcal{H}_K$ which is a vv-RKHS with mv-kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{T \times T}$, and suppose that $K \in C^{2,\gamma}(\mathbb{R}^d \times \mathbb{R}^d)$. Furthermore, for suitably regular vv-functions $u = (u_1, \ldots, u_T) : \mathbb{R}^d \to \mathbb{R}^T$ define the differential operator

$$
\mathcal{S}^{vv}[u] = (\mathcal{L}'_{\Pi_1}[u_1], \ldots, \mathcal{L}'_{\Pi_T}[u_T])^{\top}.
$$

Then, the image of $\mathcal{H}_K$ under $\mathcal{S}^{vv}$ is a vv-RKHS with reproducing kernel $K_0 : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{T \times T}$:

$$
\langle K_0(x,y) \rangle_{\mathcal{H}_K} = \sum_{s,t=1}^{d} \partial_{x}^{s} \partial_{y}^{t} K(x,y) e_{s} e_{t} + l_{s}(x) \partial_{y}^{t} K(x,y) e_{s} + l_{s}(y) \partial_{x}^{t} K(x,y) e_{t} \forall t, t' \in [T],
$$

We note that this theorem is very similar to Theorem 3.1, and recovers the kernel of (Barp et al., 2022a) when $T = 1$, provided we use the manifold analog of (11). Indeed, one advantage of (11) is that the associated Theorem C.1 can be easily extended to manifolds (more generally, we can obtain a similar result for any generators of measure-preserving diffusion given in Corollary 5.3 of Barp et al. (2021)). However, one particular disadvantage of this construction from a computational viewpoint is that it requires higher-order derivatives of the kernel $K$. It also requires the evaluation of a double sum, which significantly increases computational cost relative to our construction in the main text. For this reason, we did not explore this construction in more details.

**Proof.** We proceed as for the proof of Theorem 3.1 and shall derive a feature map for $K_0$. Recall that $g = \mathcal{S}^{vv}[u] = (\mathcal{L}'_{\Pi_1}[u_1], \ldots, \mathcal{L}'_{\Pi_T}[u_T])^{\top}$, where $\mathcal{L}'_{\Pi}$ is the second-order Stein operator, which maps scalar functions to scalar functions. Here $u$ belongs to a RKHS of $\mathbb{R}^T$-valued functions with matrix kernel $K$. From the differentiability assumption on $K$, we have $\mathcal{H}_K \subset C^2$, i.e., it is a space of twice continuously differentiable functions. Note that (here $\partial^3 = \partial^2 \partial = \frac{\partial^2}{\partial x_i \partial x_j}$)

$$
\langle \partial^3_x K(\cdot,x) e_t, u \rangle_{\mathcal{H}_K} = \partial^3_x u_t(x) = \frac{\partial^2 u_t}{\partial x_i \partial x_j}(x) \forall t \in [T],
$$

16
where \( e_i \) is the \( t^{th} \) standard basis vector of \( \mathbb{R}^T \) as before. Thus

\[
\mathcal{L}_{\Pi_i}^t(u_t(x)) = \Delta_x u_t(x) + \nabla_x \log \pi_t(x) \cdot \nabla_x u_t(x)
\]

\[
= \sum_{s=1}^d \partial_x^{ss} u_t(x) + \sum_{s=1}^d l_t(x) \partial_x^{ss} u_t(x)
\]

\[
= \sum_{s=1}^d \langle \partial_x^{ss} K(\cdot, x)e_t, u \rangle_{\mathcal{H}_K} + \sum_{s=1}^d \langle l_t(x) \partial_x^{ss} K(\cdot, x)e_t, u \rangle_{\mathcal{H}_K}
\]

\[
= \sum_{s=1}^d \langle \partial_x^{ss} K(\cdot, x)e_t + l_t(x) \partial_x^{ss} K(\cdot, x)e_t, u \rangle_{\mathcal{H}_K}
\]

\[\forall t \in [T].\]

Hence

\[
S^{vv}[u](x) = \begin{pmatrix}
\left( \sum_{s=1}^d \partial_x^{ss} K(\cdot, x)e_t + l_t(x) \partial_x^{ss} K(\cdot, x)e_t, u \right)_{\mathcal{H}_K} \\
\vdots \\
\left( \sum_{s=1}^d \partial_x^{ss} K(\cdot, x)e_T + l_T(x) \partial_x^{ss} K(\cdot, x)e_T, u \right)_{\mathcal{H}_K}
\end{pmatrix} \in \mathbb{R}^T.
\]

Note that for each \( x \in \mathbb{R}^d \), each component of the above is a bounded linear operator \( \mathcal{H}_K \to \mathbb{R} \) (i.e., the map \( u \mapsto (S^{vv}(u))(x) \) \( x \in \mathbb{R} \) to the \( s \)-component is a bounded linear operator), then we have obtained a feature map, i.e., a map \( \gamma : \mathbb{R}^d \to \mathcal{B}(\mathcal{H}_K, \mathbb{R}^T) \), where \( \mathcal{B}(\mathcal{H}_K, \mathbb{R}^T) \) denotes the space of bounded linear maps from \( \mathcal{H}_K \) to \( \mathbb{R}^T \). Specifically

\[
\gamma(x) \equiv S^{vv}[-1](x) \in \mathcal{B}(\mathcal{H}_K, \mathbb{R}^T).
\]

