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Unbiased Multi-step Estimators for the Monte Carlo Evaluation of Certain Functional Integrals

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A general class of unbiased Monte Carlo estimators for functional integrals is introduced. This class contains previously known unbiased estimators as well as some classical biased estimators improved with special correction terms. The new algorithm is applicable under weaker conditions on the functional integral. Numerical results of simulation studies are presented. The variance reduction problem in the infinite-dimensional space is considered.

1. INTRODUCTION

Functional integration on the one hand (cf. [5, 11, 17]) and Monte Carlo methods on the other hand (cf. [13, 16, 4]) play an increasing role in quantum and statistical physics. Thus, the construction of effective Monte Carlo algorithms for the evaluation of functional integrals is of considerable interest (cf. [18, 19]).

The purpose of this paper is to introduce a rather general class of unbiased estimators for certain functional integrals. This class contains the unbiased estimators proposed in [20] as well as some classical biased estimators (cf. [3]) improved with special correction terms. The new algorithm is applicable under weaker conditions on the functional integrals.

We consider functional integrals of the form

$$I_c(t_0, x_0, t, x) := E \exp\left(\int_{t_0}^{t} c(s, w(s))\, ds\right), \tag{1.1}$$

where w is the d-dimensional Brownian bridge from x_0 at the time t_0 into x at the time t, and $x_0, x \in R^d$. The symbol E denotes the mathematical expectation.

The function $c: [t_0, t] \times R^d \to R$ is supposed to be such that the integral functional of the Wiener trajectory

$$\int_{t_0}^{t} c(s, w(s))\, ds$$

is an a.s. finite random variable with a finite exponential moment (1.1).

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Functional integrals of this kind are important because of their connection with Green's function for certain partial differential equations (cf. the Feynman–Kac formula). Various parameters of quantum-mechanical systems (like the lowest energy level) can be evaluated numerically with the help of the functional integral representation of Green's function (cf. [6, 10]).

Monte Carlo methods for the evaluation of functional integrals (1.1) have been investigated in many papers (cf. the extensive reference list in [20]). They can be described as follows. First the functional of a continuous path

$$F(w) := \exp\left(\int_{t_0}^{t} c(s, w(s))\, ds\right)$$

is replaced by a functional η of a time-discrete trajectory ω. The resulting error is called the systematic error of the algorithm:

$$EF(w) = E\eta(\omega) + \text{systematic error.}$$

Then, the mathematical expectation $E\eta$ is evaluated by the empirical mean over independent samples (ω_j) of ω, generated by means of a random number generator:

$$E\eta(\omega) = (1/N) \sum_{j=1}^{N} \eta(\omega_j) + \text{statistical error.}$$

The random variable η is called an estimator for the functional integral (1.1). The estimator depends on various parameters like the probability distribution of ω.

Consequently, two main problems have to be considered in the theory of stochastic numerical algorithms for functional integrals:

the approximation problem—to estimate the systematic error in dependence on the parameters;

the variance reduction problem—to reduce the statistical error, which depends on the variance of the estimator, by an appropriate choice of the parameters.

An estimator is called unbiased if it is not connected with any systematic error, i.e., if $E\eta(\omega) = EF(w)$. Unbiased estimators are very convenient because of the simple error analysis. The statistical error can be estimated by means of confidence intervals during the process of computation.

In Section 2 we introduce the basic ideas, leading to the construction of the new type of unbiased estimators, and formulate the main results. Section 3 contains some examples illustrating the rich variety of multi-step estimators. The proof of the theorems of Section 2 are collected in Section 4. A more detailed analysis of concrete estimators is performed in Section 5. Some numerical examples are given in Section 6. Section 7 contains some reflections about the multi-step estimation scheme from the point of view of importance sampling in the infinite-dimensional space.

2. Multi-step Estimators; Basic Ideas and Results

The estimators to be introduced are based on the following three ideas:

— a measure substitution is performed in the functional integral (1.1), following the idea of the importance sampling procedure known from the finite-dimensional case (cf. the comments in Section 7);

— a mixed integration formula is derived for the transformed functional integral, using an idea by Fosdick [9];

— estimators proposed in [20] are used to estimate the inner functional integrals appearing in the mixed integration formula.

First we need some notations. Consider the set

$$T=\{(s_1, y_1, s_2, y_2): t_0 \leqq s_1 < s_2 \leqq t,\ y_1, y_2 \in R^d\},$$

where $-\infty < t_0 < t < \infty$. For any $(s_1, y_1, s_2, y_2) \in T$, we introduce the measure $m_0(s_1, y_1, s_2, y_2)$ on the space of continuous vector functions $\{v: [s_1, s_2] \to R^d\}$ generated by the corresponding conditional Wiener process subject to the conditions $w(s_1)=y_1$ and $w(s_2)=y_2$.

Further we consider the set K of measurable functions $c: [t_0, t] \times R^d \to R$ such that $\int_{s_1}^{s_2} c(s, v(s))\, ds$ is measurable and a.s. finite with respect to the measure $m_0(s_1, y_1, s_2, y_2)$, and $I_c(s_1, y_1, s_2, y_2) := \int \exp(\int_{s_1}^{s_2} c(s, v(s))\, ds)\, dm_0(s_1, y_1, s_2, y_2)(v) < \infty$, for any $(s_1, y_1, s_2, y_2) \in T$.

