Double Loop Monte Carlo Estimator with Importance Sampling for McKean-Vlasov Stochastic Differential Equation

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Abstract

This paper investigates Monte Carlo methods to estimate probabilities of rare events associated with solutions to the $d$-dimensional McKean-Vlasov stochastic differential equation. The equation is usually approximated using a stochastic interacting $P$-particle system, a set of $P$ coupled $d$-dimensional stochastic differential equations (SDEs). Importance sampling (IS) is a common technique to reduce high relative variance of Monte Carlo estimators of rare event probabilities. In the SDE context, optimal measure change is derived using stochastic optimal control theory to minimize estimator variance, which when applied to stochastic particle systems yields a $P \times d$-dimensional partial differential control equation, which is cumbersome to solve. The work in [15] circumvented this problem by a decoupling approach, producing a $d$-dimensional control PDE. Based on the decoupling approach, we develop a computationally efficient double loop Monte Carlo (DLMC) estimator. We offer a systematic approach to our DLMC estimator by providing a comprehensive error and work analysis and formulating optimal computational complexity. Subsequently, we propose an adaptive DLMC method combined with IS to estimate rare event probabilities, significantly reducing relative variance and computational runtimes required to achieve a given relative tolerance compared with standard Monte Carlo estimators without IS. The proposed estimator has $O(TOL^{-4})$ computational complexity with significantly reduced constant. Numerical experiments, which are performed on the Kuramoto model from statistical physics, show substantial computational gains achieved by our estimator.

Keywords: McKean-Vlasov stochastic differential equation, importance sampling, rare events, stochastic optimal control, decoupling approach, double loop Monte Carlo.

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1 Introduction

This paper investigates Monte Carlo (MC) methods to estimate rare event probabilities associated with solutions to the McKean-Vlasov stochastic differential equation (MV-SDE) [32]. We develop a computationally efficient MC estimator for $E[G(X(T))]$, where $G : \mathbb{R}^d \to \mathbb{R}$ is a given observable and $\{X(t) \in \mathbb{R}^d : t \in [0, T]\}$ is the solution to the MV-SDE up to finite terminal time $T$. MV-SDE was introduced in the sixties and has attracted considerable research interest. It is a special class of stochastic differential equations (SDEs) whose drift and diffusion coefficients depend on the law of the solution itself. Such SDEs arise from mean-field behaviour of stochastic interacting particle systems, commonly used to model various phenomena in pedestrian dynamics [18], collective animal behaviour [16], oscillator systems [1, 37], biological interactions [13], and financial mathematics [8]. There is a rich body of recent work regarding the existence and uniqueness of solutions to MV-SDE [19, 34], well-posedness of the associated Kolmogorov forward and backward PDEs [7, 9], and efficient numerical methods to simulate MV-SDE for certain classes of drift/diffusion coefficients [10, 14, 20, 39].

Due to the dependence of drift/diffusion on the law of the solution, the MV-SDE is often approximated using a stochastic $P$-particle system, i.e., a set of $P$ coupled $d$-dimensional SDEs. Under certain conditions, the stochastic particle system approaches the mean-field limit as the number of particles tends to infinity [38], commonly referred to as propagation of chaos. Time evolution of the particle system’s joint probability density is given by the $P \times d$-dimensional Fokker-Planck PDE, which quickly becomes infeasible to solve numerically. Hence, this work proposes MC methods and simulates approximate MV-SDE sample paths using Euler-Maruyama time-discretized stochastic particle system for bounded, Lipschitz continuous drift/diffusion coefficients [31]. MC methods using this numerical scheme have been investigated previously for smooth, non-rare observables [20], achieving $O(\text{TOL}^{-4})$ computational complexity for a prescribed error tolerance TOL. However, naïve MC methods become extremely expensive for rare events, due to the constant associated with the estimator’s computational complexity blowing up as the event becomes rarer [29].

We address the problem of estimating rare event probabilities up to relative error tolerances in the context of MV-SDEs. The importance sampling (IS) variance reduction technique [29] is crucial to overcome standard MC failure for rare event regimes. Recent studies have developed IS schemes using stochastic optimal control theory in various contexts, including stochastic reaction networks [3], and sums of independent random variables in communication system contexts [2]. In particular, several studies formulated connections between stochastic optimal control and IS for standard SDEs [23, 26, 41]. The derived optimal measure change, is often related to the solution of a Hamilton-Jacobi-Bellman (HJB) equation [27]. The curse of dimensionality, encountered in conventional numerical schemes that handle such PDEs, has been alleviated to some extent using model reduction techniques [24, 25] and neural network approaches [35].

In the MV-SDE context, drift/diffusion dependence on the law of the solution itself makes formulating the corresponding HJB control PDE challenging. Corresponding HJB PDE for stochastic particle systems would be $P \times d$-dimensional, and hence infeasible to solve numerically. This problem has been previously overcome using a decoupling approach in [15], which is the only other paper (to the best of our knowledge) that considers the
IS problem for MV-SDEs. They defined a modified, decoupled MV-SDE version where the drift/diffusion coefficients were computed using an empirical law estimated beforehand from the stochastic particle system. Thus, estimating the law is decoupled from measure changes, which are now only applied to the decoupled MV-SDE. Large deviations and the Pontryagin principle were then employed to obtain deterministic, time-dependent controls that minimize a proxy for the variance. The current paper improves on this idea by proposing a stochastic optimal control formulation to derive time and pathwise-dependent controls that minimize the IS estimator variance directly. We obtain optimal control for this SDE by solving $d$-dimensional control PDE alone, since the decoupled MV-SDE is a $d$-dimensional standard SDE for a given realization of the empirical law. Contributions from this paper include the following.

- We apply stochastic optimal control theory on the decoupled MV-SDE to derive a time and pathwise-dependent IS control that leads to a zero-variance MC estimator provided the observable does not change sign. Hence, we solve a low-dimensional control PDE using conventional finite difference schemes and obtain a control that provides considerable variance reduction.

- We introduce a double loop Monte Carlo (DLMC) estimator with IS based on the decoupling approach in MV-SDE context, since one needs to first estimate the MV-SDE law using a stochastic particle system and then define the decoupled MV-SDE given that estimated law. This is a development on the IS estimator based on the decoupling approach in [15].

- In contrast to [15], we provide estimates of bias and statistical errors for DLMC estimator and derive its optimal computational complexity. The proposed DLMC estimator achieves the same $O(TOL^{-4})$ computational complexity as for non-rare observables [20]; and when combined with the proposed IS scheme substantially reduces the associated constant, allowing feasible estimation of rare event probabilities in the MV-SDE context.

The remainder of this paper is structured as follows. Section 2 introduces MV-SDE, associated notation, and motivates MC methods to estimate expectations associated with its solution. We also review optimal measure change for importance sampling using stochastic optimal control theory for standard SDEs. Section 3 introduces the specific problem in hand and discusses the challenges to implement IS in the MV-SDE context. Section 4 introduces the proposed decoupling approach and derives an optimal control for the decoupled MV-SDE. We also define the DLMC estimator; provide a detailed error and work analysis; and formulate an optimal complexity theorem and DLMC algorithm to adaptively choose optimal parameters for feasible estimation of rare event probabilities. Section 5 applies the proposed approach to the Kuramoto model from statistical physics, and provides numerical evidence for the theoretical results. Finally Section 6 summarizes and concludes the paper, and discusses possible future research directions.
2 Preliminaries

2.1 The McKean-Vlasov stochastic differential equation

Consider the probability space \( \{ \Omega, \mathcal{F}, \{ \mathcal{F}_t \}_{t \geq 0}, P \} \), where \( \mathcal{F}_t \) is the filtration of a standard Wiener path \( \{ W(t) : t \in [0, T] \} \). For functions \( b : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^d \), \( \sigma : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^{d \times d} \), \( \kappa_1 : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \) and \( \kappa_2 : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \), we consider the following Itô SDE for stochastic process \( X : [0, T] \times \Omega \rightarrow \mathbb{R}^d \):

\[
\begin{align*}
\text{d}X(t) &= b\left(X(t), \int_{\mathbb{R}^d} \kappa_1(X(t), x) \mu_t(\text{d}x)\right) \text{d}t \\
&\quad + \sigma\left(X(t), \int_{\mathbb{R}^d} \kappa_2(X(t), x) \mu_t(\text{d}x)\right) \text{d}W(t), \quad t > 0 \tag{1}
\end{align*}
\]

where \( W : [0, T] \times \Omega \rightarrow \mathbb{R}^d \) is a standard \( d \)-dimensional Wiener process with mutually independent components; \( \mu_t \in \mathcal{P}(\mathbb{R}^d) \) is the distribution of \( X(t) \), where \( \mathcal{P}(\mathbb{R}^d) \) is the probability measure space over \( \mathbb{R}^d \); \( x_0 \in \mathbb{R}^d \) is a random initial state with distribution \( \mu_0 \in \mathcal{P}(\mathbb{R}^d) \).

Functions \( b(\cdot) \) and \( \sigma(\cdot) \) are commonly called drift and diffusion functions/coefficients, respectively. Solution existence and uniqueness for (1) can be proved under certain differentiability and boundedness conditions on \( b, \sigma, \kappa_1, \kappa_2 \) \([11, 19, 21, 34, 38]\).

Time evolution for \( \mu_t \) is given by the deterministic multi-dimensional Fokker-Planck PDE,

\[
\begin{align*}
\frac{\partial \mu(s, x; t, y)}{\partial s} &- \sum_{i=1}^{d} \frac{\partial}{\partial x_i} \left( b_i \left( x, \int_{\mathbb{R}^d} \kappa_1(x, z) \mu(s, z; t, y) \text{d}z \right) \mu(s, x; t, y) \right) \\
&\quad + \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{d} \sigma_{ik} \sigma_{jk} \left( x, \int_{\mathbb{R}^d} \kappa_2(x, z) \mu(s, z; t, y) \text{d}z \right) \\
&\quad \mu(s, x; t, y) = 0, \quad (s, x) \in (t, \infty) \times \mathbb{R}^d \tag{2}
\end{align*}
\]

where \( \mu(s, x; t, y) \) is the conditional distribution of \( X(s) \) given that \( X(t) = y \), and \( \delta_y(\cdot) \) is the Dirac measure at point \( y \). \([2]\) is a non-linear PDE due to dependency on \( b \) and \( \sigma \) on \( \mu(s, x; t, y) \) itself. This is also an integral differential equation with non-local terms because drift and diffusion functions depend on an integral over the whole \( d \)-dimensional space with respect to \( \mu(s, x; t, y) \). Solving such a non-linear integral differential equation numerically up to high tolerance can be cumbersome, particularly in higher dimensions \((d \gg 1)\).

This motivates using strong approximations to MV-SDE \([1]\), obtained by solving a system of \( P \) exchangeable Itô SDEs, also known as an interacting stochastic particle system with pairwise interaction kernels comprising \( P \) particles \([38]\). For \( p = 1, \ldots, P \), \( X^P_p(t) \) solves
the SDE,

\[
\begin{align*}
\frac{dX_p^P(t)}{dt} &= \left( X_p^P(t), \frac{1}{P} \sum_{j=1}^P \kappa_1(X_p^P(t), X_j^P(t)) \right) dt \\
+ \sigma \left( X_p^P(t), \frac{1}{P} \sum_{j=1}^P \kappa_2(X_p^P(t), X_j^P(t)) \right) dW_p(t), \quad t > 0 \tag{3}
\end{align*}
\]

where \( \{(x_0)_p\}_{p=1}^P \) are independent and identically distributed (iid) random variables sampled from the initial distribution \( \mu_0 \); \( \{W_p(t)\}_{p=1}^P \) are mutually independent \( d \)-dimensional Wiener processes, also independent of \( \{(x_0)_p\}_{p=1}^P \). Equation (3) approximates the mean-field distribution \( \mu_t \) from (1) by an empirical distribution based on \( \{X_p^P(t)\}_{p=1}^P \) particles,

\[
\mu_t(dx) \approx \mu_t^P(dx) = \frac{1}{P} \sum_{j=1}^P \delta_{X_j^P(t)}(dx),
\]

where particles \( \{X_p^P(t)\}_{p=1}^P \) are identically distributed, but not mutually independent due to pairwise interaction kernels in the drift and diffusion coefficients.

Strong convergence for the particle system has been proven for a broad class of drift and diffusion coefficients [5,6,19,33]. Given the stochastic interacting particle system (3), we can derive the PDE governing evolution of joint probability density function of \( \{X_p^P(t)\}_{p=1}^P \) using the multi-dimensional Fokker-Planck equation. For simplicity, we only include the one-dimensional case \((d = 1)\). Let \( \tilde{\mu}(t, x) \) be the joint probability density function, where \( x = [x_1, \ldots, x_P] \in \mathbb{R}^P \). Then,

\[
- \frac{\partial \tilde{\mu}(s, x; t, y)}{\partial s} - \sum_{i=1}^P \frac{\partial}{\partial x_i} \left( b \left( x_i, \frac{1}{P} \sum_{j=1}^P \kappa_1(x_i, x_j) \right) \tilde{\mu}(s, x; t, y) \right)
+ \sum_{i=1}^P \frac{1}{2} \frac{\partial^2}{\partial x_i^2} \left( \sigma^2 \left( x_i, \frac{1}{P} \sum_{j=1}^P \kappa_2(x_i, x_j) \right) \tilde{\mu}(s, x; t, y) \right) = 0, \quad (s, x) \in (t, \infty) \times \mathbb{R}^P \tag{5}
\]

where \( \tilde{\mu}(s, x; t, y) \) is the distribution of \( X^P(s) = [X^P_1(s), \ldots, X^P_P(s)] \), given that \( X^P(t) = y \).

Equation (5) is linear in \( \tilde{\mu}(t, x) \) and has no integral dependence, but it is \( P \)-dimensional in the \( d = 1 \) case and \( P \times d \)-dimensional in the general case. Thus, it is numerically infeasible to solve (5) using conventional numerical methods up to the required accuracy. This motivates using MC methods, which do not suffer from the curse of dimensionality.