In particular, as before

\[
n_0(x, y) = \gamma(x) \circ \gamma(y)^* \in \mathcal{B}(\mathbb{R}^T, \mathbb{R}^T)
\]

will thus be the kernel associated to the “feature operator” \( S^{vv} : \mathcal{H}_K \to \mathcal{H}_K \). Recall that \( \gamma(y)^* \in \mathcal{B}(\mathbb{R}^T, \mathcal{H}_K) \) is the adjoint map to \( \gamma(y) \), i.e., it satisfies for any \( a \in \mathbb{R}^T, u \in \mathcal{H}_K \):

\[
\langle \gamma(y)^*[a], u \rangle_{\mathcal{H}_K} = \gamma(y)[u] \cdot a.
\]

From this we obtain

\[
\gamma(y)^* : a \mapsto \sum_{s=1}^d \sum_{t=1}^T a_t \left( \partial_x^{ss} K(\cdot, y)e_t + l_T(y) \partial_x^{ss} K(\cdot, y)e_t \right) \in \mathcal{H}_K.
\]

From \( K_0(x, y)a = \gamma(x) \circ \gamma(y)^*[a] \) for all \( a \in \mathbb{R}^T \) and the above expressions we can finally calculate \( K_0 \). We have

\[
K_0(x, y)a = S^{vv}[\gamma(y)^*a](x) = \begin{pmatrix}
\langle \sum_{s=1}^d \partial_x^{ss} K(\cdot, x)e_t + l_t(x) \partial_x^{ss} K(\cdot, x)e_t, \gamma(y)^*a \rangle_{\mathcal{H}_K} \\
\vdots \\
\langle \sum_{s=1}^d \partial_x^{ss} K(\cdot, x)e_T + l_T(x) \partial_x^{ss} K(\cdot, x)e_T, \gamma(y)^*a \rangle_{\mathcal{H}_K}
\end{pmatrix}.
\]

We obtain that \( K_0(x, y)a \) is a vector with components:

\[
(K_0(x, y)a)_t = \sum_{r,s=1}^d \sum_{t'=1}^T a_t' \left( \partial_x^{ss} \partial_y^{rr} K(x, y) K(x, y)_{tt'} + l_t(x) \partial_x^{ss} \partial_y^{rr} K(x, y) K(x, y)_{tt'} + l_t(x) l_t'(y) \partial_x^{ss} \partial_y^{rr} K(x, y)_{tt'} \right) \forall t \in [T].
\]

Thus the components of \( K_0(x, y) \in \mathbb{R}^{T \times T} \) are

\[
(K_0(x, y))_{tt'} = \sum_{r,s=1}^d \partial_x^{ss} \partial_y^{rr} K(x, y) K(x, y)_{tt'} + l_t(x) \partial_x^{ss} \partial_y^{rr} K(x, y) K(x, y)_{tt'} + l_t(x) l_t'(y) \partial_x^{ss} \partial_y^{rr} K(x, y) K(x, y)_{tt'} \forall t, t' \in [T].
\]
Vector-Valued Control Variates

Analogously to the mv-kernel in Theorem 3.1, there are several cases of practical interest. The first is when $K(x, y) = Bk(x, y)$ is a separable kernel, in which case:

$$(K_0(x, y))_{tt'} = B_{tt'} \sum_{r,s=1}^d \partial^s_x \partial^r_y k(x, y) + l_{tt'}(y) \partial^s_x \partial^r_y k(x, y)$$

$$+ l_s(x) \partial^s_x \partial^r_y k(x, y) + l_s(x) l_{tt'}(y) \partial^s_x \partial^r_y k(x, y) \quad \forall t, t' \in [T].$$

The second is when $K$ is separable and $\Pi_1 = \ldots = \Pi_T$, in which case $l_r(x) := l_{1r}(x) = \ldots = l_{Tr}(x) \forall r \in [d]$ and:

$$(K_0(x, y))_{tt'} = B_{tt'} \sum_{r,s=1}^d \partial^s_x \partial^r_y k(x, y) + l_r(x) \partial^s_x \partial^r_y k(x, y)$$

$$+ l_s(y) \partial^s_x \partial^r_y k(x, y) + l_s(y) l_{tt'}(y) \partial^s_x \partial^r_y k(x, y) \quad \forall t, t' \in [T].$$

C.2. Alternative Constructions beyond Kernels

Although kernels are a natural way of constructing functions for multi-task problems, it is also possible to generalise constructions based on other parametric families such as polynomials or neural networks. We will not explore this avenue in detail in the present paper, but now provide brief comments on how such generalisations could be obtained.

Firstly, $u_\theta$ could be based on any additive model such as a polynomial or wavelet expansion. In that case, it is straightforward to construct vv-CVs with a separable structure as follows:

$$(u_\theta(x))_t = \sum_{t'=1}^T B_{tt'} \theta_i(x), \quad (g_\theta(x))_t = \sum_{t'=1}^T B_{tt'} S_{tt'}[\theta_i(x)] \quad \forall t \in [T],$$

where $B \in S_T^d$ and $\phi_i : \mathbb{R}^d \to \mathbb{R}$ is a (sufficiently regular) basis function. In particular, taking the basis functions to be of the form $x^\alpha$ for $\alpha \in \mathbb{N}^d$ recovers the polynomial-based CVs of (Mira et al., 2013). We also note that any model of this form leads to a quadratic MC variance objective, whose solution can be obtained in closed form under mild regularity conditions on the basis functions.

Secondly, we could use non-linear models for $u_\theta$. In that case, one approach would be to use a separable structure of the form:

$$(u_\theta(x))_t = \sum_{t'=1}^T B_{tt'} \phi_\theta(x), \quad (g_\theta(x))_t = \sum_{t'=1}^T B_{tt'} S_{tt'}[\phi_\theta(x)] \quad \forall t \in [T].$$

where $\phi_\theta(x)$ is a non-linear function of the parameters $\theta$. The above is a generalisation of the neural networks-based CVs of (Wan et al., 2019; Si et al., 2021) whenever $\phi_\theta$ is a neural network. Unfortunately the MC variance objective will usually be non-convex in those cases, and we therefore have no guarantees of recovering the optimal parameter value when using most numerical optimisers.