For any $c \in K$, we introduce the measure $m_c(s_1, y_1, s_2, y_2)$ given by its Radon–Nikodym derivative

$$\frac{dm_c(s_1, y_1, s_2, y_2)}{dm_0(s_1, y_1, s_2, y_2)}(v) = \exp\left(\int_{s_1}^{s_2} c(s, v(s))\, ds\right) I_c(s_1, y_1, s_2, y_2)^{-1}. \tag{2.1}$$

Sometimes we will use the notation

$$I_{g,c}(s_1, y_1, s_2, y_2) := \int \exp\left(\int_{s_1}^{s_2} g(s, v)\, ds\right) dm_c(s_1, y_1, s_2, y_2)(v),$$

$(s_1, y_1, s_2, y_2) \in T$, for appropriate functions g. Further, we denote $I_{g,0}(s_1, y_1, s_2, y_2) =: I_g(s_1, y_1, s_2, y_2)$.

The following theorem provides a natural interpretation of the measure m_c.

THEOREM 2.1. *The measure $m_c(s_1, y_1, s_2, y_2)$ corresponds to a Markov process with the transition density*

$$\begin{aligned} &p_c(u_1, z_1, u_2, z_2/s_2, y_2) \\ &\quad := p_0(u_1, z_1, u_2, z_2/s_2, y_2) \frac{I_c(u_1, z_1, u_2, z_2)\, I_c(u_2, z_2, s_2, y_2)}{I_c(u_1, z_1, s_2, y_2)}, \end{aligned} \tag{2.2}$$

where $p_0(.../s_2, y_2)$ *denotes the transition density of the conditional Wiener process corresponding to* $m_0(s_1, y_1, s_2, y_2)$, $(s_1, y_1, s_2, y_2) \in T$, $s_1 \leq u_1 < u_2 < s_2$, $z_1, z_2 \in R^d$.

It can be shown by simple calculations that the processes corresponding to the measures $m_c(s_1, y_1, s_2, y_2)$, $(s_1, y_1, s_2, y_2) \in T$, are compatible in the following sense. Consider (s_1, y_1, s_2, y_2), $(s_1, y_1, s_3, y_3) \in T$, $s_2 < s_3$. Then the $m_c(s_1, y_1, s_2, y_2)$-process is equivalent to the conditional $m_c(s_1, y_1, s_3, y_3)$-process under the condition that it is in y_2 at the time s_2. Therefore, it is correct to speak about the m_c-process without mentioning the index $(s_1, y_1, s_2, y_2) \in T$.

The second theorem plays the major role in the construction of the new class of unbiased estimators.

THEOREM 2.2. *Consider* $c, c_0 \in K$, (t_i): $t_0 < t_1 < \cdots < t_{n+1} := t$, $x, x_0 \in R^d$, $x_{n+1} := x$. *Then the following representation formula holds*:

$$\begin{aligned} I_c(t_0, x_0, t, x) = I_{c0}(t_0, x_0, t, x) & \\ & \times \int_{(R^d)^n} \prod_{i=0}^{n-1} p_{c0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x) \\ & \times \prod_{i=0}^{n} I_{c-c0, c0}(t_i, x_i, t_{i+1}, x_{i+1}) \\ & \times dx_1 \cdots dx_n. \end{aligned}$$

Such representation theorems are called mixed integration formulas in the literature (cf. [2, 9]). The usual way to apply them to the construction of numerical algorithms for the functional integral $I_c(t_0, x_0, t, x)$ is to approximate the inner functional integrals (like $I_{c-c0,c0}(t_i, x_i, t_{i+1}, x_{i+1})$ in Theorem 2.2) and to estimate the remaining finite-dimensional integral (cf. Example 2 in Section 3).

Instead of this, we use unbiased estimators from [20] for the inner functional integrals $I_{c-c0,c0}(t_i, x_i, t_{i+1}, x_{i+1})$ and combine them with an estimator for the finite-dimensional integral over $(R^d)^n$. We suppose the functional integral $I_{c0}(s_1, y_1, s_2, y_2)$, $(s_1, y_1, s_2, y_2) \in T$, to be known explicitly (cf. Example 1 in Section 3). According to Theorem 2.1, the transition density p_{c_0} of the process generating the measure m_{c0} is also known explicitly. Consequently, the unbiased estimators from [20] are applicable to functional integrals with respect to the measure m_{c0}.

Let $(\xi_{c-c0,c0}(s_1, y_1, s_2, y_2))$, $(s_1, y_1, s_2, y_2) \in T$, be a family of estimators such that

$$E\xi_{c-c0,c0}(s_1, y_1, s_2, y_2) = I_{c-c0,c0}(s_1, y_1, s_2, y_2).$$

The finite-dimensional integral over $(R^d)^n$ is evaluated by a standard one-point-estimator (cf., e.g., [8]). Let the distribution of $(x_1, ..., x_n)$ be given by a density $P(x_1, ..., x_n)$ satisfying the condition $P(x_1, ..., x_n) > 0$, if $\prod_{i=0}^{n-1} p_{c0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x) > 0$.

Now we define the estimator for the functional integral $I_c(t_0, x_0, t, x)$ as

$$\eta = I_{c0}(t_0, x_0, t, x) \frac{\prod_{i=0}^{n-1} p_{c0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x)}{P(x_1, ..., x_n)}$$

$$\times \prod_{i=0}^{n} \xi_{c-c_0, c_0}(t_i, x_i, t_{i+1}, x_{i+1}), \tag{2.4}$$

where the estimators $\xi_{c-c_0,c_0}(t_i, x_i, t_{i+1}, x_{i+1})$ are supposed to be independent, given the $(x_1, ..., x_n)$.

The estimators $\xi_{c-c_0,c_0}(t_i, x_i, t_{i+1}, x_{i+1})$ are given on random sequences $(t_{i,j}, x_{i,j})$, $i=0, 1, ..., n$, $j=0, 1, ..., l_i$, forming Markov chains with absorption. The chains start at $(t_{i,0}, x_{i,0}) := (t_i, x_i)$, $i=0, 1, ..., n$. Their distribution parameters are the probability of absorption

$$q_0^{(i)}(s, y),$$

and the transition density

$$q^{(i)}(s_1, y_1; s_2, y_2),$$

$$(s, y), (s_1, y_1), (s_2, y_2) \in [t_i, t_{i+1}) \times R^d.$$

The random lengths of the chains are denoted by l_i, $i=0, 1, ..., n$. We refer to [20] for more details (cf. also Example 3 in Section 3).