2.1.1 Example: Fully Connected Kuramoto Model for Synchronized Oscillators

This study focuses on a simple, one-dimensional MV-SDE (1) called the Kuramoto model, which is commonly used to describe synchronisation in statistical physics, modelling the
behaviour of large sets of coupled oscillators as systems of $P$-fully connected, synchronised oscillators. It has widespread applications in chemical and biological systems [1], neuroscience [12], and oscillating flame dynamics [37].

Consider a system of $P$-oscillators with state $\{X^P_p(t)\}_{t \geq 0}$, $p = 1, \ldots, P$ at time $t$. Then, $X^P_p(t)$ satisfies the Itô SDE

\[
\begin{align*}
  dX^P_p(t) &= \left(\nu_p + \frac{1}{P} \sum_{q=1}^{P} \sin \left( X^P_p(t) - X^P_q(t) \right) \right) dt + \sigma dW^P_p(t), \quad t > 0. \\
  X^P_p(0) &= (x^0)_p \sim \mu_0 \in \mathcal{P}({\mathbb{R}}),
\end{align*}
\]

where $\{\nu_p\}_{p=1}^P$ are iid random variables sampled from a prescribed distribution; diffusion $\sigma \in \mathbb{R}$ is constant; $\{(x^0)_p\}_{p=1}^P$ are iid random variables sampled from a prescribed distribution $\mu_0$; $\{W^P_p(t)\}_{p=1}^P$ are mutually independent one-dimensional Wiener processes; and $\{\nu_p\}_{p=1}^P, \{(x^0)_p\}_{p=1}^P, \{W_p(t)\}_{p=1}^P$ are independent. This coupled particle system reaches the mean-field limit as the number of oscillators tends to infinity. In this limit, each particle behaves according to the following MV-SDE,

\[
\begin{align*}
  dX(t) &= \left( \nu + \int_{\mathbb{R}} \sin(X(t) - x) \mu_t(dx) \right) dt + \sigma dW(t), \quad t > 0. \\
  X(0) &= x_0 \sim \mu_0 \in \mathcal{P}(\mathbb{R}),
\end{align*}
\]

where $X(t)$ denotes the state of each particle; $\nu$ is a random variable sampled from some prescribed distribution; and $\mu_t$ is the distribution for $X(t)$ at time $t$. We use this example throughout this paper as a test case for the proposed MC algorithms.

### 2.2 Importance Sampling using Stochastic Optimal Control for SDEs

Before considering MV-SDEs, we develop a framework for an IS scheme that minimizes estimator variance using stochastic optimal control for standard SDEs. The authors in [23] approach the same optimal control problem through variational characterization of thermodynamic free energy; whereas the current study achieves the same results by posing the optimal IS problem as a stochastic optimal control problem, resulting in a time and pathwise-dependent control that minimizes the IS estimator variance.

Let $Y : [0, T] \times \Omega \to \mathbb{R}^d$ be the solution to the following standard Itô SDE,

\[
\begin{align*}
  dY(t) &= b(t,Y(t)) dt + \sigma(t,Y(t)) dW(t), \quad t \in (0, T], \\
  Y(0) &= y_0, \quad y_0 \in \mathbb{R}^d,
\end{align*}
\]

where $W : [0, T] \times \Omega \to \mathbb{R}^d$ is a standard $d$-dimensional Wiener process in probability space $\{\Omega, \mathcal{F}, P\}$ with mutually independent components. We are generally interested in estimating $\mathbb{E}[G(Y(T))]$ by MC for some scalar observable $G : \mathbb{R}^d \to \mathbb{R}$, and we wish to apply a measure change to (8) such that MC estimator variance is minimized.

Let us first perform a time-discrete measure change on the Euler-Maruyama discretization of (8). We extend this later into the time-continuous setting to obtain a time-continuous
control problem. Consider time discretization $0 = t_0 < t_1 < t_2 < \ldots < t_N = T$ for the $[0, T]$ time domain with $N$ uniform time steps. Hence, $t_n = n \times \Delta t, \quad n = 0, 1, \ldots, N$ and $\Delta t = T/N$. Let $Y^N$ be the time discretized version for state $Y$ corresponding to $[8]$. Then the Euler-Maruyama time discretization for the SDE can be expressed as

$$
\begin{cases}
Y^N(t_{n+1}) = Y^N(t_n) + b(t_n, Y^N(t_n)) \Delta t \\
\quad + \sigma(t_n, Y^N(t_n)) \sqrt{\Delta t} \epsilon_n, \quad \forall n = 0, \ldots, N - 1. \\
Y^N(t_0) = Y(0) = y_0,
\end{cases}
$$

(9)

where $\epsilon_n = \epsilon(t_n) \sim \mathcal{N}(0, I_d)$; and $I_d$ is the $d$-dimensional identity matrix.

For a given time step $n \in \{0, \ldots, N - 1\}$, we perform a mean-shift measure change

$$
\hat{\epsilon}_n = \sqrt{\Delta t} \zeta_n + \epsilon_n,
$$

(10)

where $\zeta_n = \zeta(t_n, Y^N(t_n)) \in \mathbb{R}^d$ is a $d$-dimensional control. Hence, the likelihood factor $L_n$ resulting from this mean-shift at time step $n$ is

$$
L_n(\hat{\epsilon}_n) = \exp \left\{ -\frac{1}{2} \| \hat{\epsilon}_n \|^2 \right\} \exp \left\{ \frac{1}{2} \| \epsilon_n - \sqrt{\Delta t} \zeta_n \|^2 \right\}
$$

$$
= \exp \left\{ \frac{1}{2} \Delta t \| \zeta_n \|^2 - \sqrt{\Delta t} \langle \hat{\epsilon}_n, \zeta_n \rangle \right\},
$$

(11)

where $\langle \cdot, \cdot \rangle$ is the Euclidean dot product between two vectors in $\mathbb{R}^d$; and $\| \cdot \|$ is the Euclidean norm for a vector in $\mathbb{R}^d$.

Substituting (10) in (11) and setting $L_n$ as a function of $\epsilon_n$, we get

$$
L_n(\epsilon_n) = \exp \left\{ -\frac{1}{2} \Delta t \| \zeta_n \|^2 - \sqrt{\Delta t} \langle \epsilon_n, \zeta_n \rangle \right\}.
$$

(12)

Thus, the likelihood over $N$ time steps is $\prod_{n=0}^{N-1} L_n(\epsilon_n)$, and hence, the quantity of interest can be expressed as

$$
\mathbb{E} \left[ G(Y^N(T)) \right] = \mathbb{E} \left[ G(Y^N(T)) \prod_{n=0}^{N-1} L_n(\epsilon_n) \right],
$$

(13)

where $Y^N$ is subject to

$$
\begin{align*}
Y^N(t_{n+1}) &= Y^N(t_n) + \left( b(t_n, Y^N(t_n)) + \sigma(t_n, Y^N(t_n)) \zeta(t_n, Y^N(t_n)) \right) \Delta t \\
&\quad + \sigma(t_n, Y^N(t_n)) \sqrt{\Delta t} \epsilon_n, \quad \forall n = 0, \ldots, N - 1 \\
Y^N(t_0) &= Y(0) = y_0.
\end{align*}
$$

(14)

Thus, our aim is to minimize MC estimator variance, and it is sufficient to minimize the estimator’s second moment, given such a minimum exists, since (13) is an unbiased estimator,

$$
\min_{\{\zeta_n\}_{n=1}^N} \mathbb{E} \left[ G^2(Y^N(T)) \prod_{n=0}^{N-1} L_n^2(\epsilon_n) | Y^N_T(0) = y_0 \right]
$$
\[
J_{t,x}(\zeta) = \mathbb{E}\left[ \exp\left\{-\int_t^{t+\delta} \|\zeta(s,Y_{\zeta}(s))\|^2 \, ds - 2 \int_t^{t+\delta} \langle \zeta(s,Y_{\zeta}(s)), dW(s) \rangle \right\} \right.
\]
\[
\cdot u(t+\delta, Y_{\zeta}(t+\delta)) \mid Y_{\zeta}(t) = x \right].
\]
Proof. See Appendix A. □

From Lemma 1, we can derive the PDE which solves for the value function (18) and subsequently the optimal control $\zeta(\cdot, \cdot)$.

**Theorem 1** (Optimal Control to Minimize Variance for Standard SDEs). Let $\{Y(t) : t \in [0, T]\}$ solve the SDE (8), and $\{Y_\zeta(t) : t \in [0, T]\}$ solve the controlled SDE (17), where $\zeta(t, x) : [t, T] \times \mathbb{R}^d \to \mathbb{R}^d$ is the control; and assume value function $u(t, x)$ defined in (18) is bounded, smooth, and non-zero throughout its domain. Then $u(t, x)$ satisfies the following PDE

$$
\begin{align*}
\frac{\partial u}{\partial t} + \langle b(t, x), \nabla u \rangle + \frac{1}{2} \nabla^2 u : (\sigma \sigma^T)(t, x) &+ \frac{1}{8} \sigma^T \nabla u(t, x) \nabla u(t, x) \sigma \sigma^T - \frac{1}{8} \sigma^T \nabla u(t, x) \sigma \sigma^T = 0, \\
(t, x) &\in [0, T) \times \mathbb{R}^d.
\end{align*}
$$

(21)

with optimal control which minimizes the second moment defined in (16),

$$
\zeta^*(t, x) = \frac{1}{2} \sigma^T(t, x) \nabla \log u(t, x),
$$

(22)

where $\nabla \cdot$ is the gradient vector; $\nabla^2 \cdot$ is the Laplacian matrix for a scalar function; and $\cdot : \cdot$ is the Frobenius inner product between two matrix-valued functions.

Proof. See Appendix B. □

We can obtain a HJB type PDE from (21) by considering the change of variable $u(t, x) = \exp\{-2\gamma(t, x)\}$, as shown in Corollary 1.

**Corollary 1** (Hamilton-Jacobi-Bellman PDE). Let $\{Y(t) : t \in [0, T]\}$ solve the SDE (8), and $\{Y_\zeta(t) : t \in [0, T]\}$ solve the controlled SDE (17), where $\zeta(t, x) : [t, T] \times \mathbb{R}^d \to \mathbb{R}^d$ is the control; and assume the value function $u(t, x)$ defined in (18) is bounded, smooth, and non-zero throughout its domain. Then $\gamma(t, x)$ satisfies the nonlinear HJB equation

$$
\begin{align*}
\frac{\partial \gamma}{\partial t} + \langle b(t, x), \nabla \gamma \rangle + \frac{1}{2} \nabla^2 \gamma : (\sigma \sigma^T)(t, x) &+ \frac{1}{8} \sigma^T \nabla \gamma(t, x) \nabla \gamma(t, x) \sigma \sigma^T - \frac{1}{8} \sigma^T \nabla \gamma(t, x) \sigma \sigma^T = 0, \\
(t, x) &\in [0, T) \times \mathbb{R}^d.
\end{align*}
$$

(23)

with optimal control

$$
\zeta^*(t, x) = -\sigma^T(t, x) \nabla \gamma(t, x),
$$

(24)

which minimizes the second moment defined in (16).

**Remark 1.** Previous approaches formulated the same optimal control for IS, but through variational characterization of thermodynamic free energy [23], minimizing the following value function

$$
\gamma(t, x) = \inf_{\zeta \in \mathcal{Z}} \mathbb{E} \left[ \int_t^T \frac{1}{2} \|\zeta(s, Y_\zeta(s))\|^2 ds - \log(G(Y_\zeta(T))) \mid Y_\zeta(t) = x \right],
$$

(25)

where $\{Y_\zeta(t) : t \in [0, T]\}$ follows dynamics (17), which leads to the same HJB equation (23).
Various approaches have been proposed to numerically solve (23) and obtain an approximate control. The \(d\)-dimensional HJB PDE (23) has been solved using least-squares regression [22] and model reduction techniques [25] for higher dimensions. Neural networks have also been employed to solve the HJB PDE in higher dimensions with stochastic gradient [23] and cross-entropy [41] learning methods for the stochastic optimal control formulation [25].

In contrast, we use equivalency of nonlinear HJB and linear Kolmogorov backward equation (KBE). Recall that \(u(t, x)\) is the value function that minimizes the second moment. The proposed measure change with optimal control in Corollary 1 produces a zero variance estimator, provided that \(G(\cdot)\) does not change sign. We can see this by substituting \(u(t, x) = v^2(t, x)\) in (21) to obtain a PDE for \(v(t, x)\),

\[
\begin{aligned}
\frac{\partial v}{\partial t} + \langle b(t, x), \nabla v \rangle + \frac{1}{2} \nabla^2 v : (\sigma \sigma^T)(t, x) & = 0, \quad (t, x) \in [0, T) \times \mathbb{R}^d, \\
v(T, x) & = |G(x)|, \quad x \in \mathbb{R}^d
\end{aligned}
\]

with optimal control

\[
\zeta^*(t, x) = \sigma^T(t, x) \nabla \log v(t, x).
\]

Since (26) is just the KBE that solves for the conditional expectation \(\mathbb{E}[|G(Y(T))| \mid Y(t) = x]\), where \(\{Y(t) : t \in [0, T]\}\) follows dynamics (8), the second moment equals the square of the first moment, hence leading to zero variance provided \(G(\cdot)\) does not change sign. Thus, it is sufficient to solve the linear KBE (26) rather than the non-linear HJB (23) to obtain an optimal control for the zero variance estimator, provided \(G(\cdot)\) does not change sign.

For IS purposes, it is sufficient to roughly solve (26) to obtain substantial variance reduction. Hence, we employ MC methods with IS using a control derived by numerically solving (26) to estimate rare event probabilities. This is computationally much cheaper compared with directly solving the KBE to estimate the quantity of interest to achieve relative error tolerances. However, it would still be expensive to solve the multi-dimensional KBE when \(d \gg 1\). The present study does not consider high-dimensional problems, leaving them for future work.

Having formulated the optimal control for measure change in standard SDEs, we now introduce the corresponding problem in the MV-SDE context.