C.3. Polynomial vv-CVs

In Appendix C.2, we have discussed a construction for vv-CVs based on polynomials which recovers the work of (Mira et al., 2013). However, it is also possible to obtain polynomial-based vv-CVs directly through our kernel constructions in Theorem 3.1 and Appendix C.1. In particular, one option would be to take $K(x, y) = Bk(x, y)$ where $B \in S_T^d$ and $k(x, y) = (x^\top y + c)^l$ where $c \in \mathbb{R}$ and $l \in \mathbb{N}$. Firstly, using the first-order Langevin Stein operator and setting $l = 1$, we obtain:

$$(K_0(x, y))_{tt'} = B_{tt'} \sum_{r=1}^d \left[ 1 + l_{tt'}(y)y_r + l_{tt'}(x)x_r + l_r(x)l_{tt'}(y) (x^\top y + c) \right] \quad \forall t \in [T].$$

Similarly when $l = 2$, we get:

$$(K_0(x, y))_{tt'} = B_{tt'} \sum_{r=1}^d \left[ 2x_r y_r + 2 (x^\top y + c) + 2 y_r l_{tt'}(y) (x^\top y + c) + 2 x_r l_r(x) (x^\top y + c) + l_r(x) l_{tt'}(y) (x^\top y + c)^2 \right] \quad \forall t \in [T].$$

These two choices were considered in the experiments in Section 5. An alternative would be to consider this same kernel, but using the construction based on second-order Langevin Stein operators. Again, taking $l = 1$, we obtain:

$$(K_0(x, y))_{tt'} = \sum_{r=1}^d l_r(x) l_{tt'}(y) B_{tt'} \quad \forall t \in [T].$$
We now provide details of all the kernels used in the paper, as well as expressions for their derivatives.

**Squared-Exponential Kernel**

The squared-exponential kernel (sometimes called Gaussian kernel) is given by:

\[
K(x, y) = \exp\left(-\frac{(x - y)^2}{2\lambda^2}\right)
\]

Similarly, when \(l = 2\), we get:

\[
(K_0(x, y))_{t'v} = B_{t'v} \left[ 4 \left( \sum_{r=1}^{d} l_{t'v}(y) y_r + l_{t'v}(x) x_r \right) + 2 \sum_{r,s=1}^{d} l_{t'v}(x) l_{t'v}(y) (x^\top y + c) + \sum_{r,s=1}^{d} l_{t'v}(x) l_{t'v}(y) x_r y_s \right] \quad \forall t \in [T].
\]

**D. Implementation Details**

In this appendix, we focus on implementation details which may be helpful for implementing the algorithms in the main text. Firstly, in Appendix D.1 we derive the derivatives of several common kernels; this is essential for the implementation of Stein reproducing kernels. Then, in Appendix D.2, we provide details on how to select hyperparameters. Finally, in Appendix D.3, we discuss how to turn the problem of estimating \(B\) from data into a sequence of convex optimisation problems.

**D.1. Kernels and Their Derivatives**

We now provide details of all the kernels used in the paper, as well as expressions for their derivatives.

**Polynomial Kernel**

The polynomial kernel \(k_l(x, y) = (x^\top y + c)^l\) with constant \(c \in \mathbb{R}\) and power \(l \in \mathbb{N}\) has derivatives given by:

\[
\nabla_x k_l(x, y) = l(x^\top y + c)^{l-1}y, \quad \nabla_y k_l(x, y) = l(x^\top y + c)^{l-1}x,
\]

\[
\nabla_x \cdot \nabla_y k_l(x, y) = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j \partial y_j} k_l(x, y) = \sum_{j=1}^{d} \frac{\partial}{\partial x_j} \left[ \frac{(x - y) \cdot y_j}{\lambda} \right] k_l(x, y)
\]

\[
= \sum_{j=1}^{d} \frac{1}{\lambda} \left( \frac{(x - y) \cdot y_j}{\lambda} \right) k_l(x, y) = \frac{d}{\lambda} - \frac{(x - y) \cdot (x - y)}{\lambda^2} k_l(x, y).
\]

**Squared-Exponential Kernel**

The squared-exponential kernel (sometimes called Gaussian kernel) \(k(x, y) = \exp(-\frac{(x-y)^2}{2\lambda^2})\) with lengthscale \(\lambda > 0\) has derivatives given by:

\[
\nabla_x k(x, y) = -\frac{1}{\lambda} \frac{x - y}{\lambda} k(x, y), \quad \nabla_y k(x, y) = \frac{1}{\lambda} \frac{x - y}{\lambda} k(x, y),
\]

\[
\nabla_x \cdot \nabla_y k(x, y) = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j \partial y_j} k(x, y) = \sum_{j=1}^{d} \frac{\partial}{\partial y_j} \left[ \frac{(x - y) \cdot y_j}{\lambda} \right] k(x, y)
\]

\[
= \sum_{j=1}^{d} \left( \frac{1}{\lambda} \frac{x - y}{\lambda} k(x, y) + \frac{2}{\lambda^2} \frac{(x - y) \cdot y_j}{\lambda^2} k(x, y) \right)
\]

\[
= \sum_{j=1}^{d} \left( \frac{1}{\lambda} \frac{x - y}{\lambda} k(x, y) + \frac{2}{\lambda^2} \frac{(x - y) \cdot y_j}{\lambda^2} k(x, y) \right)
\]

\[
= k(x, y) \left( \frac{4\lambda^2 (x - y) \cdot y}{\lambda^2 (1 + |x|^2)} + \frac{2\alpha (x - y) \cdot y}{\lambda^2 (1 + |x|^2)} \right) = \frac{4\lambda^2 (x - y) \cdot y}{\lambda^2 (1 + |x|^2)} + \frac{2\alpha (x - y) \cdot y}{\lambda^2 (1 + |x|^2)} + \frac{d}{\lambda} - \frac{(x - y) \cdot (x - y)}{\lambda^2}.
\]
Product of Kernels  Finally, some of our examples will also use products of well-known kernels. Consider the kernel
\[ k(x, y) = \prod_{j=1}^{d} k_j(x_j, y_j). \]