The estimator (2.4) depends on the parameters c_0, (t_i), appearing in the mixed integration formula (2.3), on the concrete form of the estimators ξ, and on P, $(q_0^{(i)}, q^{(i)})$, defining the probability distribution of the discrete trajectory $\omega = ((x_i), (t_{i,j}, x_{i,j}))$. Therefore, we use the term "the class of estimators (2.4)" as well as the term "the estimator (2.4)."

The main property of the estimator (2.4) is the subject of the following theorem.

THEOREM 2.3. *Let the estimator η be given in the form* (2.4). *The condition*

$$E|\eta| < \infty \tag{2.5}$$

is necessary and sufficient for η to be unbiased, i.e.,

$$E\eta = I_c(t_0, x_0, t, x).$$

A more detailed investigation of the estimator (2.4) will be performed in Section 5.

3. EXAMPLES

We consider some special cases (concrete values of the parameters) in order to demonstrate the rich variety of the class of estimators (2.4).

EXAMPLE 1. We suppose $n=0$. The estimator (2.4) takes the form

$$\eta = I_{c0}(t_0, x_0, t, x)\, \xi_{c-c0,c0}(t_0, x_0, t, x). \tag{3.1}$$

Thus (for $c_0=0$), the whole variety of estimators proposed in [20] is contained in the class of multi-step estimators (2.4). We call the estimators of the form (3.1) one-step estimators. They have one more degree of freedom, compared with the estimators from [20]. This is the function c_0.

The values $I_{c0}(s_1, y_1, s_2, y_2)$, $(s_1, y_1, s_2, y_2) \in T$, are known explicitly in the case of quadratic c_0 (cf. [17]), where the corresponding m_{c0}-processes are Gaussian. We give the explicit formulas for the case

$$c_0(s, y) = -a^2 y^2/2, \qquad y \in R,\ a>0.$$

The transition density $p_{c0}(s_1, y_1, s_2, y_2/t, x)$ is Gaussian with mean

$$y_1 \frac{\sinh(a(t-s_2))}{\sinh(a(t-s_1))} + x \frac{\sinh(a(s_2-s_1))}{\sinh(a(t-s_1))}$$

and variance

$$\frac{\sinh(a(s_2-s_1))\sinh(a(t-s_2))}{\sinh(a(t-s_1))}.$$

We call the corresponding process the harmonic oscillator process because of its relation to the quantum-mechanical harmonic oscillator having the potential c_0. A similar example was considered in [7], where a special estimator of the type (3.1) also was used for the numerical solution of Schrödinger's equation.

Before turning to the next example, we remember a "shift procedure," which was used in [20] for the purpose of variance reduction. It is based on the following simple transformation of the functional integrals,

$$\begin{aligned} &I_{c-c0,c0}(t_i, x_i, t_{i+1}, x_{i+1}) \\ &\quad = \exp(d_i(t_{i+1}-t_i)) \times I_{c-c0-d_i,c0}(t_i, x_i, t_{i+1}, x_{i+1}), \end{aligned}$$

where $d_i := d(t_i, x_i, t_{i+1}, x_{i+1})$, $i=0, 1, ..., n$, and d is an appropriate measurable function. Replacing $\xi_{c-c0,c0}(t_i, x_i, t_{i+1}, x_{i+1})$ by $\exp(d_i(t_{i+1}-t_i)) \times \xi_{c-c0-d_i,c0}(t_i, x_i, t_{i+1}, x_{i+1})$, the estimator (2.4) can be modified,

$$\begin{aligned} \eta = {} & I_{c0}(t_0, x_0, t, x) \frac{\prod_{i=0}^{n-1} p_{c0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x)}{P(x_1, ..., x_n)} \\ & \times \exp\left(\sum_{i=0}^{n} d_i(t_{i+1}-t_i)\right) \prod_{i=0}^{n} \xi_{c-c0-d_i,c0}(t_i, x_i, t_{i+1}, x_{i+1}). \end{aligned} \tag{3.2}$$

EXAMPLE 2. We suppose the parameter d to be

$$d_i = ((c-c_0)(t_i, x_i) + (c-c_0)(t_{i+1}, x_{i+1}))/2, \tag{3.3}$$

$i=0, 1, ..., n$. Then, the estimator (3.2) is closely related to well-known biased estimators based on Chorin's approximation formula (cf. [3, 14, 1, 12]). Suppose $c_0 = 0$. Then, Chorin's estimators are obtained from (3.2) by omitting the product $\prod_{i=0}^{n}$,

$$\eta = \frac{\prod_{i=0}^{n-1} p_0(t_i, x_i, t_{i+1}, x_{i+1}/t, x)}{P(x_1, ..., x_n)} \times \exp\left(\sum_{i=0}^{n} (c(t_i, x_i) + c(t_{i+1}, x_{i+1}))(t_{i+1} - t_i)/2\right). \tag{3.4}$$

In Chorin's approximation formula, the terms $\exp((c(t_i, x_i) + c(t_{i+1}, x_{i+1}))/2)$ are used as deterministic approximations of the inner functional integrals

$$I_c(t_i, x_i, t_{i+1}, x_{i+1}) = \int \exp\left(\int_{t_i}^{t_{i+1}} c(s, v(s))\, ds\right) \times dm_0(t_i, x_i, t_{i+1}, x_{i+1})(v),$$

$i=0, 1, ..., n$. Thus, the multi-step estimator (3.2), with the parameter d given in (3.3), can be interpreted as Chorin's estimator with a correction term that makes it unbiased.