3 Problem Setting

Let \(T > 0\) be some finite terminal time and \(\{X(t) : t \in [0, T]\}\) be the solution to MV-SDE (1) as defined in Section 2.1. Let \(G : \mathbb{R}^d \to \mathbb{R}\) be a given scalar observable function. Our objective is to build a computationally efficient estimator, \(A\), of \(\mathbb{E}[G(X(T))]\) for some given tolerance \(\text{TOL} > 0\) that satisfies

\[
\mathbb{P}[|A - \mathbb{E}[G(X(T))]| < \text{TOL}] > 1 - \alpha,
\]

where \(\alpha\) is the confidence level.

It is often relevant that the MC estimator satisfies a relative error tolerance \(\text{TOL}_r\) rather than a global error tolerance \(\text{TOL}\) when dealing with rare event probabilities, where
TOL = TOLr \times \mathbb{E}[G(X(T))]. The KBE provides a deterministic PDE that can be used to estimate \( \mathbb{E}[G(X(T))] \). Existence and uniqueness for KBE solutions for (1) for general drift/diffusion functions are not straightforward problems due to drift/diffusion dependencies on the law \( \mu_t \). This problem can be avoided by formulating the KBE for stochastic \( P \)-particle system (3). Computational costs for solving the corresponding \( P \times d \)-dimensional KBE numerically for a given TOL scales exponentially with the dimension. Conventional numerical schemes also do not handle relative error tolerances, which makes error control challenging even in one dimensional problems. We overcome this issue by using MC methods.

Naive MC approaches quickly become infeasible in the rare event context, since the number of sample paths required to satisfy a given statistical error tolerance scales inversely with the probability of the event to be estimated. Thus, we combine IS with MC as a variance reduction technique to produce computationally feasible estimates for rare event probabilities. Section 2.2 derives the method for optimal IS for standard SDEs. However, there are two main difficulties deriving and solving the variance minimization problem in MV-SDE context.

1. It is not straightforward to derive variance minimization for MV-SDE (1), because drift and diffusion functions depend on \( \mu_t \), the probability density for the solution. Any measure change will lead to changes in the drift \( b(\cdot, \cdot) \) and diffusion \( \sigma(\cdot, \cdot) \) coefficients.

2. Suppose we use the stochastic \( P \)-particle approximation (3) instead and wish to apply a measure change on it. Solving a variance minimization problem in this context will result in a HJB PDE in \( P \times d \) dimensions, and numerical methods to solve such an equation suffer from the curse of dimensionality when \( P \times d \gg 1 \).

Therefore, we use a decoupling approach \cite{15} rather than considering measure change on the stochastic particle system.

4 Double Loop Monte Carlo with Importance Sampling

4.1 Decoupling Approach for MV-SDEs

The decoupling approach was introduced in \cite{15} as a method to efficiently implement IS in the context of MV-SDEs. The idea is to first approximate the MV-SDE law \( \mu_t \) empirically and then use that as an input to define a standard "decoupled" SDE to which a change in measure is applied. Essentially, the approach is to decouple the computation of the MV-SDE law and the probability measure change required for IS. This ensures that the MV-SDE (1) is converted into a standard SDE with random coefficients, for which measure change can be applied as in Section 2.2. We first formally introduce the general scheme of the decoupling approach.

1. Since we do not have direct access to \{\mu_t : t \in [0,T]\} for the MV-SDE, we approximate it using the empirical measure \{\mu^P_t : t \in [0,T]\} from (4) using \{X^P_p(t) : t \in [0,T]\} from (5).
2. Given the empirical law \( \{\mu_t^P : t \in [0, T]\} \), we define the "decoupled" MV-SDE that solves for \( X^P : [0, T] \times \Omega \to \mathbb{R}^d \)

\[
\begin{align*}
d\bar{X}^P(t) &= b(\bar{X}^P(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_1(\bar{X}^P(t), X_j^P(t)) ) \, dt \\
&\quad + \sigma(\bar{X}^P(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_2(\bar{X}^P(t), X_j^P(t)) ) \, d\bar{W}(t), \quad t \in [0, T] \\
\bar{X}^P(0) &= \bar{x}_0 \sim \mu_0, \quad \bar{x}_0 \in \mathbb{R}^d,
\end{align*}
\]

where superscript \( P \) in \( \bar{X}^P(t) \) indicates the drift and diffusion functions in (29) are computed using the empirical law \( \{\mu_t^P : t \in [0, T]\} \) derived from the stochastic \( P \)-particle system; drift and diffusion coefficients \( b \) and \( \sigma \) are the same as defined in Section 2.1; \( \{\bar{W}(t) : t \in [0, T]\} \) is a standard \( d \)-dimensional Wiener process that is independent of Wiener processes \( \{W_p(t)\}_{p=1}^{P} \) used in (3); \( \bar{x}_0 \in \mathbb{R}^d \) is a random initial state sampled from the \( \mu_0 \) distribution as defined in (1) and independent from \( \{(x_0)_p\}_{p=1}^{P} \) used in (3). (29) is a standard SDE with random coefficients, where randomness arises from drift and diffusion dependencies on empirical measure \( \{\mu_t^P : t \in [0, T]\} \). Solution existence and uniqueness for such SDEs have been shown previously [40].

3. We introduce a copy space to distinguish (29) from the stochastic \( P \)-particle system [15]. Suppose (3) is defined on the probability space \( (\Omega, \mathcal{F}, \mathbb{P}) \). We define a copy space \( (\bar{\Omega}, \bar{\mathcal{F}}, \bar{\mathbb{P}}) \), and (29) is defined on the product space \( (\Omega, \mathcal{F}, \mathbb{P}) \times (\bar{\Omega}, \bar{\mathcal{F}}, \bar{\mathbb{P}}) \). Thus, \( \bar{\mathbb{P}} \) is a probability measure induced by \( \{\mu_t^P : t \in [0, T]\} \) randomness and \( \bar{\mathbb{P}} \) is the measure due to Wiener process randomness driving (29) conditioned on \( \{\mu_t^P : t \in [0, T]\} \).

4. Thus, we approximate our quantity of interest as

\[
\mathbb{E}[G(X(T))] \approx \mathbb{E}_{\mathbb{P} \otimes \bar{\mathbb{P}}}[G(\bar{X}^P(T))] = \mathbb{E}_\mathbb{P}\left[\mathbb{E}_{\bar{\mathbb{P}}}[G(\bar{X}^P(T)) | \{\mu_t^P : t \in [0, T]\}]\right],
\]

where we omit the probability measure henceforth when taking the nested expectation for ease of notation. \( \mathbb{E}[G(\bar{X}^P(T))] \) means that expectation is taken with respect to all randomness sources in the decoupled MV-SDE (29). First, we estimate the inner expectation \( \mathbb{E}[G(\bar{X}^P(T)) | \{\mu_t^P : t \in [0, T]\}] \), and then we estimate the outer expectation using MC sampling over different \( \mu_t^P \) realizations.

The inner expectation \( \mathbb{E}[G(\bar{X}^P(T)) | \{\mu_t^P : t \in [0, T]\}] \) can be obtained from the KBE associated with (29). However, obtaining an analytical solution is not always possible and conventional numerical methods do not handle relative error tolerances even in the \( d = 1 \) case, which are relevant for rare event regimes. Even if we could solve the KBE accurately, we would need to solve it multiple times for each \( \mu_t^P \) realization, which could quickly become a bottleneck. Therefore, we propose to use MC methods coupled with IS, even for the one-dimensional case, to estimate the nested expectation.
Remark 2 (Time Extension for the Empirical Law). In practice, one only has access to time-discretized $\{\mu^P_t : t \in [0,T]\}$ from the Euler-Maruyama time discretization of (3). However, $\mu^P_t$ must be defined continuously throughout the time domain for the decoupled MV-SDE to be well-defined. Therefore, we used the continuous Euler time extension for the discretized law to extend the $\mu^P_t$ over the whole time domain.

4.2 Optimal Importance Sampling for Decoupled MV-SDE using Stochastic Optimal Control

We introduced the decoupled MV-SDE for given $\{\mu^P_t : t \in [0,T]\}$ to implement IS measure change on a standard lower-dimensional SDE and hence reduce MC estimator variance for rare event probabilities. Since (29) is a standard SDE for fixed $\{\mu^P_t : t \in [0,T]\}$, we follow the procedure in Section 2.2 to derive optimal measure change.

This section only discusses the important results required for this formulation. We use Lemma 1 and the procedure in Section 2.2 to obtain the HJB PDE that provides optimal control for the decoupled MV-SDE.

Theorem 2 (HJB PDE for decoupled MV-SDE). Let $\{\bar{X}^P(t) : t \in [0,T]\}$ solve (31) and $\{\bar{X}_\xi^P(t) : t \in [0,T]\}$ solve the following controlled SDE with control $\zeta(t,x) : [t,T] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$

$$\begin{align*}
\text{d}\bar{X}_\xi^P(t) &= \left( b\left(\bar{X}_\xi^P(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_1(\bar{X}_\xi^P(t), X_j^P(t))\right) \\
&\quad + \sigma\left(\bar{X}_\xi^P(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_2(\bar{X}_\xi^P(t), X_j^P(t))\right) \zeta(t,\bar{X}_\xi^P(t))\right)dt \\
&\quad + \sigma\left(\bar{X}_\xi^P(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_2(\bar{X}_\xi^P(t), X_j^P(t))\right) \text{d}W(t), \quad 0 < t < T \tag{31}
\end{align*}$$

Assume that (3) is used to compute $\mu^P_t$ in (29) and (31), and define the value function $u(t,x)$ that minimizes the second moment as

$$u(t,x) = \min_{\zeta \in \mathcal{Z}} \mathbb{E}\left[ G^2(\bar{X}_\xi^P(T)) \exp\left\{- \int_t^T \|\zeta(s,\bar{X}_\xi^P(s))\|^2 - 2 \int_t^T \langle \zeta(s,\bar{X}_\xi^P(s)), dW(s)\rangle\right\} \mid \bar{X}_\xi^P(t) = x, \{\mu^P_t : t \in [0,T]\}\right]. \tag{32}$$

Assume $u(t,x)$ is bounded, smooth, and non-zero throughout its domain. Define a new function $\gamma(t,x)$, such that

$$u(t,x) = \exp\{-2\gamma(t,x)\}. \tag{33}$$
Then $\gamma(t, x)$ satisfies the nonlinear HJB equation,

$$
\begin{aligned}
\frac{\partial \gamma}{\partial t} + \langle b \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_1(x, X_j^P(t)) \right), \nabla \gamma \rangle + \frac{1}{2} \nabla^2 \gamma : (\sigma \sigma^T) \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) & - \frac{1}{4} \left\| \sigma^T \nabla \gamma \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) \right\|^2 = 0, \\
(\gamma, t, x) & \in [0, T) \times \mathbb{R}^d
\end{aligned}
$$

(34)

with optimal control

$$
\zeta^*(t, x) = -\sigma^T \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) \nabla \gamma(t, x),
$$

(35)

which minimizes the second moment $[32]$. The HJB PDE that solves for $u(t, x)$ leads to a zero variance estimator for a given empirical $\mu^P_t$, provided $G(\cdot)$ does not change sign. Hence, we can recover the linear KBE as shown in Section 2.2 and obtain the following control PDE in the MV-SDE context,

$$
\begin{aligned}
\frac{\partial v}{\partial t} + \langle b \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_1(x, X_j^P(t)) \right), \nabla v \rangle & + \frac{1}{2} \nabla^2 v : (\sigma \sigma^T) \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) = 0, \\
(\gamma, t, x) & \in [0, T) \times \mathbb{R}^d
\end{aligned}
$$

(36)

with optimal control

$$
\zeta^*(t, x) = \sigma^T \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) \nabla \log v(t, x).
$$

(37)

This paper solves the one-dimensional ($d = 1$) KBE arising from the Kuramoto Model [6] numerically using finite differences. Model reduction techniques [24, 25] or solving the minimization problem (32) using stochastic gradient methods [23] are appropriate for higher-dimensional ($d \gg 1$) problems. We do not have closed-form solutions for the inner or outer expectations, and it is infeasible to obtain numerical solutions for both that satisfy relative error tolerance even in the one-dimensional case. This necessitates the use of a DLMC estimator in this context. The following steps describe how the DLMC estimator is constructed.

1. Approximate the $\mu_t$ in [1] by empirical $\mu^P_t$ using [2]. In practice, we obtain discretized empirical law with $N_1$ time steps from Euler-Maruyama time discretization of the
3. Given the approximate $0 = t_0 < t_1 < t_2 < \ldots < t_{N_1} = T$ for the $[0, T]$ time domain with $N_1$ equal time steps. Hence, $t_n = n \times \Delta t_1$, $n = 0, 1, \ldots, N_1$; and $\Delta t_1 = T/N_1$. Let $X_p^{P|N_1}$ be the time-discretized version for state $X_p$ corresponding to $\{3\}$.

2. Let $\mu^{P|N_1}$ be the discrete law obtained from above step, then

\[
\mu^{P|N_1}(t_n) = \frac{1}{P} \sum_{j=1}^{P} \delta_{X_j^{P|N_1}(t_n)}, \quad \forall n = 0, \ldots, N_1.
\tag{38}
\]

To define a time-continuous extension for the empirical law, we extend the time-discrete stochastic particle system to all $t \in [0, T]$ using the continuous-time Euler extension.

3. Given the approximate $\mu^{P|N_1}$ from (38), we use (36) and (37) to obtain optimal control $\zeta(\cdot, \cdot)$ for IS of (29).