The derivatives of this kernel can be expressed in terms of the components of the product and their derivatives as follows:
\[
\nabla_x k(x, y) = \left( \frac{\partial k_1(x, y_1)}{\partial x_1}, \ldots, \frac{\partial k_d(x, y_d)}{\partial x_d} \right) \prod_{j \neq d} k_j(x_j, y_j)
\]
\[
\nabla_y k(x, y) = \left( \frac{\partial k_1(x_1, y)}{\partial y_1}, \ldots, \frac{\partial k_d(x_d, y_d)}{\partial y_d} \right) \prod_{j \neq d} k_j(x_j, y_j)
\]
\[
\nabla_y \cdot \nabla_x k(x, y) = \sum_{j=1}^{d} \frac{\partial^2 k_j(x, y)}{\partial y_j \partial x_j} \prod_{i \neq j} k_i(x_i, y_i)
\]

D.2. Hyper-parameters Selection  Most kernels (whether scalar- or matrix-valued) will have hyperparameters which we will have to select. For example, the squared-exponential kernel will often have a lengthscale or amplitude parameter, and these will have a significant impact on the performance.

We propose to select kernel hyperparameters through a marginal likelihood objective by noticing the equivalence between the optimal vv-CV based on the objective in (8) and the posterior mean of a zero-mean Gaussian process model with covariance matrix \( K_0(x, y) \); see (Oates et al., 2017) for a discussion in the sv-CV case. Unfortunately, computing the marginal likelihood in the general case can be prohibitively expensive due to the need to take inverses of large kernel matrices; the exact issue we were attempting to avoid through the use of the stochastic optimisation approaches. For simplicity, we instead maximise the marginal likelihood corresponding to \( B = I_T \):

\[
\nu^* := \arg \max_\nu -\frac{1}{2} \sum_{t=1}^{T} \left( \sum_{i,j=1}^{n_t} f_t(x_{ij}) (K_{\Pi_t}(\nu) + \lambda M_i)_{ij}^{-1} f_t(x_{ij}) + \log \det[K_{\Pi_t}(\nu) + \lambda M_i] \right).
\]

where \( K_{\Pi_t}(\nu) \) is a matrix with entries \( K_{\Pi_t}(\nu)_{ij} = k_t(x_{ij}, x_{ij}; \nu) \) where \( k_t \) is a Stein reproducing kernel of the form in (3) specialised to \( \Pi_t \) which has hyperparameters given by some vector \( \nu \). This form is not optimal when \( B \neq I_T \), but we found that it tend to perform well in our numerical experiments. The regularisation parameter \( \lambda \) can also be selected through the marginal likelihood. However, in practice we are in an interpolation setting and therefore choose \( \lambda \) as small as possible whilst still being large enough to guarantee numerically stable computation of the matrix inverses above.

D.3. Convex Optimisation for Estimating \( B \)  As discussed in Section 4, estimating the matrix \( B \) for a separable kernel from data leads to a non-convex optimisation problem. Thankfully, we can approximate the optimum using a sequence of convex problems by extending the work of Dinuzzo et al. (2011); Ciliberto et al. (2015) together with Theorem 4.1 above. For this, we will require that the kernel \( K_0 \) is separable, and shall thus restrict ourselves to the case where we have a single target distribution (i.e. special case II).

**Theorem D.1.** Suppose that \( \Pi_t = \Pi \) for \( t \in [T] \) and \( K(x, y) = Bk(x, y) \) so that \( K_0(x, y) = Bk_0(x, y) \) where \( k_0 \) is defined in (3). Then the following objective is convex in \( (\theta, \beta, B) \) for any value of \( \delta > 0 \):

\[
I^{\nu}_m(\theta, \beta, B) = J_m(\theta, \beta, I_T) + \lambda \sum_{t,t'=1}^{T} \sum_{j=1}^{m_t} \sum_{j'=1}^{m_{t'}} \text{Tr} \left[ B^\dagger \left( k_0(x_{ij}, x_{t'j'}) \theta_{ij} \theta_{t'j'}^\top + \delta^2 I_T \right) \right] + \|B\|^2,
\]

and for each \( \beta \) and any sequence \( \delta_t \to 0 \), the associated sequence of minimisers \( (\theta_t, B_t) \) converges to \( (\theta_*, B_*) \) s.t., \( (\theta_*, B_*) \) minimises the objective in (10).

**Proof.** Since the kernel \( K_0 \) is separable, the objective (10) may be written in the form of Ciliberto et al. (2015, Problem (Q)). Has shown therein, \( \sum_{t,t'=1}^{T} \sum_{j=1}^{m_t} \sum_{j'=1}^{m_{t'}} \text{Tr} \left[ B^\dagger \left( k_0(x_{ij}, x_{t'j'}) \theta_{ij} \theta_{t'j'}^\top \right) \right] \) is jointly convex in \( B \) and \( \theta \), and since the first term in \( I^{\nu}_m(\theta, \beta, B) \) is convex in \( \beta \) and \( \theta \) jointly, \( I^{\nu}_m(\theta, \beta, B) \) is jointly convex in \( (\theta, B, \beta) \). Moreover, by Theorem 3.1 & 3.3 in (Ciliberto et al., 2015), when \( \delta \to 0 \), \( (\theta, B) \) converges in Frobenius norm to \( (\theta_*, B_*) \), where \( (\theta_*, B_*) \) a minimiser of (10), where \( B_\dagger \) denotes the pseudo-inverse of \( B_* \).