EXAMPLE 3. Finally, we consider a special choice of the distribution parameters P, $(q_0^{(i)}, q^{(i)})$, and two concrete inner estimators ξ (cf. [20]). We use the parameters

$$P(x_1, ..., x_n) = \prod_{i=0}^{n-1} p_{c_0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x), \tag{3.5}$$

$$q_0^{(i)}(s, y) = \exp(-\gamma(t_{i+1} - s)), \quad (s, y) \in [t_i, t_{i+1}) \times R^d, \tag{3.6}$$

$$\begin{aligned} q^{(i)}(s_1, y_1; s_2, y_2) = {} & p_{c_0}(s_1, y_1, s_2, y_2/t_{i+1}, x_{i+1}) \\ & \times \exp(\gamma(t_{i+1} - s_2))/(\exp(\gamma(t_{i+1} - s_1)) - 1), \\ & (s_1, y_1) \in [t_i, t_{i+1}) \times R^d, \\ & (s_2, y_2) \in (s_1, t_{i+1}) \times R^d, \qquad \gamma > 0. \end{aligned} \tag{3.7}$$

The estimators are

$$\xi^{(1)}_{c-c_0-d_i, c_0}(t_i, x_i, t_{i+1}, x_{i+1})((t_{i,j}, x_{i,j})) = \exp(\gamma(t_{i+1} - t_i))\, \gamma^{-l_i} \prod_{j=1}^{l_i} ((c-c_0)(t_{i,j}, x_{i,j}) - d_i) \tag{3.8}$$

and

$$\xi^{(2)}_{c-c_0-d_i,c_0}(t_i, x_i, t_{i+1}, x_{i+1})((t_{i,j}, x_{i,j}))$$
$$=1+\sum_{k=1}^{l_i} \exp(\gamma(t_{i,k}-t_i))\,\gamma^{-k}\prod_{j=1}^{k}((c-c_0)(t_{i,j}, x_{i,j})-d_i). \tag{3.9}$$

The trajectory $\omega=((x_i), (t_{i,j}, x_{i,j}))$ defined by the parameters (3.5)–(3.7) is closely connected with the m_{c_0}-process. First, the random moments $(t_{i,j})$ are to be generated with a distribution that can easily be obtained from (3.6), (3.7). Then, the random points (x_i), $(x_{i,j})$ are to be chosen independently of $(t_{i,j})$ as the values of a trajectory of the m_{c_0}-process at the moments (t_i) and $(t_{i,j})$, respectively.

Thus, the parameters (3.5)–(3.7) allow a rather clear interpretation of various classes of estimators. Biased estimators (cf. (3.4)) use the trajectory of the basic process at some deterministic moments (t_i). The systematic error can be avoided by using the trajectory of the basic process at random moments. The one-step estimators use this trajectory exclusively at random moments, the multi-step estimators, at some deterministic and some random moments.

4. Proofs of the Theorems of Section 2

First we prove a useful technical assertion.

Lemma 4.1. *Consider $c\in K$, $(s_1, y_1, s_2, y_2)\in T$, and (u_i), $i=0, 1, ..., n+1$, such that $s_1=: u_0<u_1<\cdots<u_{n+1}:=s_2$. Let f and g be measurable functions such that the integral*

$$J:=\int f(v(u_1), ..., v(u_n))\exp\left(\int_{s_1}^{s_2} g(s, v(s), v(u_1), ..., v(u_n))\,ds\right)$$
$$\times\, dm_c(s_1, y_1, s_2, y_2)(v)$$

exists. Then the equality

$$J=\int_{(R^d)^n} f(z_1, ..., z_n)\prod_{i=0}^{n-1} p_0(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2)$$
$$\times\prod_{i=0}^{n} I_c(u_i, z_i, u_{i+1}, z_{i+1})\, I_c(s_1, y_1, s_2, y_2)^{-1}$$
$$\times\prod_{i=0}^{n}\int\exp\left(\int_{u_i}^{u_{i+1}} g(s, v(s), z_1, ..., z_n)\,ds\right)$$
$$\times\, dm_c(u_i, z_i, u_{i+1}, z_{i+1})(v)\, dz_1\cdots dz_n,$$

holds with $z_0:=y_1$ and $z_{n+1}:=y_2$.

Proof. First we substitute the measure m_c by the measure m_0 according to (2.1):

$$J = I_c(s_1, y_1, s_2, y_2)^{-1} \int f(v(u_1), ..., v(u_n))$$
$$\times \exp\left(\int_{s_1}^{s_2} (g(s, v(s), v(u_1), ..., v(u_n)) + c(s, v(s)))\, ds\right)$$
$$\times\, dm_0(s_1, y_1, s_2, y_2)(v).$$

Now we write the expectation with respect to the Wiener process as an integral over the conditional expectations with the condition $w(u_1) = z_1, ..., w(u_n) = z_n$. It follows that

$$J = I_c(s_1, y_1, s_2, y_2)^{-1} \int_{(R^d)^n} \prod_{i=0}^{n-1} p_0(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2) f(z_1, ..., z_n)$$
$$\times E\left\{\prod_{i=0}^{n} \exp\left(\int_{u_i}^{u_{i+1}} (g(s, w(s), z_1, ..., z_n) + c(s, w(s)))\, ds\right)\right/$$
$$\left. w(u_1) = z_1, ..., w(u_n) = z_n\right\} dz_1 ... dz_n.$$

The factors inside the conditional expectation are independent. Consequently, we obtain

$$J = I_c(s_1, y_1, s_2, y_2)^{-1} \int_{(R^d)^n} \left\{ f(z_1, ..., z_n)\right.$$
$$\times \prod_{i=0}^{n-1} p_0(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2)$$
$$\times \prod_{i=0}^{n} \int \exp\left(\int_{u_i}^{u_{i+1}} (g(s, v(s), z_1, ..., z_n) + c(s, v(s)))\, ds\right)$$
$$\left.\times\, dm_0(u_i, z_i, u_{i+1}, z_{i+1})(v)\right\} dz_1 \cdots dz_n.$$

Substituting the measures $m_0(u_i, z_i, u_{i+1}, z_{i+1})$, $i = 0, 1, ..., n$, by the corresponding m_c-measures, one obtains the assertion of the lemma.