4. Given the approximate $\mu^{P|N_1}$ from (38) and control $\zeta : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$, we solve (31) for $\{\bar{X}_\zeta^{P|N_1}(t) : t \in [0, T]\}$. Equation (31) can be expressed with modified notation, indicating the drift and diffusion coefficients come from the time extended version for $\mu^{P|N_1}$ obtained using $P$ particles and $N_1$ time steps,

\[
\begin{align*}
\text{d} \bar{X}_\zeta^{P|N_1}(t) &= \left( b \left( \bar{X}_\zeta^{P|N_1}(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_1(\bar{X}_\zeta^{P|N_1}(t), X_j^{P|N_1}(t)) \right) \\
&+ \sigma \left( \bar{X}_\zeta^{P|N_1}(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_2(\bar{X}_\zeta^{P|N_1}(t), X_j^{P|N_1}(t)) \right) \zeta(t, \bar{X}_\zeta^{P|N_1}(t)) \right) \text{d}t \\
&+ \sigma \left( \bar{X}_\zeta^{P|N_1}(t), \frac{1}{P} \sum_{j=1}^{P} \kappa_2(\bar{X}_\zeta^{P|N_1}(t), X_j^{P|N_1}(t)) \right) \text{d}W(t), \quad 0 < t < T \\
\bar{X}_\zeta^{P|N_1}(0) &= \bar{x}_0 \sim \mu_0.
\end{align*}
\tag{39}
\]

5. Since there is no closed form solution to (39), we use Euler-Maruyama time discretization with $N_2$ time steps and notation to indicate the three discretization parameters used: $P, N_1, N_2$. Consider a new time discretization $0 = \bar{t}_0 < \bar{t}_1 < \bar{t}_2 < \ldots < \bar{t}_{N_2} = T$ for the $[0, T]$ time domain with $N_2$ equal time steps. Hence, $\bar{t}_n = n \times \Delta t_2$, $n = 0, 1, \ldots, N_2$ and $\Delta t_2 = \frac{T}{N_2}$.

- For time step $n = 0$,

\[
\bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_0) = \bar{x}_0.
\]

- For $n = 1, \ldots, N_2 - 1$

\[
\bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_{n+1}) = \bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_n) + \left( b \left( \bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_n), \frac{1}{P} \sum_{j=1}^{P} \kappa_1(\bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_n), X_j^{P|N_1}(\bar{t}_n)) \right) \\
+ \sigma \left( \bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_n), \frac{1}{P} \sum_{j=1}^{P} \kappa_2(\bar{X}_\zeta^{P|N_1|N_2}(\bar{t}_n), X_j^{P|N_1}(\bar{t}_n)) \right) \text{d}W(\bar{t}_n), \quad 0 < \bar{t} < T
\]

15
where \( \epsilon_n \sim \mathcal{N}(0, I_d) \).

6. Given \( \{\tilde{X}_\zeta^{p|n_1|n_2}(t_n)\}_{n=1}^{N_2} \), we can express the quantity of interest with IS as

\[
E \left[ G(\tilde{X}_\zeta^{p|n_1|n_2}(T)) \right] = E \left[ G(\tilde{X}_\zeta^{p|n_1|n_2}(T))L^{p|n_1|n_2} \right],
\]

where, similar to (12), the likelihood factor can be expressed as

\[
L^{p|n_1|n_2} = \prod_{n=0}^{N_2-1} \exp \left\{ -\frac{1}{2} \gamma t^2 \left\| \zeta(t_n, \tilde{X}_\zeta^{p|n_1|n_2}(t_n)) \right\|^2 - \sqrt{\Delta t} \langle \epsilon_n, \zeta(t_n, \tilde{X}_\zeta^{p|n_1|n_2}(t_n)) \rangle \right\}.
\]

Hence, \( L^{p|n_1|n_2} = 1 \) when \( \zeta(t, x) = 0, \ (t, x) \in [0, T] \times \mathbb{R}^d \).

We provide a general DLMC algorithm (Algorithm 1) to estimate the required quantity of interest using Steps 1–6 above.

**Algorithm 1:** General DLMC algorithm for decoupled MV-SDE

**Inputs:** \( P, N_1, N_2, M_1, M_2; \)
for \( m_1 = 1, \ldots, M_1 \) do
Generate realization of law \((\mu^{p|n_1})^{(m_1)}\) with \( P \)-particle system and \( N_1 \) time steps using (38);
Given \((\mu^{p|n_1})^{(m_1)}\) solve KBE (36) to obtain control \((\zeta(\cdot, \cdot))^{(m_1)}\);
for \( m_2 = 1, \ldots, M_2 \) do
Given \((\mu^{p|n_1})^{(m_1)}\) and \((\zeta(\cdot, \cdot))^{(m_1)}\), solve decoupled MV-SDE with \( N_2 \) time steps using (40);
Compute \( G \left( \tilde{X}_\zeta^{p|n_1|n_2}(T) \right)^{(m_1,m_2)} \);
Compute \( (L^{p|n_1|n_2})^{(m_1,m_2)} \) using (42);
end
Approximate \( E \left[ G(\tilde{X}_\zeta^{p|n_1|n_2}(T)) \right] \) by \( \frac{1}{M_2} \sum_{m_2=1}^{M_2} G \left( \tilde{X}_\zeta^{p|n_1|n_2}(T) \right)^{(m_1,m_2)} (L^{p|n_1|n_2})^{(m_1,m_2)} \); end
Approximate \( E \left[ G(\tilde{X}_\zeta^{p|n_1|n_2}(T)) \right] \) by \( \frac{1}{M_1} \sum_{m_1=1}^{M_1} \frac{1}{M_2} \sum_{m_2=1}^{M_2} G \left( \tilde{X}_\zeta^{p|n_1|n_2}(T) \right)^{(m_1,m_2)} (L^{p|n_1|n_2})^{(m_1,m_2)} \);
The output of Algorithm 1 is our DLMC estimator, defined as follows

\[ A_{MC} = \frac{1}{M_1} \sum_{m_1=1}^{M_1} \frac{1}{M_2} \sum_{m_2=1}^{M_2} G \left( \left( \tilde{X}^{P|N_1|N_2}(T) \right)^{(m_1,m_2)} \right) \left( L^{P|N_1|N_2} \right)^{(m_1,m_2)}. \]  

(43)

4.2.1 Error Analysis

We bound the global error introduced by the DLMC estimator \( A_{MC} \) as

\[ |\mathbb{E}[G(X(T))] - A_{MC}| \leq \left| \mathbb{E}[G(X(T))] - \mathbb{E}\left[ G\left( \tilde{X}^{P|N_1|N_2}(T) \right) \right] \right| = \epsilon_b, \text{ Bias Error} \\
+ \left| \mathbb{E}\left[ G\left( \tilde{X}^{P|N_1|N_2}(T) \right) \right] - A_{MC} \right| = \epsilon_s, \text{ Statistical Error} \]

(44)

Although \( A_{MC} \) should satisfy a given TOL in the sense of (28), this study imposes the more restrictive conditions

Bias Constraint: \( \epsilon_b \leq \theta \text{TOL} \),  
Statistical Constraint: \( \mathbb{P}[\epsilon_s \leq (1 - \theta) \text{TOL}] \leq \alpha \),  

(45, 46)

for a given tolerance splitting parameter \( \theta \in (0, 1) \) and confidence level \( \alpha \).

Let us first analyze bias error, which can be split into two terms,

\[ \epsilon_b = \left| \mathbb{E}[G(X(T))] - \mathbb{E}\left[ G\left( \tilde{X}^{P|N_1|N_2}(T) \right) \right] \right| \leq \left| \mathbb{E}[G(X(T))] - \mathbb{E}\left[ G\left( \tilde{X}^{P}(T) \right) \right] \right| + \left| \mathbb{E}\left[ G\left( \tilde{X}^{P}(T) \right) \right] - \mathbb{E}\left[ G\left( \tilde{X}^{P|N_1|N_2}(T) \right) \right] \right|, \]

Decoupling Error

Time Discretization Error

(47)

and make the following assumptions,

**Assumption 1** (Decoupling Error).

\[ |\mathbb{E}[G(X(T))] - \mathbb{E}\left[ G\left( \tilde{X}^{P}(T) \right) \right]| \leq C_p P^{-1}, \]

and

**Assumption 2** (Time Discretization Error).

\[ \left| \mathbb{E}\left[ G\left( \tilde{X}^{P}(T) \right) \right] - \mathbb{E}\left[ G\left( \tilde{X}^{P|N_1|N_2}(T) \right) \right] \right| \leq C_{n_1} N_1^{-1} + C_{n_2} N_2^{-1}. \]

In Assumption 1, the constant \( C_p \) depends only on \( T \) and the smoothness and boundedness of \( b(\cdot, \cdot), \sigma(\cdot, \cdot) \) and \( G(\cdot) \). This assumption is motivated by the weak convergence with respect to the number of particles (see [19]). In Assumption 2, the constants \( C_{n_1}, C_{n_2} \) are independent of the number of particles \( P \) and number of time steps \( N_1, N_2 \) and only depend on \( T \) and the smoothness and boundedness of \( b(\cdot, \cdot), \sigma(\cdot, \cdot) \) and \( G(\cdot) \) and their derivatives. Assumption 2 is motivated by the weak convergence of the Euler-Maruyama scheme.
for standard SDEs [28]. These assumptions will be verified numerically for the Kuramoto
Model (6) in Section 5.

Substituting Assumptions 1 and 2 into (47), the bias bound can be expressed as

$$
\epsilon_b \leq \frac{C_p}{P} + \frac{C_{n1}}{N_1} + \frac{C_{n2}}{N_2}.
$$

(48)

Consider the statistical constraint (46). We can approximate the statistical error \(\epsilon_s\) using the Central Limit Theorem as

$$
\epsilon_s \approx C_\alpha \sqrt{\text{Var}[A_{MC}]} \leq (1 - \theta)\text{TOL},
$$

(49)

where \(C_\alpha\) is the \((1 - \alpha)\)-quantile for the standard normal distribution. Hence, (49) can be expressed as

$$
\text{Var}[A_{MC}] \leq \left( \frac{(1 - \theta)\text{TOL}}{C_\alpha} \right)^2.
$$

(50)

to obtain a constraint on the estimator variance.

For notational convenience, let \(Y^{P|N_1|N_2} = G\left(\bar{X}_\zeta^{P|N_1|N_2}(T)\right)\) \((L^{P|N_1|N_2})\) and \(\{Y_{m_1,m_2}^{P|N_1|N_2}\}\) be random samples for \(Y^{P|N_1|N_2}\). Thus, the DLMC estimator variance be expressed as

$$
\text{Var}[A_{MC}] = \text{Var} \left[ \frac{1}{M_1} \sum_{m_1=1}^{M_1} \frac{1}{M_2} \sum_{m_2=1}^{M_2} Y_{m_1,m_2}^{P|N_1|N_2} \right] = \frac{1}{M_1} \text{Var} \left[ \frac{1}{M_2} \sum_{m_2=1}^{M_2} Y_{1,m_2}^{P|N_1|N_2} \right].
$$

(51)

Using the law of total variance, we get

$$
\text{Var}[A_{MC}] = \frac{1}{M_1} \text{Var} \left[ \mathbb{E} \left[ \frac{1}{M_2} \sum_{j=1}^{M_2} Y_{1,j}^{P|N_1|N_2} | \mu^{P|N_1} \right] \right] + \frac{1}{M_1} \mathbb{E} \left[ \text{Var} \left[ \frac{1}{M_2} \sum_{j=1}^{M_2} Y_{1,j}^{P|N_1|N_2} | \mu^{P|N_1} \right] \right]
$$

\[= \frac{1}{M_1} \text{Var} \left[ \mathbb{E} \left[ Y^{P|N_1|N_2} | \mu^{P|N_1} \right] \right] + \frac{1}{M_1 M_2} \mathbb{E} \left[ \text{Var} \left[ Y^{P|N_1|N_2} | \mu^{P|N_1} \right] \right],
$$

(52)

where \(\{Y_{1,j}^{P|N_1|N_2}\}_{j=1}^{M_2}\) are conditionally independent samples given \(\mu^{P|N_1}\).

We make the following assumptions

**Assumption 3.**

$$
V_{1}^{P|N_1|N_2} = \text{Var} \left[ \mathbb{E} \left[ Y^{P|N_1|N_2} | \mu^{P|N_1} \right] \right] \leq C_1 P^{-1}
$$

and

**Assumption 4.**

$$
V_{2}^{P|N_1|N_2} = \mathbb{E} \left[ \text{Var} \left[ Y^{P|N_1|N_2} | \mu^{P|N_1} \right] \right] \leq C_2,
$$

where \(C_1\) and \(C_2\) are positive constants independent of \(N_1, N_2,\) and \(P\).

Assumption 3 was motivated by convergence of \(\mu^{P|N_1}\) to a deterministic law as \(P \to \infty\). Since the outer variance is with respect to \(\mu^{P|N_1}\) randomness, variance in Assumption 3 vanishes as the number of particles increases. Assumption 4 was motivated by inner
variance boundedness with respect to randomness generated by the Wiener paths used in (29). These assumptions are verified numerically for (6) in Section 5.

Substituting Assumptions 3 and 4 in (52), the constraint (50) can be expressed as

$$\frac{C_1}{PM_1} + \frac{C_2}{M_1M_2} \leq \left( \frac{(1 - \theta)\text{TOL}}{C_\alpha} \right)^2. \quad (53)$$

### 4.2.2 Work Analysis

This section analyzes the cost to run each DLMC Algorithm 1 step once.

1. Computational cost = $N_1 \times P^2$ for one realization of empirical law using the Euler-Maruyama time-stepping scheme with $N_1$ time steps.

2. Computational cost = $N_3 \times P \times h^{-d\Gamma}$ to solve (36) numerically with discretization parameter $h$ in space domain and $N_2$ time steps with solver work rate $\Gamma$.

3. Computational cost = $P \times N_2$ for one (40) realization using the Euler-Maruyama time-stepping scheme with $N_2$ time steps.