This theorem could therefore be used to construct an approach based on convex optimisation algorithms which are used iteratively for a decreasing sequence of penalisation parameters in order to converge to an optimum approaching the global optimum. However, this approach is limited to the case where all distributions are identical, and is hence not as widely applicable as Algorithm 1.
E. Additional Details for the Experimental Study

This last Appendix provides additional experiments including: an illustration plot of matrix-valued Stein reproducing kernel in Appendix E.1; a synthetic example from (South et al., 2022b) when the Stein kernel matches the smoothness of integrands in Appendix E.2; extra experiments for physical modelling of waterflow when having unbalanced datasets in Appendix E.4.2.

Meanwhile, additional details of our numerical experiments in Section 5 of the main paper are provided: multifidelity univariate step functions in Appendix E.3; multifidelity modelling of waterflow in Appendix E.4, model evidence for dynamic systems in Appendix E.5 and Bayesian inference of Lotka-Volterra system in Appendix E.6.

E.1. Illustration of Matrix-valued Stein Kernels

An illustration of matrix-valued Stein kernels $K_0$ is demonstrated in Figure 3 for the case $T = 2$. As observed, the choice of kernel $k$ can have significant impacts on $K_0$. Moreover, $K_0$ possesses a well-known property of Stein kernels: even when $k$ is translation-invariant (see the top row) this may not be the case for $K_0$. This is due to the fact that $K_0$ depends on $l$. Finally, we can also observe that the two outputs of $1^T K_0(x, y)$ are correlated, a property which will be key when it comes to vv-CVs.

![Matrix-valued Stein reproducing kernel](image)

Figure 3. Illustration of a separable mv-kernel $K_0$ for $T = 2$ through projections with $\Pi = (1, 1)$. Here, $\Pi_1 = \mathcal{N}(0, 1), \Pi_2 = \mathcal{N}(0, 1.25), B_{11} = B_{22} = 1$ and $B_{12} = B_{21} = 0.1$. The first row corresponds to taking $k$ to be a squared-exponential kernel, whereas the second and third row correspond to taking a polynomial kernel $k(x, y) = (x^T y + 1)^l$ with $l = 1$ and $l = 2$ respectively.

E.2. Additional Experiment: A Synthetic Example

Here is a synthetic example selected from (South et al., 2022b) (denoted $f_2$), and to make the problem fit into our framework we introduced another similar integrand (denoted $f_1$):

$$f_1(x) = 1.5 + x + 1.5x^2 + 1.75 \sin(\pi x) \exp(-x^2),$$
$$f_2(x) = 1 + x + x^2 + \sin(\pi x) \exp(-x^2).$$

For this problem, we trained all CVs through stochastic optimisation and use $m = (50, 50)$ MC samples. This synthetic example was originally used by (South et al., 2022b) to show one of the drawbacks of kernel-based CVs, namely that the fitted CV will usually tend to $\beta$ in parts of the domain where we do not have any function evaluations. This phenomenon
Vector-Valued Control Variates can be observed on the red lines in Figure 4 (left and center) which gives a CV based on a squared-exponential kernel. This behaviour is clearly one of the biggest drawbacks of existing kernel-based approaches. However, the blue curve, representing a kernel-based vv-CV with separable kernel where $B$ was inferred through optimisation, partially overcomes this issue by using evaluations of both integrands, hence clearly demonstrating potential advantages of sharing function values across integration tasks.

The right-most plot in Figure 4 presents several box plots for the sum of squared errors for each integration problem calculated over 100 repetitions of the experiment. The different box plots show the impact of the difference in $\Pi_1$ and $\Pi_2$. As we observed, vv-CVs tend to outperform CVs, although this difference in performance is more stark when $\Pi_2$ has a larger tail than $\Pi_1$. This reinforces the previous point, since a more disperse $\Pi_2$ means that the second integrand will be evaluated more often at more extreme areas of the domain, which will help obtain a better vv-CV by improving the fit at the tails of the distribution.

In this experiment, the choice of $k$ as a squared-exponential kernel was motivated by the fact that this makes $k_0$ infinitely differentiable, and hence matching the smoothness of both $f_1$ and $f_2$.

The experiment was replicated 100 times for all methods. The exact details of the implementation are as follows.

• CV
  - Sample size: 50.
  - Hyper-parameter tuning: batch size 5; learning rate 0.05; total number of epochs 30.
  - Base kernel: squared exponential kernel
  - Optimisation: $\lambda = 0.001$; batch size is 5; learning rate is 0.001; total number of epochs 400.

• vv-CV (estimated $B$)
  - Sample size: (50, 50) from ($\Pi_1$, $\Pi_2$) for ($f_1$, $f_2$).
  - Hyper-parameter tuning: batch size 5 (10 in total for ($f_1$, $f_2$)); learning rate 0.05; total number of epochs 30.
  - Base kernel: squared exponential kernel
  - Optimisation: $B^{(0)}$ is initialized at the identity matrix $I_2$. $\lambda = 0.001$; batch size is 5 (10 in total for ($f_1$, $f_2$)); learning rate is 0.001; total number of epochs 400.