Now we are able to prove Theorem 2.1.

Proof of Theorem 2.1. First we prove that p_c satisfies the conditions of a Markov transition density. Lemma 4.1 with $(f, g, c, n) = (1, c, 0, 1)$ provides the equality

$$I_c(s_1, y_1, s_2, y_2) = \int_{R^d} p_0(s_1, y_1, u_1, z_1/s_2, y_2)$$
$$\times I_c(s_1, y_1, u_1, z_1)\, I_c(u_1, z_1, s_2, y_2)\, dz_1, \tag{4.1}$$

which implies the normalization condition for $p_c(.../s_2, y_2)$. To prove the Chapman–Kolmogorov property we consider $s_1 \leqq u_1 < u_2 < u_3 < s_2$, $z_1, z_3 \in R^d$, and write down $p_c(u_1, z_1, u_3, z_3/s_2, y_2)$ according to its definition (2.2). Applying formula (4.1) to $I_c(u_1, z_1, u_3, z_3)$ we obtain

$$\begin{aligned} p_c(u_1, z_1, u_3, z_3/s_2, y_2) = p_0(u_1, z_1, u_3, z_3/s_2, y_2) &\frac{I_c(u_3, z_3, s_2, y_2)}{I_c(u_1, z_1, s_2, y_2)} \\ &\times \int_{R^d} p_0(u_1, z_1, u_2, z_2/u_3, z_3)\, I_c(u_1, z_1, u_2, z_2) \\ &\times I_c(u_2, z_2, u_3, z_3)\, dz_2. \end{aligned}$$

Now we use the property of conditional Markov transition densities

$$p_0(u_1, z_1, u_2, z_2/u_3, z_3) = \frac{p_0(u_1, z_1, u_2, z_2/s_2, y_2)\, p_0(u_2, z_2, u_3, z_3/s_2, y_2)}{p_0(u_1, z_1, u_3, z_3/s_2, y_2)}. \tag{4.2}$$

Finally we obtain the desired equality:

$$\begin{aligned} p_c(u_1, z_1, u_3, z_3/s_2, y_2) &= \frac{I_c(u_3, z_3, s_2, y_2)}{I_c(u_1, z_1, s_2, y_2)} \\ &\quad \times \int_{R^d} p_0(u_1, z_1, u_2, z_2/s_2, y_2)\, p_0(u_2, z_2, u_3, z_3/s_2, y_2) \\ &\quad \times I_c(u_1, z_1, u_2, z_2)\, I_c(u_2, z_2, u_3, z_3)\, dz_2 \\ &= \int_{R^d} p_c(u_1, z_1, u_2, z_2/s_2, y_2)\, p_c(u_2, z_2, u_3, z_3/s_2, y_2)\, dz_2. \end{aligned}$$

It remains to show that $p_c(.../s_2, y_2)$ generates the finite-dimensional distributions of the $m_c(s_1, y_1, s_2, y_2)$-process. We consider (u_i): $s_1 =: u_0 < u_1 < \cdots < u_{n+1} := s_2$, and a bounded measurable function f. According to Lemma 4.1, we find

$$\begin{aligned} &\int f(v(u_1), ..., v(u_n))\, dm_c(s_1, y_1, s_2, y_2)(v) \\ &= \int_{(R^d)^n} f(z_1, ..., z_n) \prod_{i=0}^{n-1} p_0(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2) \\ &\quad \times \prod_{i=0}^{n} I_c(u_i, z_i, u_{i+1}, z_{i+1})/I_c(s_1, y_1, s_2, y_2)\, dz_1 \cdots dz_n \\ &= \int_{(R^d)^n} f(z_1, ..., z_n) \prod_{i=0}^{n-1} p_c(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2)\, dz_1 \cdots dz_n. \end{aligned}$$

Thus, Theorem 2.1 is established.

Now we prove the mixed integration formula.

Proof of Theorem 2.2. Performing the transformation from the measure m_0 to the measure m_{c_0}, we obtain

$$I_c(s_1, y_1, s_2, y_2) = I_{c-c_0, c_0}(s_1, y_1, s_2, y_2)\, I_{c_0}(s_1, y_1, s_2, y_2), \qquad (s_1, y_1, s_2, y_2) \in T. \tag{4.3}$$

Using (2.2), the assertion of Lemma 4.1 can be written in the form

$$\begin{aligned}
&\int f(v(u_1), ..., v(u_n)) \exp\left(\int_{s_1}^{s_2} g(s, v(s), v(u_1), ..., v(u_n))\, ds\right) dm_c(s_1, y_1, s_2, y_2)(v) \\
&= \int_{(R^d)^n} \left\{ f(z_1, ..., z_n) \prod_{i=0}^{n-1} p_c(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2) \right. \\
&\quad \times \prod_{i=0}^{n} \int \exp\left(\int_{u_i}^{u_{i+1}} g(s, v(s), z_1, ..., z_n)\, ds\right) \\
&\quad \left. \times\, dm_c(u_i, z_i, u_{i+1}, z_{i+1})(v) \right\} dz_1 \cdots dz_n.
\end{aligned} \tag{4.4}$$

In particular, with $(f, g, c) = (1, c - c_0, c_0)$, we obtain the formula

$$\begin{aligned}
I_{c-c_0, c_0}(s_1, y_1, s_2, y_2) = \int_{(R^d)^n} & \prod_{i=0}^{n-1} p_{c_0}(u_i, z_i, u_{i+1}, z_{i+1}/s_2, y_2) \\
& \times \prod_{i=0}^{n} I_{c-c_0, c_0}(u_i, z_i, u_{i+1}, z_{i+1})\, dz_1 \cdots dz_n.
\end{aligned} \tag{4.5}$$

The assertion of Theorem 2.2 follows immediately from (4.3) and (4.5).