The above steps assume a naive method (with computational cost $O(P)$) to compute the empirical mean for drift and diffusion coefficients in (3) and (40). Hence, total computational work for Algorithm 1 can be expressed as

$$W = M_1 \left\{ P^2N_1 + N_3Ph^{-d\Gamma} + M_2 \{PN_2\} \right\}. \quad (54)$$

Thus, solving (36) $M_1$ times would become a significant bottleneck. We overcome this problem in our revised Algorithm 2 by solving (36) offline, just once, using drift and diffusion coefficients obtained from one (38) realization, with some large $P, \bar{N}$. This implies that we impose a deterministic control that is independent of the different stochastic $P$-particle system realizations in Algorithm 1 rather than a stochastic control. We motivate this choice from the $\mu^P|\bar{N}$ convergence in the drift and diffusion coefficients to $\mu_t$ for (1) as $P, \bar{N}$ tend to infinity. The computational work for Algorithm 2 can be expressed as

$$W = M_1 \left\{ P^2N_1 + M_2 \{PN_2\} \right\}, \quad (55)$$

where we exclude the cost to solve (36) in (55) because this is done offline and only once. Given constraints (45) and (53), we need to find optimal parameters $P, N_1, N_2, M_1, M_2$ to ensure minimal (55). This can be posed as the following optimization problem,

$$\begin{align*}
\min_{\{P,N_1,N_2,M_1,M_2\}} & \quad W = M_1N_1P^2 + M_1M_2N_2P \\
\text{s.t.} & \quad \frac{C_p}{P} + \frac{C_{n_1}}{N_1} + \frac{C_{n_2}}{N_2} \approx \theta\text{TOL}, \\
& \quad C_\alpha \left( \frac{C_1}{PM_1} + \frac{C_2}{M_1M_2} \right) \approx (1 - \theta)^2\text{TOL}^2, \quad (56)
\end{align*}$$
with the solution formulated in Theorem 3.

**Algorithm 2:** Revised general DLMC algorithm for decoupled MV-SDE

**Offline:**
Generate realisation of law $\mu^{P|\bar{N}}$ with $\bar{P}$-particle system and $\bar{N}$ time steps using (38) with some large $\bar{P}$, $\bar{N}$;

Given $\mu^{P|\bar{N}}$, solve KBE (36) to obtain control $\zeta(\cdot, \cdot)$; Inputs: $P, N_1, N_2, M_1, M_2, \zeta(\cdot, \cdot)$;

for $m_1 = 1, \ldots, M_1$ do
  Generate realization of law $(\mu^{P|N_1})^{(m_1)}$ with $P$-particle system and $N_1$ time steps using (38);
  for $m_2 = 1, \ldots, M_2$ do
    Given $(\mu^{P|N_1})^{(m_1)}$ and $\zeta(\cdot, \cdot)$, solve decoupled MV-SDE with $N_2$ time steps using (40);
    Compute $G\left(\bar{X}^{P|N_1|N_2}(T)^{(m_1,m_2)}\right)$;
    Compute $(\mathbb{L}^{P|N_1|N_2})^{(m_1,m_2)}$ using (42);
  end
Approximate $\mathbb{E}\left[G\left(\bar{X}^{P|N_1|N_2}(T)^{(m_1,m_2)}\right)\right]$ by
\[
\frac{1}{M_2} \sum_{m_2=1}^{M_2} G\left(\bar{X}^{P|N_1|N_2}(T)^{(m_1,m_2)}\right) \left(\mathbb{L}^{P|N_1|N_2}\right)^{(m_1,m_2)};
\]
end
Approximate $\mathbb{E}\left[G\left(\bar{X}^{P|N_1|N_2}(T)^{(m_1,m_2)}\right)\right]$ by
\[
\frac{1}{M_1} \sum_{m_1=1}^{M_1} \frac{1}{M_2} \sum_{m_2=1}^{M_2} G\left(\bar{X}^{P|N_1|N_2}(T)^{(m_1,m_2)}\right) \left(\mathbb{L}^{P|N_1|N_2}\right)^{(m_1,m_2)};
\]

**Theorem 3** (Optimal DLMC Complexity). Consider the DLMC estimator in (43), arising from Algorithm 2. For any TOL > 0, there exist optimal parameters $\{P, N_1, N_2, M_1, M_2\}$ such that (45), (53) hold and optimal computational work is
\[
W = M_1 N_1 P^2 + M_1 M_2 N_2 P = O(TOL^{-4}). \tag{57}
\]

*Proof*. See Appendix C.

**Remark 3.** Introducing DLMC for this problem crucially guarantees $O(TOL^{-4})$ complexity of proposed estimator. From (56) and Theorem 3, using a single realization for the particle system ($M_1 = 1$), as done in [15], leads to complexity $O(TOL^{-5})$. Moreover, the proposed IS scheme for the DLMC estimator also considerably reduces the associated constant for rare event probabilities compared with previous MC estimators [20]. Section 5 validates this numerically.

### 4.2.3 Adaptive double loop Monte Carlo algorithm

We formulate a DLMC algorithm that adaptively chooses optimal parameters $P, N_1, N_2, M_1, M_2$. Define the hierarchies
- $P_{\ell} = P_0 \times \tau^\ell$, $\ell = 0, \ldots, L$
\( (N_1)_\ell = (N_2)_\ell = N_\ell = N_0 \times \tau^\ell, \ell = 0, \ldots, L \)

For simplicity, set \( N_1 = N_2 \) and \( \tau = 2 \), since optimal \( N_1, N_2 \) are both \( O(\text{TOL}^{-1}) \) (Appendix C). Let some level \( L \) satisfy (45), and then find optimal parameters \( M_1, M_2 \) that satisfy (50). This can be posed as the optimization problem

\[
\min_{\{M_1, M_2\}} \mathcal{W} = M_1 N_L P_L^2 + M_1 M_2 N_L P_L \\
\quad C_\alpha^2 \left( \frac{V_{1L}}{M_1} + \frac{V_{2L}}{M_1 M_2} \right) \approx (1 - \theta)^2 \text{TOL}^2.
\]

where \( V_{1L} = V_{1L}[N_L|N_L] \) and \( V_{2L} = V_{2L}[N_L|N_L] \). Solving (58),

\[
M_1 = \left( V_{1L} + \sqrt{\frac{V_{1L} V_{2L}}{P_L}} \right) \frac{C_\alpha^2}{(1 - \theta)^2 \text{TOL}^2}, \quad M_2 = \sqrt{\frac{V_{2L} P_L}{V_{1L}}}.
\]

In principle, the number of samples \( M_1, M_2 \) obtained in (59) are real-valued. However, practically we use the next highest integer values for \( M_1, M_2 \). From (59), we need only to estimate the constants \( V_{1L} \) and \( V_{2L} \) to obtain a DLMC estimator that satisfies (50). The proposed adaptive algorithm uses an heuristic estimator for these constants (Appendix 5).

Next, we choose \( L \) that satisfies (45). For convenience, set \( G = G(X(T)) \) and its discretization at level \( \ell \) as \( \hat{G}_\ell = G\left( \bar{X}_\ell(N_L|N_L) \right) \). The likelihood factor \( \mathbb{L}_\ell = \mathbb{L}[P_L[N_L|N_L] \) at level \( \ell \) is computed using (42). The bias for level \( \ell \) can be expressed as

\[
\epsilon_b = |E[G - G_\ell]| \leq \frac{C_p}{P_\ell} + \frac{C_\alpha}{N_\ell}.
\]

We use the Richardson extrapolation technique [30] to estimate bias for \( \tau = 2 \) at level \( \ell \) as

\[
|E[G - G_\ell]| \approx 2|E[G_{\ell+1} - G_\ell]|.
\]

**Remark 4 (Robust Bias Estimation).** We use MC estimate of \( E[\Delta G_{\ell+1}] = E[G_{\ell+1} - G_\ell] \) for the bias, following Algorithm [3] which incorporates an antithetic sampler [20] to estimate the bias using sufficiently correlated samples of \( G_{\ell+1} \) and \( G_\ell \). More details regarding antithetic sampler can be found in Algorithm [3].

It is more relevant to satisfy relative tolerance \( \text{TOL}_r \) rather than absolute tolerance \( \text{TOL} \), where \( \text{TOL} = E[G(X(T))] \times \text{TOL}_r \), for rare event observables. The proposed adaptive algorithm keeps updating an heuristic estimate for \( E[G(X(T))] \) (the quantity of interest). Hence, we now have all the components required to formulate an adaptive DLMC algorithm, as shown in Algorithm [4]. Algorithm [4] also defines external parameters \( \{\hat{M}_1, \hat{M}_2\} \) and \( \{\tilde{M}_1, \tilde{M}_2\} \), selected to ensure robust estimates for \( V_{1\ell}, V_{2\ell} \), and bias. Selecting these
parameters is discussed in more detail in Section 5.

Algorithm 3: Estimating $\mathbb{E}[\Delta G_{\ell}]$ with an antithetic sampler

**Inputs:** $\ell, M_1, M_2, \zeta(\cdot, \cdot)$

for $m_1 = 1, \ldots, M_1$ do

Generate $\left(\mu^{P|\nu_0}\right)^{(m_1)}$ realization with $P_\ell$-particle system and $N_\ell$ time steps using (38);

Generate two realizations in level $\ell - 1$, $\left(\mu^{P_{\ell-1}|\nu_{\ell-1}}\right)^{(m_1)}_1$, $\left(\mu^{P_{\ell-1}|\nu_{\ell-1}}\right)^{(m_1)}_2$ by partitioning $P_\ell$ particles into two sets of $P_{\ell-1}$ particles and using the same Wiener path as above for each partition on the coarser time grid with $N_{\ell-1}$ steps;

for $m_2 = 1, \ldots, M_2$ do

Given $\left(\mu^{P|\nu_0}\right)^{(m_1)}$ and $\zeta(\cdot, \cdot)$, solve decoupled MV-SDE with $N_\ell$ time steps using (40);

Compute $\left(G_\ell\right)^{(m_1,m_2)}$;

Compute $\left(\mathbb{L}_\ell\right)^{(m_1,m_2)}$;

Given $\zeta(t,x)$ and $\left(\mu^{P_{\ell-1}|\nu_{\ell-1}}\right)^{(m_1)}_1$, $\left(\mu^{P_{\ell-1}|\nu_{\ell-1}}\right)^{(m_1)}_2$ respectively, solve decoupled MV-SDE using the same Wiener path as above with $N_{\ell-1}$ time steps using (40);

Compute $\left(G_{\ell-1}\right)^{(m_1,m_2)}_1$ and $\left(G_{\ell-1}\right)^{(m_1,m_2)}_2$ respectively;

Compute $\left(\mathbb{L}_{\ell-1}\right)^{(m_1,m_2)}_1$ and $\left(\mathbb{L}_{\ell-1}\right)^{(m_1,m_2)}_2$ respectively;

end

end

Approximate $\mathbb{E}\left[G_\ell - G_{\ell-1}\right]$ by

$$\frac{1}{M_1} \sum_{m_1=1}^{M_1} \frac{1}{M_2} \sum_{m_2=1}^{M_2} \left(\left(G_\ell\mathbb{L}_\ell\right)^{(m_1,m_2)} - \left(G_{\ell-1}\mathbb{L}_{\ell-1}\right)^{(m_1,m_2)}_1 + \left(G_{\ell-1}\mathbb{L}_{\ell-1}\right)^{(m_1,m_2)}_2\right);$$

Algorithm 4: Adaptive DLMC algorithm for decoupled MV-SDE

**Offline:**

Generate $\mu^{P|\nu}$ realisation with $\bar{P}$-particle system and $\bar{N}$ time steps with arbitrarily large $\bar{P}, \bar{N}$;

Given $\mu^{P|\nu}$, solve KBE (36) to obtain control $\zeta(\cdot, \cdot)$;

**Input:** $P_0, N_0, \text{TOL}, \zeta(\cdot, \cdot)$;

$\ell = 0;

\text{Estimate } \hat{\alpha} = \mathbb{E}[G_0] \text{ using } P_0, N_0, \bar{M}_1, \bar{M}_2, \zeta(\cdot, \cdot) \text{ in Algorithm 2};$

while $\text{Bias} > \theta \text{TOL} \cdot \hat{\alpha}$ do

$P_\ell = P_0 \times 2^\ell$, $N_\ell = N_0 \times 2^\ell$;

Estimate $V_{1\ell}$ and $V_{2\ell}$ using $P_\ell, N_\ell, \bar{M}_1, \bar{M}_2, \zeta(\cdot, \cdot)$ in Algorithm 5;

Compute optimal $M_1, M_2$ with estimated $V_{1\ell}, V_{2\ell}$ using (59);

Estimate Bias $= 2\mathbb{E}[\Delta G_{\ell+1}]$ with $P_\ell, N_\ell, \bar{M}_1, \bar{M}_2, \zeta(\cdot, \cdot)$ in Algorithm 3;

Update $\hat{\alpha} = \mathbb{E}[G_\ell]$ using $P_\ell, N_\ell, M_1, M_2, \zeta(\cdot, \cdot)$ in Algorithm 2;

$\ell \leftarrow \ell + 1$;

end

$A_{MC} = \hat{\alpha}.$
5 Numerical Results

This section provides numerical evidence for the various assumptions and work complexities defined in Section 4. Reported results focus on (5) with $\sigma = 0.4$, $T = 1$, $(x_0)_p \sim \mathcal{N}(0,0.2)$, and $\nu_p \sim \mathcal{U}(-0.2,0.2)$ for all $p = 1,\ldots,P$. We implemented our DLMC Algorithm on both non-rare and rare event observables. We demonstrate the effectiveness of this variance reduction method over naive MC.

5.1 Objective function $G(x) = \cos x$

We implemented the proposed DLMC algorithm for the non-rare observable $G(x) = \cos x$. Since this is not a rare event observable, we do not require IS in the algorithms, i.e., $\zeta(t,x) = 0, \forall (t,x) \in [0,T] \times \mathbb{R}^d$.