E.3. Experimental details of Multi-fidelity Univariate Step Functions

The experiment is replicated 100 times for all methods. Details of their implementation is given below:
Vector-Valued Control Variates

Table 4. Prior Distributions for the inputs of the Borehole function.

| Random variable | Distributions                  | Random variable | Distributions                  |
|-----------------|--------------------------------|-----------------|--------------------------------|
| $r_w$           | Normal$(0.1, 0.0161812^2)$     | $r$             | Normal$(100, 0.01)$           |
| $T_u$           | Normal$(89335, 20)$            | $T_l$           | Normal$(89.55, 1)$           |
| $H_u$           | Normal$(1050, 1)$              | $H_l$           | Normal$(760, 1)$              |
| $L$             | Normal$(1400, 10)$             | $K_w$           | Normal$(10950, 30)$           |

- Squared-exponential kernel
  - CV
    * Sample size: 40.
    * Base kernel: squared exponential kernel.
    * Hyper-parameter tuning: batch size is 10; learning rate 0.02; total number of epochs 15.
    * Optimisation: $\lambda = 1e - 5$; batch size is 10; learning rate is $3e - 4$; total number of epochs 400.
  - vvCV (estimated B/fixed B)
    * Sample size: $(40, 40)$ from $(\text{Normal}(0, 1), \text{Normal}(0, 1))$ for $(f_L, f_H)$.
    * Hyper-parameter tuning: batch size is 5 (10 in total for $(f_L, f_H)$); learning rate 0.02; total number of epochs 15.
    * Base kernel: squared exponential kernel.
    * Optimisation: When $B$ is fixed, we set $B_{11} = B_{22} = 0.5, B_{12} = B_{21} = 0.01$; otherwise, $B^{(0)}$ is initialized at the identity matrix $I_2$, $\lambda = 1e - 5$; batch size is 5 (10 in total for $(f_L, f_H)$); learning rate is $3e - 4$; total number of epochs 400.

- First-order polynomial kernel
  - CV
    * Sample size: 40.
    * Base kernel: first order polynomial kernel.
    * Optimisation: $\lambda = 10^{-5}$; batch size is 10; learning rate is $3 \times 10^{-4}$; total number of epochs 400.
  - vv-CV (estimating B/fixed B)
    * Sample size: $(40, 40)$ from $(\text{Normal}(0, 1), \text{Normal}(0, 1))$ for $(f_L, f_H)$.
    * Base kernel: first order polynomial kernel.
    * Optimisation: When $B$ is fixed, we set $B_{11} = B_{22} = 0.5, B_{12} = B_{21} = 0.01$; otherwise, $B^{(0)}$ is initialized at the identity matrix $I_2$, $\lambda = 10^{-5}$; batch size is 5 (10 in total for $(f_L, f_H)$); learning rate is $3 \times 10^{-4}$; total number of epochs 400.

The empirical computational cost for all tasks is as follows. Scalar-valued CVs take approximately 2.4 seconds for either choice of kernels; vv-CVs with fixed $B$ take around 3.3 seconds with a squared-exponential kernel or around 3.1 seconds with a 1st order polynomial kernel; vv-CVs with estimated $B$ take around 6.6 seconds with a squared-exponential kernel or around 6.2 seconds with a 1st order polynomial kernel.

E.4. Experimental Details of the Physical Modelling (Borehole) of Waterflow

In this section, we provide details on the Borehole example from the main paper, and provide complementary experiments. The distributions with respect to which the integral is taken is an eight-dimensional Gaussian with independent marginals provided in Table 4. The low-fidelity model and high-fidelity model of water flow (Xiong et al., 2013) is given by,

\[
\begin{align*}
  f_L(x) &= \frac{5T_\omega(H_u - H_l)}{\log\left(\frac{T_\omega}{T_l}\right)\left(1 + \frac{2\Delta L}{\log\left(\frac{T_\omega}{T_l}\right)^2 K_w + \frac{2\lambda}{\Delta T}}\right)}, \\
  f_H(x) &= \frac{2\pi T_\omega(H_u - H_l)}{\log\left(\frac{T_\omega}{T_l}\right)\left(1 + \frac{2\Delta L}{\log\left(\frac{T_\omega}{T_l}\right)^2 K_w + \frac{2\lambda}{\Delta T}}\right)},
\end{align*}
\]

where $x = (r_w, r, T_u, T_l, H_u, H_l, L, K_w)$. 

23
E.4.1. Experiment in the main text: Balanced vv-CVs

The number of replications is 100 for all methods. Details of their implementation is given below:

- **Base kernel**: Instead of using \( k(x, x') = \exp(-\|x - x'\|^2/2\nu) \) with \( l > 0 \) which implicitly assumes that the length-scales are identical in all directions, we now allow that each dimension can have its own length-scale. That is,

\[
k(x, x') := \prod_{j=1}^d k_j(x_j, x'_j) \quad \text{where} \quad k_j(x_j, x'_j) = \exp\left(-\frac{(x_j - x'_j)^2}{2\nu_j}\right).
\]

Each of the components has its own length-scale \( \nu_j > 0 \) to be determined.

- Since \( \pi(x) = \prod_{j=1}^d \pi_j(x_j) \), the score function is \( \nabla_x \log \pi(x) = \left(\frac{\partial \log \pi_1(x)}{\partial x_1}, \ldots, \frac{\partial \log \pi_d(x)}{\partial x_d}\right)^\top \).

- **Hyper-parameter tuning**: batch size 5 (10 in total for \((f_L, f_H)\)); learning rate of tuning 0.05; epochs of tuning 20.