Fosdick's mixed integration formula [9] is obtained from Theorem 2.2 for $c_0 = 0$. It remains to prove Theorem 2.3.

Proof of Theorem 2.3. Condition (2.5) is necessary and sufficient for the existence of a finite mathematical expectation $E\eta$. Suppose (2.5) to be fulfilled. Using simple properties of the conditional expectation, we obtain

$$\begin{aligned}
E\eta = EE\{\eta/(x_i)\} &= I_{c_0}(t_0, x_0, t, x) \\
&\times \int_{(R^d)^n} \prod_{i=0}^{n-1} p_{c_0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x) \\
&\times \prod_{i=0}^{n} E\{\xi_{c-c_0, c_0}(t_i, x_i, t_{i+1}, x_{i+1})/(x_i)\}\, dx_1 \cdots dx_n.
\end{aligned}$$

The assertion follows immediately from Theorem 2.2.

5. Further Results on Multi-step Estimators

Theorem 2.3 gives a general answer to the approximation problem. The multi-step estimator (2.4) is unbiased, if its mathematical expectation is finite (condition (2.5)). Now, we use the concrete form (3.2), (3.5)–(3.8) of the multi-step estimator in order to specify the condition (2.5). We look for a more explicit form of this condition in terms of the parameters of the estimator.

Proposition 5.1. *Consider the estimator η in the form* (3.2), (3.5)–(3.8). *Then*

$$E|\eta| = \int \exp\left(\int_{t_0}^{t} (|(c-c_0)(s, v(s)) - g(s, v)| + c_0(s, v(s)) + g(s, v))\, ds\right) \times dm_0(t_0, x_0, t, x)(v),$$

where

$$g(s, v) := \sum_{i=0}^{n} 1_{(t_i, t_{i+1})}(s)\, d(t_i, v(t_i), t_{i+1}, v(t_{i+1}))$$

and 1_A denotes the indicator function of a set A.

Proof. We know from [20] that

$$\begin{aligned} E|\xi_{c-c_0, c_0}(t_i, x_i, t_{i+1}, x_{i+1})| &= \int \exp\left(\int_{t_i}^{t_{i+1}} (|(c-c_0)(s, v(s)) - d_i| + d_i)\, ds\right) \\ &\quad \times dm_{c_0}(t_i, x_i, t_{i+1}, x_{i+1}), \end{aligned}$$

with $d_i := d(t_i, x_i, t_{i+1}, x_{i+1})$. Consequently, applying Lemma 4.1 in the form (4.4), we obtain

$$\begin{aligned} E|\eta| &= EE\{|\eta|/(x_i)\} = I_{c_0}(t_0, x_0, t, x) \\ &\quad \times \int_{(R^d)^n} \left\{\prod_{i=0}^{n-1} p_{c_0}(t_i, x_i, t_{i+1}, x_{i+1}/t, x)\right. \\ &\quad \times \prod_{i=0}^{n} \int \exp\left(\int_{t_i}^{t_{i+1}} (|(c-c_0)(s, v(s)) - d_i| + d_i)\, ds\right) \\ &\quad \left.\times dm_{c_0}(t_i, x_i, t_{i+1}, x_{i+1})(v)\right\} dx_1 \cdots dx_n \\ &= I_{c_0}(t_0, x_0, t, x) \int \exp\left(\int_{t_0}^{t} (|(c-c_0)(s, v(s)) - g(s, v)| \right. \\ &\quad \left. + g(s, v))\, ds\right) dm_{c_0}(t_0, x_0, t, x)(v). \end{aligned}$$

Substituting the measure m_{c0} by m_0 according to (2.1), we obtain the desired expression.

It can be shown that $E|\xi^{(2)}| \leqq E|\xi^{(1)}|$. Thus, Proposition 5.1 also provides sufficient conditions for the estimator (3.2), (3.5)–(3.7), (3.9) to be unbiased.

In the following, we suppose $d = 0$. Given any $c_0 \in K$, we consider the class K_{c0} of functions $c \in K$, for which the estimator (3.2), (3.5)–(3.8) is unbiased. Theorem 2.3 and Proposition 5.1 imply

$$K_{c0} = \{c \in K: I_{|c-c0|+c0}(t_0, x_0, t, x) < \infty\}.$$

We show, how the remaining parameter c_0 influences the class K_{c0}.

PROPOSITION 5.2. *The sets* K_{c0} *have the following properties*:

(i) $K_{c0} \subset K_{c_1}$, *for any* $c_0, c_1 \in K$ *such that* $c_0 \geqq c_1$;

(ii) $K_{c0} = K_{c_1}$, *for any* $c_0, c_1 \in K$ *such that* $c_0 - c_1$ *is bounded*;

(iii) $K_{c0} \supset \{c \in K: c - c_0$ *is bounded from below*$\}$.

Proof. (i) For $c \in K_{c0}$ and any argument, we have the inequality $|c - c_1| + c_1 \leqq |c - c_0| + |c_0 - c_1| + c_1 = |c - c_0| + c_0$. Consequently, $I_{|c-c1|+c_1}(t_0, x_0, t, x) = I_{|c-c0|+c0}(t_0, x_0, t, x)$, and $c \in K_{c_1}$.