First, we verified Assumption 1. Since we do not know $\mathbb{E}[G(X(T))]$ exactly, we used Richardson extrapolation to obtain the following estimate that can be numerically computed

$$\mathbb{E}[G(\bar{X}^{2P}(T)) - \mathbb{E}[G(\bar{X}^{P}(T))] = \frac{C_P}{2P} + \text{h.o.t.} \quad (62)$$

To get a robust estimate, we couple the expectation computations in (62) using the antithetic sampler (Algorithm 3). Assumption 2 was verified using the following three estimates for the time discretization error with respect to parameters $N_1, N_2$:

$$\mathbb{E}[G(\bar{X}^{P|2N_1|N_2}(T))] - \mathbb{E}[G(\bar{X}^{P|N_1|N_2}(T))] = \frac{C_{n_1}}{2N_1} + \text{h.o.t.} \quad (63)$$

$$\mathbb{E}[G(\bar{X}^{P|N_1|2N_2}(T))] - \mathbb{E}[G(\bar{X}^{P|N_1|N_2}(T))] = \frac{C_{n_2}}{2N_2} + \text{h.o.t.} \quad (64)$$

$$\mathbb{E}[G(\bar{X}^{P|2N_1|2N_2}(T))] - \mathbb{E}[G(\bar{X}^{P|N_1|N_2}(T))] = \frac{C_n}{2N} + \text{h.o.t.} \quad (65)$$

Figure 1 verifies the proposed orders of error convergence for the bias with respect to $P, N_1, N_2$. Figure 2 shows estimated $V_1^{P|N_1|N_2}$ and $V_2^{P|N_1|N_2}$ from Algorithm 5. $V_1^{P|N_1|N_2}$ converges with $O(P^{-1})$ and $V_2^{P|N_1|N_2}$ is almost constant. Figures 1 and 2 confirm that the assumptions in Section 4 were well-founded.

We tested the adaptive DLMC algorithm (Algorithm 4) on the Kuramoto model (6) using $P_0 = 5, N_0 = 4$ as input to the algorithm. We used Algorithm 5 with $M_1 = 100$ and $M_2 = 3000$ samples to estimate $V_1$ and $V_2$ for each level $\ell$; and Algorithm 3 with $M_1 = M_1$ and $M_2 = M_2$ samples to estimate the bias, where $M_1$ and $M_2$ are optimal number of samples obtained from (59).

Figure 3a shows computational runtime for Algorithm 4 for different error tolerances. Runtimes for sufficiently small tolerances follow the predicted theoretical rate $O(\text{TOL}^{-4})$ derived in Theorem 3.

Figure 3b shows the exact DLMC estimator error for separate Algorithm 4 runs for different prescribed error tolerances TOL, where the exact error was computed using reference DLMC approximation with TOL = $10^{-3.5}$. Figure 3b clearly shows that Algorithm 4 satisfied the DLMC estimator error constraints.
(a) Verifying (62): DLMC estimate for $|E[G(X^{2P}(T))]|$ using Algorithm 2 with inputs $N_1 = N_2 = 128, M_1 = 100, M_2 = 10^3$ with respect to number of particles $P$.

(b) Verifying (63): DLMC estimator for $|E[G(X^{P|2N_1|N_2}(T))]|$ using Algorithm 2 with inputs $P = 80, N_1 = 256, M_1 = 10^2, M_2 = 10^3$ with respect to number of time steps $N_1$.

(c) Verifying (64): DLMC estimator for $|E[G(X^{P|N_1|2N_2}(T))]|$ using Algorithm 2 with inputs $P = 80, N_1 = 256, M_1 = 10^2, M_2 = 10^3$ with respect to number of time steps $N_2$.

(d) Verifying (65): DLMC estimator for $|E[G(X^{P|2N_2|N}(T))]|$ using Algorithm 2 with inputs $P = 80, M_1 = 10^2, M_2 = 10^3$ with respect to number of time steps $N$.

Figure 1: Verifying Assumptions 1 and 2 for Kuramoto model (6) for $G(x) = \cos x$. 
(a) Verifying Assumption 3: DLMC estimator for $V_{P|N_1|N_2} = \text{Var} \left[ \mathbb{E} \left[ Y | \mu^P \right] \right]$ using Algorithm 5 with inputs $N_1 = N_2 = 128, M_1 = 10^2, M_2 = 10^4$ with respect to number of particles $P$.

(b) Verifying Assumption 4: DLMC estimator for $V_{P|N_1|N_2} = \mathbb{E} \left[ \text{Var} \left[ Y | \mu^P \right] \right]$ using Algorithm 5 with inputs $N_1 = N_2 = 256, M_1 = 10^2, M_2 = 10^4$ with respect to number of particles $P$.

Figure 2: Verifying Assumptions 3 and 4 for Kuramoto model (6).

(a) Runtime with respect to TOL.

(b) Global Error with respect to TOL.

Figure 3: Adaptive DLMC Algorithm 4 applied to Kuramoto example (6) for $G(x) = \cos x$. 

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5.2 Objective function \( G(x) = \mathbb{1}_{\{x > K\}} \)

For sufficiently large \( K \), \( G(x) = \mathbb{1}_{\{x > K\}} \) corresponds to the probability for a rare event. Figures 4–5 use threshold \( K = 2 \), corresponding to probability of approximately \( 2 \times 10^{-4} \). We used the IS scheme (Section 4) with IS control \( \zeta(\cdot,\cdot) \) for the one-dimensional Kuramoto model (6) obtained by solving (36) numerically using finite differences (see Appendix E for more details about the numerical solver) and linear interpolation throughout the domain.

Two numerical experiments were conducted to verify variance reduction from IS. In the first experiment shown in Figure 4a, we verified variance reduction on the MC estimator of the inner expectation conditioned on an empirical law \( \mu^{P|N_1} \). To generate Figure 4a, we obtained \( \mu^{P|N_1} \) empirically using the stochastic \( P \)-particle system with \( P = 200 \) using \( N_1 = 32 \) time steps. We used this law to both obtain the IS control \( \zeta(\cdot,\cdot) \) as well as an input to all realizations of the decoupled MV-SDE (29). We simulated decoupled MV-SDE using \( N_2 = 32 \) time steps.

Figure 4a compares sample means and squared coefficients of variation for the MC estimator of the inner conditional expectation with and without IS with respect to the number of sample paths \( M \) for the decoupled MV-SDE. The plots verify that \( \mathbb{P}\{\bar{X}(T) > K\} \approx 2.2 \times 10^{-4} \) with and without IS, whereas the squared coefficient of variation for the estimator reduced approximately 6,000 fold with IS.

In the second experiment, we used \( \bar{P} = 200 \) particles and \( \bar{N} = 100 \) time steps in the stochastic particle system to estimate empirical \( \mu^{\bar{P}|\bar{N}} \) and hence obtain optimal IS control. Then we set \( P = 100, N_1 = N_2 = 32, M_1 = 10^3 \), and varied \( M_2 \) as inputs to Algorithm 2. Figure 4b shows sample mean and squared coefficient of variation of the DLMC estimator with respect to \( M_2 \). We observe estimator convergence with and without IS with significantly reduced variance (approximately \( 10^3 \) fold) for the IS case.

We applied Algorithm 4 to the Kuramoto model (6) with \( \bar{P} = 1000 \) particles and \( \bar{N}_1 = 100 \) time steps to estimate empirical \( \mu^{\bar{P}|\bar{N}} \) using the stochastic particle system and obtain control \( \zeta(\cdot,\cdot) \). We used \( P_0 = 5, N_0 = 4 \) and a relative error tolerance \( \text{TOL}_r \) as inputs to Algorithm 4. The following heuristics were employed to ensure the proposed algorithm’s robustness.

- We used \( \tilde{M}_1 = 10^3 \) and \( \tilde{M}_2 = 10^2 \) to obtain an initial rough estimate for the required quantity to help quantify the required tolerance.
- Algorithm 5 was employed to estimate \( V_{1\ell} \) and \( V_{2\ell} \) with \( \tilde{M}_1 = 50 \) and \( \tilde{M}_2 = 10^3 \) for the first three levels, i.e., \( \ell = 1, 2, 3 \). Assumptions 3 and 4 were employed for subsequent levels to linearly extrapolate \( V_{1\ell}, V_{2\ell} \).
- Algorithm 3 with \( \tilde{M}_1 = \max(M_1, 100) \) and \( \tilde{M}_2 = \max(M_2, 50) \) was used to estimate bias, with \( \tilde{M}_1, \tilde{M}_2 \) the computed optimal sample sizes. Estimated bias was compared with extrapolated bias from the last two levels and the maximum over the three values was taken, to ensure bias estimate robustness for \( \ell > 3 \).

We see in Figure 5a that \( K = 2 \) corresponds to a probability of around \( 2.53 \times 10^{-4} \). Figure 5b shows the exact error of our DLMC estimator for different runs of Algorithm 4 over various prescribed relative error tolerances. We used a reference DLMC approximation computed with \( \text{TOL}_r = 1.5\% \). One can see in Figure 5c that the computational runtime
(a) Left: MC estimator for $\mathbb{P}[\bar{X}(T) > K]$ conditional on fixed empirical $\mu_{P|N_1}$ with and without IS with respect to number of sample paths $M$. Right: MC estimator squared coefficient of variation for $\mathbb{P}[\bar{X}(T) > K]$ conditional on fixed empirical $\mu_{P|N_1}$ with respect to number of sample paths $M$.

(b) Left: DLMC estimator for $\mathbb{P}[\bar{X}(T) > K]$ with and without IS with respect to number of sample paths in inner loop $M_2$. Right: DLMC estimator squared coefficient of variation for $\mathbb{P}[\bar{X}(T) > K]$ with respect to number of sample paths in inner loop $M_2$.

Figure 4: DLMC estimator variance reduction using importance sampling on Kuramoto example (6) for $G(x) = 1_{\{x > K\}}$. 

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Figure 5: Algorithm 4 applied to Kuramoto example (6) for $G(x) = 1_{\{x>K\}}$.

closely follows the predicted theoretical rate of $\mathcal{O}(\text{TOL}^{-4})$ for small relative tolerances. Figure 5d clearly shows the outperformance of our IS scheme with respect to crude DLMC. In addition to the runtime, we also compared the estimated computational work, given by (55), for the IS and crude DLMC methods. Since it is not feasible to run crude DLMC for rare events, we used a heuristic estimate of the computational work of crude DLMC without actually running the algorithm. Figure 5d provides numerical evidence that the IS estimator reduced the computational work to achieve a prescribed relative error tolerance by multiple orders (3 orders of magnitude in this case), implying that our IS estimator dramatically reduced the constant associated with rare event probabilities.

Table 1 shows the number of samples required to reach a given relative tolerance with and without IS for different thresholds $K$. The number of samples required to satisfy a given relative tolerance increases for DLMC without IS as the probability reduces [29]. IS, however, reduces both $M_1$ and $M_2$, although the scheme only acts on the DLMC estimator’s inner expectation. In fact, the required number of samples for IS is significantly less
Table 1: Naive DLMC and DLMC+IS methods estimating rare event probabilities to satisfy \( TOL_r \) for different thresholds \( (K) \).

| K   | \( \mathcal{A}_{MC} \) | \( TOL_r \) | \( \ell \) | \( M_1 \) | \( M_2 \) | \( M_1 \) | \( M_2 \) |
|-----|-----------------|-----------|-----|-----|-----|-----|-----|
| 1   | \( 5.6 \times 10^{-2} \) | 20% | 3   | 59  | 12  | 157 | 65  |
|     |                 | 10% | 4   | 111 | 27  | 284 | 131 |
|     |                 | 5%  | 5   | 167 | 58  | 456 | 297 |
| 1.5 | \( 6.8 \times 10^{-3} \) | 20% | 4   | 41  | 24  | 230 | 325 |
|     |                 | 10% | 5   | 64  | 48  | 386 | 700 |
|     |                 | 5%  | 6   | 105 | 102 | 662 | 1491|
| 2   | \( 2.53 \times 10^{-4} \) | 20% | 5   | 17  | 48  | 477 | 3629|
|     |                 | 10% | 6   | 33  | 90  | 913 | 6929|
|     |                 | 5%  | 7   | 57  | 186 | 1711| 14864|

than without IS, and also remains of the same order regardless of the event rarity. Thus, the proposed DLMC estimator with IS numerically achieved the bounded relative error property [4].

6 Conclusion

This work has shown both theoretically and numerically, under certain assumptions which could be verified numerically, the effectiveness of the novel DLMC estimator with IS based on the decoupling approach [15] when used to estimate rare event probabilities associated with a stochastic particle system in the mean-field limit. For this, we used stochastic optimal control theory to derive the optimal IS change of measure for the decoupled MV-SDE (29). Our numerical experiments show that the above obtained IS control reduces DLMC estimator variance substantially. In the rare event regime, where the standard DLMC approach fails, our approach yields accurate estimates of rare event probabilities with reduced computational effort. Our novel DLMC estimator has a computational cost of \( O(TOL^{-4}) \) which is exactly the same complexity as that of the MC estimator introduced in [20] for smooth, non-rare observables, while substantially reducing the associated constant for rare event probabilities.

Future work includes extending the proposed IS scheme to the multi-dimensional case by using model reduction techniques or stochastic gradient based learning methods, leading to a more generalized and efficient algorithm. The presence of multiple discretization parameters in the decoupled MV-SDE hints towards the use of multi-level and multi-index MC methods coupled with IS to further reduce work complexity of the DLMC estimator.

A Proof for Lemma 1

Assume the minimizer for \( C_{t,x} \) can be attained. Then we prove the equality in (19) by proving both inequalities \( \geq \) and \( \leq \). First, consider \( \geq \):
Let $\zeta^*(t, x) \in \mathcal{Z}$ be the optimal control for $s \in (t, T)$ that minimizes the second moment. From the value function definition \[18\],

$$u(t, x) = \mathbb{E} \left[ G^2(Y_{\zeta^*}(T)) \exp \left\{ - \int_t^T \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds 
- 2 \int_t^T \left( \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \right) \right\} \mid Y_{\zeta^*}(t) = x \right]$$

(66)

$$= \mathbb{E} \left[ G^2(Y_{\zeta^*}(T)) \exp \left\{ - \int_{t+\delta}^{t+\delta} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_{t+\delta}^{t+\delta} \left( \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \right) \right\} \mid Y_{\zeta^*}(t) = x\right]$$

(67)

$$= \mathbb{E} \left[ \mathbb{E} \left[ G^2(Y_{\zeta^*}(T)) \exp \left\{ - \int_t^{t+\delta} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_t^{t+\delta} \left( \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \right) \right\} \mid Y_{\zeta^*}(t) = x\right] \left| Y_{\zeta^*}(t) = x, \mathcal{F}_{t+\delta} \right. \right]$$

(68)

where we recall that $\mathcal{F}_{t+\delta}$ is the Wiener process filtration until time $t + \delta$.