- Optimisation (estimated B/pre-fixing B): When \( B \) is fixed, we set \( B_{11} = B_{22} = 5e - 4, B_{12} = B_{21} = 5e - 5 \); otherwise, \( B^{(0)} \) is initialized at \( 1e - 5 \times I_2, \lambda = 1e - 5 \); batch size 5 (10 in total for \((f_L, f_H)\)); learning rate for the cases when sample sizes are \((10, 20, 50, 100, 150)\) are \((0.09, 0.06, 0.012, 0.0035, 0.002)\), respectively.

The empirical computational cost (measured in seconds) of this example is: when \( m = (10, 10) \), it takes CF, vv-CVs with fixed B and vv-CVs with estimated B around 0.03, 1.2 and 2.6 seconds, respectively; when \( m = (20, 20) \), it takes CF, vv-CVs with fixed B and vv-CVs with estimated B around 0.1, 3 and 5 seconds, respectively; when \( m = (50, 50) \), it takes CF, vv-CVs with fixed B and vv-CVs with estimated B around 0.7, 7.5 and 13.5 seconds, respectively; when \( m = (100, 100) \), it takes CF, vv-CVs with fixed B and vv-CVs with estimated B around 2.7, 17 and 27.6 seconds, respectively; when \( m = (150, 150) \), it takes CF, vv-CVs with fixed B and vv-CVs with estimated B around 6, 29 and 49 seconds, respectively.

E.4.2. Additional experiment: unbalanced data-sets for physical modelling of water flow

In Figure 5, we present the results of vv-CVs when the sample sizes are unbalanced; that is, we have a different number of samples for the low-fidelity and high-fidelity models. The exact setup is given below, and we replicated the experiment 100 times.

- **Sample size**: \( m_H \) is fixed to be 20, while \( m_L \in \{20, 40, 60\} \).

- **Base kernel**: product of squared exponential kernels. \( k(x, x') := \prod_{j=1}^d k_j(x_j, x'_j) \), where each \( k_j(x_j, x'_j) = \exp(- (x_j - x'_j)^2/2\nu_j) \) has its own length-scale \( \nu_j > 0 \) to be determined.

- **Hyperparameter tuning**: batch size of tuning 5 (10 in total for \((f_L, f_H)\)); learning rate of tuning is 0.05; epochs of tuning is 20.

- Optimisation (estimated B/pre-fixing B): When \( B \) is fixed, we set \( B_{11} = B_{22} = 5 \times 10^{-4}, B_{12} = B_{21} = 5 \times 10^{-5} \); otherwise, \( B^{(0)} \) is initialized at \( 10^{-5} \times I_2, \lambda = 10^{-5} \); learning rate is \((0.06, 0.04, 0.02)\) when \( m_L \in \{20, 40, 60\} \), respectively.

Interestingly, we notice that not much is gained when increasing the number of samples for the low-fidelity model. In fact, in the case of a fixed \( B \), the performance tends to decrease with a larger \( m_L \). This is likely due to the “negative transfer” phenomenon which is well-known in machine learning. This phenomenon can occur when two tasks are not similar enough to provide any gains in accuracy. In this case, there is clearly no advantage in using a larger \( m_L \) since this increases computational cost and does not provide any gains in accuracy.

E.5. Experimental Details of the Computation of the Model Evidence through Thermodynamic Integration

To implement our vv-CVs, we need to derive the corresponding score functions. For a power posterior, the score function is of the form:

\[
\nabla_\theta \log p(\theta|y, t) = t \nabla_\theta \log p(y|\theta) + \nabla_\theta \log p(\theta)
\]
Vector-Valued Control Variates

Figure 5. Performance of vv-CVs with unbalanced sample sizes. Here we fix $m_H = 20$, and changing $m_L$ to be 20, 40, 60. Each experiment is repeated 100 times.

where $\nabla_\theta \log p(\theta)$ is the score function corresponding to the prior. In our case, the prior is a log-normal distribution $\log \theta \sim \mathcal{N}(\mu, \sigma^2)$ (where $\sigma = 0.25$), and its score function is given by:

$$\nabla_\theta \log p(\theta) = -\frac{1}{\theta} - \frac{\log \theta - \mu}{\sigma^2}.$$ 

The score functions for all temperatures are plotted in Figure 6; as observed, temperatures consecutive score functions are very similar to one another.

In order to keep the computational cost manageable, we split the $T = 62$ integration problems into groups of closely related problems. In particular, we jointly estimate the means in terms of 4 consecutive temperatures on the ladder ( group 1 is $\mu_1, \mu_2, \mu_3, \mu_4$, group 2 is $\mu_5, \mu_6, \mu_7, \mu_8$, etc...). Since 31 is not divisible by 4, our last group consists of three means $\mu_{29}, \mu_{30}, \mu_{31}$. Then, the same approach is taken to create groups of 4 (or 3 for the last group) variances.

The number of replications was 20 for each method. Details are given below:

- CV
  * Base kernel: Preconditioned squared-exponential kernel (Oates et al., 2017).
  * Hyperparameter tuning: we use the values $(0.1, 3)$ in (Oates et al., 2017).
  * Optimisation: $\lambda = 10^{-3}$; batch size is 5; total number of epochs is 400.

- vv-CV(estimated B)
  * Base kernel: Preconditioned squared-exponential kernel (Oates et al., 2017).
  * Hyperparameter tuning: we use the values $(0.1, 3)$ in (Oates et al., 2017).
  * Optimisation: $\lambda = 10^{-3}$; batch size is 5; learning rate is 0.01; number of epochs is 400.