(ii) First we show that $K_{c0+a} \subset K_{c0}$, for any constant a. We have $|c - c_0| + c_0 \leqq |c - c_0 - a| + |a| + c_0 + a - a$, which implies $I_{|c-c0|+c0} \leqq I_{|c-c0-a|+c0+a} \exp((|a| - a)(t - t_0))$. Thus, the assertion follows for c_0, c_1 such that $c_0 - c_1$ is constant. Consider now c_0, c_1 such that $-a \leqq c_0 - c_1 \leqq a$, $a = \text{const}$. With (i), we find $K_{c0} \supset K_{c1+a} = K_{c_1}$ and $K_{c0} \subset K_{c_1-a} = K_{c_1}$, which implies the assertion.

(iii) Consider $c \in K$ such that $c - c_0 \geqq a$, $a = \text{const}$. We have $I_{|c-c0-a|+c0+a} = I_c < \infty$ and find $c \in K_{c0+a} = K_{c0}$, via (ii).
This completes the proof.

The set K_0 consists of all functions $c \in K$ satisfying the condition $I_{|c|}(t_0, x_0, t, x) < \infty$ known from [20]. Proposition 5.2 allows us to answer the question whether this condition on c can be weakened by an appropriate choice of the parameter c_0.

The class K_{c0}, $c_0(s, y) = -a^2y^2/2$, $y \in R$, $a > 0$ (cf. Example 1 in Section 3), is really wider than K_0, for sufficiently large t. It contains K_0 according to Proposition 5.2(i). The function c_0 itself is in K_{c0}, for arbitrary (t_0, x_0, t, x). But c_0 is not in K_0 for (t_0, x_0, t, x) such that $(t - t_0) > \pi/a$ (cf. the explicit formulas for Gaussian functional integrals in [17]). According to Proposition 5.2(ii), the same is true for functions of the form $c_0 + c$, where c is bounded.

In the following, we consider the second moment of the estimator (3.2), (3.5)–(3.8).

PROPOSITION 5.3. *Consider the estimator* (3.2), (3.5)–(3.8). *Then*

$$E\eta^2 = I_{c_0}(t_0, x_0, t, x) \int \exp\left(\int_{t_0}^{t} \{((c-c_0)(s, v(s)) - g(s, v))^2/\gamma + c_0(s, v(s)) + \gamma + 2g(s, v)\}\, ds\right) \times dm_0(t_0, x_0, t, x)(v),$$

where the function g is defined as in Proposition 5.1.

Proof. We know from [20] that

$$E\xi^{(1)}_{c-c_0-d_i, c_0}(t_i, x_i, t_{i+1}, x_{i+1})^2 = \int \exp\left(\int_{t_i}^{t_{i+1}} (((c-c_0)(s, v(s)) - d_i)^2/\gamma + \gamma)\, ds\right) \times dm_{c_0}(t_i, x_i, t_{i+1}, x_{i+1})(v).$$

Proceeding analogously to the proof of Proposition 5.1, we obtain the assertion.

In particular, Proposition 5.3 shows that the estimator (3.2), (3.5)–(3.8) has a finite second moment, if the parameter c_0 is chosen in such a way that $|c - c_0|$ is bounded. Thus, we found another useful property of the parameter c_0 beside its influence on the estimator to be unbiased. The parameter c_0 enables us to handle functional integrals (1.1) with a function c of the form "quadratic term plus bounded perturbation."

6. NUMERICAL EXAMPLES

First, we consider the example of the harmonic oscillator

$$c(s, y) = -0.5\, y^2, \; y \in R. \tag{6.1}$$

TABLE I

Example 6.2 and One-Step Estimators

t	Confidence intervals	l	Example 6.1
3.0	0.616 +/− 0.008 0.617 +/− 0.006	0.3	0.547
4.0	0.452 +/− 0.007 0.454 +/− 0.005	0.4	0.383
5.0	0.322 +/− 0.006 0.324 +/− 0.004	0.5	0.260

TABLE II

Example 6.2 with $t=3.0$ and Chorin's Estimator

n	N	Confidence intervals
3	4000	0.665 +/− 0.011
6	2000	0.636 +/− 0.014
12	1000	0.618 +/− 0.019

The choice $c_0 = c$ leads to an exact estimator η, since the inner functional integrals equal one. This property of our scheme to provide exact estimators for quadratic functions c is analogous to the corresponding property of quadrature formulas to be exact for certain polynomials.

As a second example, we consider the perturbed harmonic oscillator

$$c(s, y) = -0.5y^2 + 0.1 \sin|y|, \qquad y \in R,\ t_0 = 0,\ x_0 = 0,\ x = 0. \tag{6.2}$$

The results obtained by means of one-step estimators with the parameter $c_0(s, y) = -0.5y^2$ are shown in Table I. The parameter γ is chosen to be 0.1. The number of independent samples is $N = 5000$. The empirical means are calculated simultaneously for the estimators (3.2), (3.5)–(3.8) and (3.2), (3.5)–(3.7), (3.9) on the same trajectories. Confidence intervals are constructed with the confidence level 0.01 (cf. [20] for details). The upper results in the column "confidence intervals" correspond to the estimator (3.8), the lower results to the estimator (3.9). The empirical mean length l is also given. The results for the unperturbed harmonic oscillator (6.1) are contained in the last column.

Some results concerning the biased Chorin's estimator (3.4), (3.5), and the example (6.2) with $t = 3$, are shown in Table II.