Considering Markovianity for process $Y_{\zeta^*}$, \[68\] can be expressed as

$$u(t, x) = \mathbb{E} \left[ G^2(Y_{\zeta^*}(T)) \exp \left\{ - \int_{t+\delta}^{t+\delta} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds 
- 2 \int_{t+\delta}^{t+\delta} \left( \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \right) \right\} \mid Y_{\zeta^*}(t + \delta) \right]$$

(69)

$$= \mathbb{E} \left[ \exp \left\{ - \int_t^{t+\delta} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_t^{t+\delta} \left( \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \right) \right\} \mid Y_{\zeta^*}(t) = x\right] \right] \right]$$

(70)

Since $\zeta^*$ may not be an optimal control from time $t + \delta$ to $T$ given $Y_{\zeta^*}(t + \delta)$, we can write from the definition of the value function \[18\] that,

$$C_{t+\delta,x(t+\delta)}(\zeta^*) \geq u(t + \delta, x(t + \delta)).$$

(71)
Substituting (71) into (70),

\[ u(t, x) \geq \mathbb{E} \left[ \exp \left\{ - \int_{t}^{t+\delta} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_{t}^{t+\delta} \langle \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \rangle \right\} \right] \]

\[ u(t+\delta, x(t+\delta)) \mid Y_{\zeta^*}(t) = x \] \quad (72)

and taking the minimum over all controls \( \zeta^*(t, x) \) in \([t, t+\delta]\)

\[ u(t, x) \geq \min_{\zeta^*:[t,t+\delta] \rightarrow \mathbb{R}^d} \mathbb{E} \left[ \exp \left\{ - \int_{t}^{t+\delta} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_{t}^{t+\delta} \langle \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \rangle \right\} \right] \]

\[ u(t+\delta, x(t+\delta)) \mid Y_{\zeta^*}(t) = x \] \quad (73)

Now consider the second inequality \( \leq \). Let \( \zeta^+(t, x) \) be some arbitrary control from \( t \) to \( t+\delta \). Given \( Y_{\zeta^*}(t+\delta) \), let \( \zeta^+(t, x) \) be the optimal control from \( t+\delta \) to \( T \), and define a new control \( \zeta'(t, x) = (\zeta^+, \zeta^+) \) over \([t, T]\). From (18),

\[ u(t, x) \leq G_{t,x}(\zeta') \] \quad (74)

\[ \leq \mathbb{E} \left[ G^2(Y_{\zeta'}(T)) \exp \left\{ - \int_{t}^{T} \| \zeta'(s, Y_{\zeta'}(s)) \|^2 ds - 2 \int_{t}^{T} \langle \zeta'(s, Y_{\zeta'}(s)), dW(s) \rangle \right\} \right] \]

\[ \mid Y_{\zeta'}(t) = x \] \quad (75)

\[ \leq \mathbb{E} \left[ G^2(Y_{\zeta'}(T)) \exp \left\{ - \int_{t}^{t+\delta} \| \zeta^+(s, Y_{\zeta^+}(s)) \|^2 ds - 2 \int_{t}^{t+\delta} \langle \zeta^+(s, Y_{\zeta^+}(s)), dW(s) \rangle \right\} \right] \]

\[ \exp \left\{ - \int_{t+\delta}^{T} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_{t+\delta}^{T} \langle \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \rangle \right\} \mid Y_{\zeta^*}(t) = x \] \quad (76)

\[ \leq \mathbb{E} \left[ \mathbb{E} \left[ G^2(Y_{\zeta'}(T)) \exp \left\{ - \int_{t}^{t+\delta} \| \zeta^+(s, Y_{\zeta^+}(s)) \|^2 ds - 2 \int_{t}^{t+\delta} \langle \zeta^+(s, Y_{\zeta^+}(s)), dW(s) \rangle \right\} \right] \right. \]

\[ \exp \left\{ - \int_{t+\delta}^{T} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds - 2 \int_{t+\delta}^{T} \langle \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \rangle \right\} \]

\[ \mid Y_{\zeta^*}(t) = x, \mathcal{F}_{t+\delta} \] \quad (77)

and we can express (77) as

\[ u(t, x) \leq \mathbb{E} \left[ G^2(Y_{\zeta'}(T)) \exp \left\{ - \int_{t+\delta}^{T} \| \zeta^*(s, Y_{\zeta^*}(s)) \|^2 ds \right\} \right] \]
\begin{align*}
-2 \int_{t+\delta}^{T} \langle \zeta^*(s, Y_{\zeta^*}(s)), dW(s) \rangle \bigg\} \bigg| Y_{\zeta^*}(t + \delta) \bigg| Y_{\zeta^*}(t) = x \bigg].
\end{align*}

Considering optimality of control $\zeta^*$ in $[t + \delta, T]$, we can express (78) as

\begin{align*}
u(t, x) \leq \mathbb{E} \left[ \exp \left\{ - \int_{t}^{t+\delta} \| \zeta^+(s, Y_{\zeta^*}(s)) \|^{2} ds - 2 \int_{t}^{t+\delta} \langle \zeta^+(s, Y_{\zeta^*}(s)), dW(s) \rangle \right\} \right. \\
u(t + \delta, x(t + \delta)) \bigg| Y_{\zeta^*}(t) = x \bigg].
\end{align*}

Taking the minimum over all controls $\zeta^+ \in \mathcal{Z}$ over $[t, t + \delta]$,

\begin{align*}
u(t, x) \leq \min_{\zeta^+ : [t, t+\delta] \rightarrow \mathbb{R}^d} \mathbb{E} \left[ \exp \left\{ - \int_{t}^{t+\delta} \| \zeta^+(s, Y_{\zeta^*}(s)) \|^{2} ds - 2 \int_{t}^{t+\delta} \langle \zeta^+(s, Y_{\zeta^*}(s)), dW(s) \rangle \right\} \right. \\
u(t + \delta, x(t + \delta)) \bigg| Y_{\zeta^*}(t) = x \bigg].
\end{align*}

Equations (73) and (80) prove the equality (19). This completes the proof.

\section*{B \ Proof for Theorem 1}

From Lemma 1, the value function defined in (18) satisfies

\begin{align*}
u(t, x) = \min_{\zeta \in \mathcal{Z}} \mathbb{E} \left[ \exp \left\{ - \int_{t}^{t+\delta} \| \zeta(s, Y_{\zeta}(s)) \|^{2} ds \right\} \exp \left\{ -2 \int_{t}^{t+\delta} \langle \zeta(s, Y_{\zeta}(s)), dW(s) \rangle \right\} \right. \\
u(t + \delta, Y_{\zeta}(t + \delta)) \bigg| Y_{\zeta}(t) = x \bigg].
\end{align*}

We then use the truncated Taylor series expansion on function $\exp\{x\}$ for small $\delta$,

\begin{align*}
\exp\left\{ - \int_{t}^{t+\delta} \| \zeta(s, Y_{\zeta}(s)) \|^{2} ds \right\} = 1 - \int_{t}^{t+\delta} \| \zeta(s, Y_{\zeta}(s)) \|^{2} ds \\
+ \frac{1}{2} \left( \int_{t}^{t+\delta} \| \zeta(s, Y_{\zeta}(s)) \|^{2} ds \right)^{2} + \text{h.o.t},
\end{align*}

\begin{align*}
\exp\left\{ -2 \int_{t}^{t+\delta} \langle \zeta(s, Y_{\zeta}(s)), dW(s) \rangle \right\} = 1 - 2 \int_{t}^{t+\delta} \langle \zeta(s, Y_{\zeta}(s)), dW(s) \rangle \\
+ 2 \left( \int_{t}^{t+\delta} \langle \zeta(s, Y_{\zeta}(s)), dW(s) \rangle \right)^{2} + \text{h.o.t}.
\end{align*}
Next, we write down Itô’s formula for \( u(t + \delta, x(t + \delta)) \),
\[
    u(t + \delta, x(t + \delta)) = u(t, x) + \int_t^{t+\delta} \left( \partial_t u + \langle b + \sigma \zeta, \nabla u \rangle + \frac{1}{2} (\sigma \sigma^T) : \nabla^2 u \right) \ dt \\
    + \int_t^{t+\delta} \langle \sigma \nabla u, dW(s) \rangle;
\]
\[\text{(84)}\]

Substituting (82), (83), and (84) in (81) and considering only the leading terms,
\[
    u(t, x) = \min_{\zeta \in \mathbb{Z}} \left\{ u(t, x) + \mathbb{E} \left[ \int_t^{t+\delta} \| \zeta \|² dt \mid Y_\zeta(t) = x \right] \\
    + \mathbb{E} \left[ \int_t^{t+\delta} \left( \partial_t u + \langle b + \sigma \zeta, \nabla u \rangle + \frac{1}{2} (\sigma \sigma^T) : \nabla^2 u \right) dt \mid Y_\zeta(t) = x \right] \\
    + \mathbb{E} \left[ \int_t^{t+\delta} \langle \sigma \nabla u, dW_s \rangle \mid Y_\zeta(t) = x \right] - 2\mathbb{E} \left[ \int_t^{t+\delta} \langle \sigma \zeta, \nabla u \rangle dt \mid Y_\zeta(t) = x \right] + \text{h.o.t.} \right\}. 
\]
\[\text{(85)}\]

Assuming continuity of conditional expectation on \( Y_\zeta(t) = x \) as \( \delta \) tends to 0,
\[
    0 = \min_{\zeta \in \mathbb{Z}} \left\{ \| \zeta \|² u + \partial_t u + \langle b, \nabla u \rangle + \frac{1}{2} (\sigma \sigma^T) : \nabla^2 u - \langle \sigma \zeta, \nabla u \rangle \right\} \\
    = \partial_t u + \langle b, \nabla u \rangle + \frac{1}{2} (\sigma \sigma^T) : \nabla^2 u + \min_{\zeta \in \mathbb{Z}} \left\{ \| \zeta \|² u - \langle \sigma \zeta, \nabla u \rangle \right\}. 
\]
\[\text{(86)}\]

Assuming \( u(t, x) > 0, \forall (t, x) \in [0, T] \times \mathbb{R}^d \), we obtain the minimizer for (86) as in (22). Substituting the optimal control \( \zeta^*(t, x) \) in (86), produces (21), which solves for value function \( u \).

\[\text{C Proof for Theorem 3}\]

We used the Lagrangian multiplier method to solve (56), with corresponding Lagrangian
\[
    \mathcal{L} = M_1 N_1 P^2 + M_1 M_2 N_2 P + \lambda_1 \left( \frac{C_P}{P} + \frac{C_{n_1}}{N_1} + \frac{C_{n_2}}{N_2} - \theta \text{TOL} \right) \\
    + \lambda_2 \left( C_\alpha^2 \left( \frac{C_1}{P M_1} + \frac{C_2}{M_1 M_2} \right) - (1 - \theta)^2 \text{TOL}^2 \right), \tag{87}\]

where \( \lambda_1 \) and \( \lambda_2 \in \mathbb{R} \) are Lagrangian multipliers. Hence, we obtain optimality conditions for (87),
\[
    \frac{\partial \mathcal{L}}{\partial M_1} = 0 \implies N_1 P^2 + M_2 N_2 P = \lambda_2 C_\alpha^2 \left( \frac{C_1}{P M_1} + \frac{C_2}{M_1 M_2} \right), \\
    \frac{\partial \mathcal{L}}{\partial M_2} = 0 \implies M_1 N_2 P = \frac{\lambda_2 C_2 C_\alpha^2}{M_1 M_2^2}, 
\]
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\[
\frac{\partial L}{\partial N_1} = 0 \Rightarrow \frac{\lambda_1 C_{n_1}}{N_1^2} = M_1 P^2,
\]
\[
\frac{\partial L}{\partial N_2} = 0 \Rightarrow \frac{\lambda_1 C_{n_2}}{N_2^2} = M_1 M_2 P,
\]
\[
\frac{\partial L}{\partial P} = 0 \Rightarrow 2M_1 N_1 P + M_1 M_2 N_2 = \frac{\lambda_1 C_p}{P^2} + \frac{\lambda_2 C_2^2 C_1}{M_1 P^2},
\]
\[
\frac{\partial L}{\partial \lambda_1} = 0 \Rightarrow \frac{C_p}{P} + \frac{C_{n_1}}{N_1} + \frac{C_{n_2}}{N_2} = \theta \text{TOL},
\]
\[
\frac{\partial L}{\partial \lambda_2} = 0 \Rightarrow C_2^2 \left( \frac{C_1}{PM_1} + \frac{C_2}{M_1 M_2} \right) = (1 - \theta)^2 \text{TOL}^2.
\]
Solving the above equations for \(P, N_1, N_2, M_1, M_2, \lambda_1, \) and \(\lambda_2,\)

\[
P = \left( \frac{C_p + \beta C_{n_1}}{\alpha + \beta C_{n_2}} \right) = \mathcal{O}(\text{TOL}^{-1}),
\]
\[
N_1 = \left( \frac{\alpha C_p + C_{n_1} + \alpha C_{n_2}}{\theta \text{TOL}} \right) = \mathcal{O}(\text{TOL}^{-1}),
\]
\[
N_2 = \left( \frac{C_p + C_{n_1} + C_{n_2}}{\theta \text{TOL}} \right) = \mathcal{O}(\text{TOL}^{-1}),
\]
\[
M_1 = \frac{\theta}{(1 - \theta)^2} \frac{C_2^2 \left( C_1 + \frac{C_2}{\gamma} \right)}{\left( C_p + \frac{\beta C_{n_1}}{\alpha} + \beta C_{n_2} \right) \text{TOL}} = \mathcal{O}(\text{TOL}^{-1}),
\]
\[
M_2 = \left( \gamma C_p + \frac{\gamma \beta C_{n_1}}{\alpha} + \beta \gamma C_{n_2} \right) = \mathcal{O}(\text{TOL}^{-1}),
\]

where constants

\[
\alpha = \left( \frac{C_2}{C_1} \right)^{\frac{1}{2}} \left( \frac{C_{n_1}}{C_{n_2}} \right)^{\frac{3}{2}},
\]
\[
\gamma = \left( \frac{C_2}{C_1} \right)^{\frac{2}{3}} \left( \frac{C_{n_1}}{C_{n_2}} \right)^{\frac{1}{3}},
\]
\[
\beta = \frac{\left( \alpha^2 \frac{C_p}{C_{n_1}} \right)}{(\alpha + \gamma)}.
\]
Substituting optimal parameters (88) into (55),

\[
W = M_1 N_1 P^2 + M_1 M_2 N_2 P = \mathcal{O}(\text{TOL}^{-4}).
\]
D Estimating $V_{1L}$ and $V_{2L}$ for adaptive DLMC