E.6. Experimental Details of the Lotka-Volterra System

We implement log-exp transform on model parameters and avoid constrained parameters on the ODE directly. Lotka—Volterra system can be re-parameterized as,

$$\frac{dv_1(s)}{ds} = \tilde{\alpha} v_1(s) - \tilde{\beta} v_1(s)v_2(s),$$

$$\frac{dv_2(s)}{ds} = \tilde{\delta} v_1(s)v_2(s) - \tilde{\gamma} v_2(s),$$
Figure 6. Score functions corresponding to the power posteriors at different temperatures on the temperature ladder.
where

\[ \tilde{\alpha} = \exp(\alpha), \tilde{\beta} = \exp(\beta), \]
\[ \tilde{\delta} = \exp(\delta), \tilde{\gamma} = \exp(\gamma), \]

where \( v_1 \) and \( v_2 \) represents the number of preys and predators, respectively.

The model is,

\[ y_{10} \sim \text{Log-Normal}(\log \tilde{v}_1(0), \tilde{\sigma}_{y_1}) \]
\[ y_{20} \sim \text{Log-Normal}(\log \tilde{v}_2(0), \tilde{\sigma}_{y_2}) \]
\[ y_{1s} \sim \text{Log-Normal}(\log v_1(s), \tilde{\sigma}_{y_1}) \]
\[ y_{2s} \sim \text{Log-Normal}(\log v_2(s), \tilde{\sigma}_{y_2}) \]

where

\[ \tilde{v}_1(0) := \exp(v_1(0)), \tilde{v}_2(0) := v_2(0) \]
\[ \tilde{\sigma}_{y_1} := \exp(\sigma_{y_1}), \tilde{\sigma}_{y_2} = \exp(\sigma_{y_2}). \]

By doing so, \( x := (\alpha, \beta, \delta, \gamma, v_1(0), v_2(0), \sigma_x, \sigma_y)^\top \) can be defined on the whole \( \mathbb{R}^8 \) as the exponential transformation will make sure they larger than zero, and thus can be assigned priors on \( \mathbb{R}^8 \), e.g., Gaussian. As a result, the expectations associated with \( \pi(x) \) are defined on \( \mathbb{R}^8 \) and Stan will return the scores of these parameters directly as these 8 parameters themselves are unconstrained through manually reparameterisation.

Priors are,

\[ \alpha, \gamma \sim \text{Normal}(0, 0.5^2) \]
\[ \beta, \delta \sim \text{Normal}(-3, 0.5^2) \]
\[ \sigma_x, \sigma_y \sim \text{Normal}(-1, 1^2) \]
\[ v_1(0), v_2(0) \sim \text{Normal}(\log 10, 1^2) \]

The fitting for predators \( y_{1s} \) and \( v_1(s) \) at points \( s_1, \ldots, s_m \) are shown in Figure 7. The fitting for predators \( y_{2s} \) and \( v_2(s) \) at points \( s_1, \ldots, s_m \) are shown in Figure 8.

![Figure 7. Bayesian inference of abundance of preys of Lotka-Volterra system. Dots are observations; lines are the posterior means while dotted lines are the corresponding 95\% credible intervals. Tasks are chosen in the area between the two vertical red lines.](image-url)
Tasks $\Pi[f_t]$ at time $s'_1, \ldots, s'_T$ (the base unit is 1 year):

* $T = 2$: 1913.1, 1913.2;
* $T = 5$: 1912.1, 1912.2, 1912.4, 1912.6, 1912.8;
* $T = 10$: 1912.1, 1912.2, 1912.4, 1912.6, 1912.8, 1913.1, 1913.2, 1913.4, 1913.6, 1913.8.

Base kernel: same one as in E.4: product of squared-exponential kernels.

Hyperparameter tuning: batch size is 10; learning rate 0.01; total number of epochs 10.

Optimisation: $\lambda = 10^{-5}$; batch size 10; learning rate $10^{-3}$; total number of epochs 400.

The empirical computational cost (measured in seconds) of this example is: when $T = 2$, it takes CF, scalar-valued CVs, vv-CVs with fixed $B$ and vv-CVs with estimated $B$ around 67, 80, 150 and 159 seconds respectively for all $T$ tasks; when $T = 5$, it takes CF, scalar-valued CVs, vv-CVs with fixed $B$ and vv-CVs with estimated $B$ around 170, 200, 854 and 882 seconds respectively for all $T$ tasks; when $T = 10$, it takes CF, scalar-valued CVs, vv-CVs with fixed $B$ and vv-CVs with estimated $B$ around 340, 400, 3435 and 3469 seconds respectively for all $T$ tasks.

### E.6.1. ADDITION EXPERIMENTS FOR BAYESIAN INFERENCE OF ABUNDANCE OF PREYS OF LOTKA-VOLTERA SYSTEM

We present additional experiments in Table 5 under the same settings as those in the above section. We consider to estimate $\Pi[f_t]$ at time $s'_1, \ldots, s'_T$ (the base unit is 1 year),

* $T = 2$: 1915.1, 1915.2;
* $T = 5$: 1915.1, 1915.2, 1915.4, 1915.6, 1915.8;
* $T = 10$: 1914.1, 1914.2, 1914.4, 1914.6, 1914.8, 1915.1, 1915.2, 1915.4, 1915.6, 1915.8.

#### Table 5. Additional Experiments for the Bayesian inference of the Lotka-Volterra system: Sum of mean absolute error of each task.

| $T$ | $m$ | vv-CV- Estimated B | vv-CV-Fixed B | CF | MC |
|-----|-----|-------------------|---------------|----|----|
| 2   | 500 | 0.169             | 0.144         | 0.242 | 0.275 |
| 5   | 500 | 0.322             | 0.245         | 1.246 | 0.661 |
| 10  | 500 | 0.916             | 0.792         | 5.835 | 1.797 |