TABLE III

Example 6.3, Multi-step Estimators, and Chorin's Estimator

n	N	Confidence intervals	l	Confidence intervals
1	5000	1.145 +/− 0.015 1.145 +/− 0.012	0.3	1.000 +/− 0.000
3	4000	1.140 +/− 0.026 1.143 +/− 0.008	2.3	1.112 +/− 0.002
6	2000	1.154 +/− 0.039 1.144 +/− 0.009	5.3	1.132 +/− 0.003
12	1000	1.163 +/− 0.055 1.151 +/− 0.010	11.3	1.142 +/− 0.004

Finally, we use the example

$$c(s, y) = 0.1 \sin|y|, \qquad y \in R,\ t_0 = 0,\ t = 3,\ x_0 = 0,\ x = 0, \tag{6.3}$$

to illustrate the relation between the biased Chorin's estimator (3.4), (3.5) and the multi-step estimators (3.2) (3.5)–(3.9) (cf. Table III). The parameter γ is 0.1 again.

7. Comments and Outlook

Unbiased Monte Carlo algorithms for the numerical evaluation of finite-dimensional integrals are well-known (cf. [8] or any other monograph on Monte Carlo theory). A direct generalization of these methods to the case of functional integrals

$$I_c(t_0, x_0, t, x) = \int \exp\left(\int_{t_0}^{t} c(s, v(s))\, ds\right) dm_0(t_0, x_0, t, x)(v) \tag{7.1}$$

is impossible. The corresponding one-point estimator would be

$$F(v) := \exp\left(\int_{t_0}^{t} c(s, v(s))\, ds\right), \tag{7.2}$$

depending on an infinite-dimensional object v, distributed according to m_0.

The construction of one-step estimators in [20] was a first attempt to establish a theory of unbiased estimators for infinite-dimensional integrals. Multi-step estimators proposed in this paper are a further contribution to such a theory. The class of unbiased estimators has been extended considerably. The parameters c_0, (t_i), and P appear as additional degrees of freedom of the unbiased estimation scheme. The scheme is applicable under weaker conditions now (cf. Proposition 5.2).

The main problem to be considered in the future is the variance reduction problem. Its solution is only at the beginning. However, the introduction of the parameters c_0, (t_i), and P represents necessary advancement toward importance sampling in the infinite-dimensional space.

The basic principle of the importance-sampling technique is (in terms of the "estimator" (7.2)) to generate the random object v according to a measure having a density $D(v)$ with respect to m_0 and to use the estimator $F(v)/D(v)$ instead of (7.2). The density D is to be chosen similar to the functional F.

Although we do not use the estimator (7.2), we are able to implement this principle within the unbiased estimation scheme, via the parameters c_0, (t_i), and P.

The parameter c_0, which corresponds to the measure m_{c0}, can be chosen (in the class of quadratic functions) in order to be similar to c. The effect can be remarkable, as example (6.2) shows. This example could not be handled without the parameter c_0.

In this paper, we did not use the variance reduction procedure proposed in [20], which is based on an appropriate choice of the parameters $q^{(i)}$ and $q_0^{(i)}$, according to their optimal forms. Simulation studies with one-step estimators (cf. [20]) showed that this procedure works very efficiently on relatively small time intervals. On larger time intervals, it turns out to be insufficient.

Within the multi-step estimation scheme, the one-step estimators are used on smaller time intervals. They serve as correction terms for some biased estimators for finite-dimensional approximations to the functional integral. These correction terms cause an additional variance compared with the biased estimator (cf. example (6.3)). This additional variance could be reduced by means of techniques developed in [20].

On the other hand, variance reduction techniques for finite-dimensional integrals (cf. [14] concerning Chorin's estimator) can be used via the parameters (t_i) and P within the unbiased estimation scheme now. Moreover, we even conjecture that it might be possible to adapt the principle of the Metropolis algorithm [15] to the unbiased estimation scheme via the parameter P.

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References

1. G. L. Blankenship and J. S. Baras, *SIAM J. Appl. Math.* **41**, 518 (1981).
2. R. H. Cameron, *Duke Math. J.* **18**, 111 (1951).
3. A. J. Chorin, *Math. Comput.* **27**, 1 (1973).
4. H. DeRaedt and A. Lagendijk, *Phys. Rep.* **127**, 233 (1985).
5. C. DeWitt-Morette, A. Maheshwari, and B. Nelson, *Phys. Rep.* **50**, 255 (1979).
6. M. D. Donsker and M. Kac, *J. Res. Nat. Bur. Standards* **44**, 551 (1950).
7. I. G. Dyatkin and S. A. Zhukova, *Zh. Vychisl. Mat. Mat. Fiz.* **8**, 222 (1968).
8. S. M. Ermakov, *Monte Carlo Method and Related Questions* (Nauka, Moscow, 1975). [Russian]
9. L. D. Fosdick, *Math. Comput.* **19**, 225 (1965).
10. L. D. Fosdick, *SIAM Rev.* **10**, 315 (1968).
11. J. Glimm and A. Jaffe, *Quantum Physics: A Functional Integral Point of View* (Springer, New York, 1981).
12. O. H. Hald, University of California Preprint PAM–303, 1985 (unpublished).
13. M. H. Kalos (Ed.), *Monte Carlo Methods in Quantum Problems* (Reidel, Boston, 1984).
14. F. H. Maltz and D. L. Hitzl, *J. Comput. Phys.* **32**, 345 (1979).
15. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).
16. H. Mitter and L. Pittner (Eds.), *Stochastic Methods and Computer Techniques in Quantum Dynamics* (Springer, New York, 1984).
17. L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
18. E. V. Shuryak and O. V. Zhirov, *Nucl. Phys. B* **242**, 393 (1984).
19. M. Takahashi and M. Imada, *J. Phys. Soc. Japan.* **53**, 3765 (1984).
20. W. Wagner, *J. Comput. Phys.* **71**, 21 (1987).