**Algorithm 5:** Estimating constants $V_{1L}$ and $V_{2L}$ for adaptive DLMC algorithm

**Inputs:** $P_L, N_L, M_1, M_2, \zeta(\cdot, \cdot)$; for $m_1 = 1, \ldots, M_1$ do 
  Generate $(\mu_{P_L|N_L}^{(m_1)})$ realization with $P_L$-particle system and $N_L$ time steps using (38); 
  for $m_2 = 1, \ldots, M_2$ do 
    Given $(\mu_{P_L|N_L}^{(m_1)})$ and $\zeta(\cdot, \cdot)$, solve decoupled MV-SDE with $N_L$ time steps using (40); 
    Compute $\overline{G} \left( \left( \bar{X}_{\zeta}^{P_L|N_L|N_L}(T) \right)^{(m_1,m_2)} \right);$ 
    Compute $(\mathbb{L}_{P_L|N_L}^{(m_1,m_2)} N_L)$ using (42); 
  end 
  Approximate $\mathbb{E} \left[ G \left( X_{\zeta}^{P_L|N_L|N_L}(T) \right) \mathbb{L}_{P_L|N_L|N_L} \mid (\mu_{P_L|N_L}^{(m_1)}) \right]$ by 
  $\frac{1}{M_2} \sum_{m_2=1}^{M_2} G \left( \left( X_{\zeta}^{P_L|N_L|N_L}(T) \right)^{(m_1,m_2)} \right) \mathbb{L}_{P_L|N_L|N_L}^{(m_1,m_2)}$; 
  Approximate $\text{Var} \left[ G \left( X_{\zeta}^{P_L|N_L|N_L}(T) \right) \mathbb{L}_{P_L|N_L|N_L} \mid (\mu_{P_L|N_L}^{(m_1)}) \right]$ by sample variance of 
  $\left\{ G \left( \left( X_{\zeta}^{P_L|N_L|N_L}(T) \right)^{(m_1,m_2)} \right) \mathbb{L}_{P_L|N_L|N_L}^{(m_1,m_2)} \right\}_{m_2=1}^{M_2}$; 
end 
Approximate $V_{1L}$ by sample variance of 
\[ \left\{ \mathbb{E} \left[ G \left( X_{\zeta}^{P_L|N_L|N_L}(T) \right) \mathbb{L}_{P_L|N_L|N_L} \mid (\mu_{P_L|N_L}^{(m_1)}) \right] \right\}_{m_1=1}^{M_1} ; \]
Approximate $V_{2L}$ by \[ \frac{1}{M_1} \sum_{m_1=1}^{M_1} \text{Var} \left[ G \left( X_{\zeta}^{P_L|N_L|N_L}(T) \right) \mathbb{L}_{P_L|N_L|N_L} \mid (\mu_{P_L|N_L}^{(m_1)}) \right] ; \]

E Building Numerical PDE Solver for Optimal IS Control

We consider the one-dimensional KBE version of (36)

\[
\begin{aligned}
\frac{\partial v}{\partial t} + b \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_1(x, X_j^P(t)) \right) \frac{\partial v}{\partial x} \\
+ \frac{1}{2} \sigma^2 \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) \frac{\partial^2 v}{\partial x^2} = 0, \quad (t, x) \in [0, T) \times \mathbb{R}
\end{aligned}
\]

with optimal control

\[
\zeta(t, x) = \sigma^T \left( x, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x, X_j^P(t)) \right) \frac{\partial \log v}{\partial x}(t, x).
\]
The goal is to estimate control $\zeta(t, x)$ given $\mu^P_t$. Let $G \equiv -b \frac{\partial}{\partial x} - \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2}$. Then (90) can be expressed as
\[
\begin{aligned}
\{ & \partial_t v(t, x) = Gv(t, x), (t, x) \in [0, T) \times \mathbb{R} \\
& v(T, x) = |G(x)|, x \in \mathbb{R}. \}
\end{aligned}
\]

In order to discretize the PDE using finite-differences (FD), the $x$-space as well as the time space has to be discretized. This is done by introducing the grids
\[
0 = t_0 < t_1 < \ldots < t_{N_t} = T, \quad \text{and} \quad (92)
\]
\[
-x_b = x_0 < x_1 < \ldots < x_{N_x} = x_b. \quad (93)
\]

Note that, for the space dimension $x$, we approximate the domain $\mathbb{R}$ by an appropriately chosen $[-x_b, x_b]$. We use uniform grids in both dimensions.
\[
t_n = n \Delta t, \quad n = 0, \ldots, N_t \quad \text{and} \quad (94)
\]
\[
x_i = -x_b + i \Delta x, \quad i = 0, \ldots, N_x. \quad (95)
\]

Let $v^n_i \equiv v(t_n, x_i) \equiv v(n \Delta t, -x_b + i \Delta x)$. Then perform discretization in $x$ using central differences,
\[
\frac{\partial v^n_i}{\partial x} = \frac{v^n_{i+1} - v^n_{i-1}}{2 \Delta x} + O(\Delta x^2). \quad (96)
\]
\[
\frac{\partial^2 v^n_i}{\partial x^2} = \frac{v^n_{i+1} - 2v^n_i + v^n_{i-1}}{\Delta x^2} + O(\Delta x^2). \quad (97)
\]

Therefore, the $G$ operator applied to $v$ at time $t_n$ can be expressed as
\[
G v \big|_{i}^{n} = -b \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_1(x_i, X^P_j(t_n)) \right) \frac{\partial v^n_i}{\partial x} - \frac{\sigma^2}{2} \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x_i, X^P_j(t_n)) \right) \frac{\partial^2 v^n_i}{\partial x^2} \big|_{i}^{n}
\]
\[
= -b \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_1(x_i, X^P_j(t_n)) \right) \frac{v^n_{i+1} - v^n_{i-1}}{2 \Delta x}
\]
\[
- \frac{\sigma^2}{2} \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x_i, X^P_j(t_n)) \right) \frac{v^n_{i+1} - 2v^n_i + v^n_{i-1}}{\Delta x^2} + O(\Delta x^2). \quad (98)
\]

Grouping the coefficients together,
\[
G v \big|_{i}^{n} = \left( \frac{b \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_1(x_i, X^P_j(t_n)) \right)}{2 \Delta x} - \frac{\sigma^2 \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x_i, X^P_j(t_n)) \right)}{2 \Delta x^2} \right) v^n_{i-1} = \eta^n_{i-1}
\]

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\[-\left( b \left( x_i, \frac{1}{\Delta x} \sum_{j=1}^{P} \kappa_1(x_i, X_j(t_n)) \right) \frac{\sigma_2}{2 \Delta x} \right) v_{i+1}^n + \sigma_2 \left( x_i, \frac{1}{\Delta x} \sum_{j=1}^{P} \kappa_2(x_i, X_j(t_n)) \right) \varepsilon_{i+1}^n \]

\[= d_{u,i}^n v_{i+1}^n + d_n v_i^n + d_n v_{i+1}^n + O(\Delta x^2). \]  

(99)

We can formulate a linear system for each time step using (99). Let \( \mathbf{v}^n \equiv (v_0^n, \ldots, v_{N_x}^n)^T \). Then, the finite difference can be expressed as

\[(G \mathbf{v}^n)_{i=0}^{N_x} = G^n \mathbf{v}^n + O(\Delta x^2), \]

where \( G^n \in \mathbb{R}^{N_x \times N_x} \) is the discretization operator at time \( t_n \),

\[
G^n = \begin{pmatrix}
d_{0}^n & d_{u,0}^n & 0 & 0 & \cdots & 0 \\
d_{u,1}^n & d_{1}^n & d_{u,1}^n & 0 & \cdots & 0 \\
0 & \ddots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & 0 \\
0 & 0 & \cdots & d_{l,N-1}^n & d_{N-1}^n & d_{u,N-1}^n \\
0 & 0 & \cdots & d_{l,N}^n & d_{N}^n & d_{u,N}^n
\end{pmatrix}. \]

(101)

We used the generic \( \theta \) time-discretization scheme family,

\[
\frac{v_i^n - v_i^{n-1}}{\Delta t} = \theta \mathbf{g}_i^n \mathbf{v}_i^n + (1 - \theta) \mathbf{g}_i^{n-1} \mathbf{v}_i^{n-1}, \]

(102)

where \( \mathbf{g}_i^n \in \mathbb{R}^{1 \times N_x} \) is the \( i \)-th row for \( G^n \). Hence, time step update in matrix-vector form can be expressed as

\[
\mathbf{v}^{n-1} = (I + (1 - \theta) \Delta t G^n)^{-1} (I - \theta \Delta t G^n) \mathbf{v}^n. \]

(103)

Different \( \theta \) values correspond to different time-stepping schemes. This study used \( \theta = 0.5 \) corresponding to the Crank-Nicholson scheme, with convergence \( O(\Delta t^2) \). We have terminal time condition at \( t = T \),

\[
\mathbf{v}^N_t = (G(x_i))_{i=0}^{N_x} = (G(-x_b + i \Delta x))_{i=0}^{N_x}. \]

(104)

However, (90) does not specify boundary conditions. To circumvent this problem, we use non-reflective boundary conditions at \( x = -x_b \) and \( x = x_b \) to emulate that the actual domain is not bounded at the boundaries, i.e., \( v_0^n \) and \( v_0^n \) are extrapolated from known values,

\[
v_0^n \approx v_2^n + \frac{x_2 - x_0}{x_2 - x_1} (v_1^n - v_2^n) = 2v_1^n - v_2^n, \]

(105)
\[ v^n_{N_x} \approx v^{n-2}_{N_x} + \frac{x_{N_x} - x_{N_x-2}}{x_{N_x-1} - x_{N_x-2}}(v^n_{N_x-1} - v^n_{N_x-2}) = 2v^n_{N_x-1} - v^n_{N_x-2}. \]  

(106)

We then prescribe (105) and (106) as Dirichlet boundary conditions. This also modifies some \( G^n \) elements,

\[
Gv|_1^n = d^n_{t,1} v^n_0 + d^n_{11} v^n_1 + d^n_{u,1} v^n_2
\]

\[
\approx 2v^n_{N_x-1} - v^n_{N_x-2}
\]

\[ \Rightarrow g^n_1 = (0, 2d^n_{t,1} + d^n_{11}, d^n_{u,1} - d^n_{t,1}, 0, \ldots, 0). \]  

(107)

\[
Gv|_{N_x-1}^n = d^n_{t,N_x-1} v^n_{N_x-2} + d^n_{N_x-1} v^n_{N_x-1} + d^n_{u,N_x-1} v^n_{N_x} \approx 2v^n_{N_x-1} - v^n_{N_x-2}
\]

\[ \Rightarrow g^n_{N_x-1} = (0, \ldots, 0, d^n_{t,N_x-1} - d^n_{u,N_x-1}, d^n_{N_x-1} + 2d^n_{u,N_x-1}, 0). \]  

(108)

Hence, the modified discretization matrix \( G^n \) can now include boundary conditions

\[
G^n = \begin{pmatrix}
1 & 0 & 0 & 0 & \ldots & 0 \\
0 & d^n_1 & d^n_{u,1} & 0 & \ldots & 0 \\
0 & d^n_{t,2} & d^n_{u,2} & \ddots & \vdots & \\
\vdots & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & d^n_{t,N_x-1} & d^n_{u,N_x-1} & 0 \\
0 & 0 & \ldots & 0 & 0 & 1
\end{pmatrix}.
\]  

(109)

Since the boundary conditions are fixed by Dirichlet conditions, the computation needs to only be done in the inner \( \mathbb{R}^{(N_x-2) \times (N_x-2)} \) sub-matrix. Having obtained the numerical solution for \( v(t, x) \), we can apply central differences to (91) to obtain numerical solutions to optimal control,

\[
\zeta(t_n, x_i) \approx \sigma^T \left( x_i, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x_i, X_j^P(t_n)) \right) \frac{\log v^n_{i+1} - \log v^n_{i-1}}{2\Delta x}.
\]  

(110)

The boundary points use one-sided finite difference formulae,

\[
\zeta(t_n, x_0) \approx \sigma^T \left( x_0, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x_0, X_j^P(t_n)) \right) \frac{\log v^n_0 - \log v^n_1}{\Delta x}.
\]  

(111)

\[
\zeta(t_n, x_{N_x}) \approx \sigma^T \left( x_{N_x}, \frac{1}{P} \sum_{j=1}^{P} \kappa_2(x_{N_x}, X_j^P(t_n)) \right) \frac{\log v^n_{N_x} - \log v^n_{N_x-1}}{\Delta x}.
\]  

(112)
We now have optimal control at grid points (92) and (93). We can extend this control throughout the $[0,T] \times \mathbb{R}$ domain using linear interpolation in both time and space. Since (90) is advection-diffusion type, choosing the ratio $\frac{\Delta t}{\Delta x}$ is important to ensure stable solutions. For (6) we choose $\frac{\Delta t}{\Delta x} = 0.2$.

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