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OPTIMAL CHOICES OF CORRELATION OPERATORS IN BROWNIAN SIMULATION METHODS*

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Abstract. We analyze Brownian simulation methods for systems of partial differential equations coupled to convection-diffusion equations. In many situations the spatial correlation of Brownian noise can be viewed as a free parameter. We formulate the choice of the noise correlation as an optimization problem for mean error minimization. In contrast to earlier work which was restricted to systems of finite dimensions, our formulation is performed in function space. We then provide an approximation theorem that reduces the problem into the solution of finite-dimensional semidefinite programming problems. Examples are given to illustrate our main results.

Key words. Brownian simulations, SPDEs, spatial correlations, semidefinite programming

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1. Introduction.

Brownian simulation is a technique for solving partial differential equations (PDEs) using random simulations of stochastic systems of equations. The prominent forerunner in this context is Chorin's method of random vortex methods, which approximates solutions of the Navier–Stokes equations in the regime of slightly viscous flows [3]. In this system, the fluid is represented by a finite collection of point vortices, whose motion is primarily determined by the induced flow field. Viscous dissipation is incorporated by the addition of a Brownian velocity component to each point vortex. Thus, the positions of the point vortices satisfy a system of stochastic differential equations (SDEs), and the induced (stochastic) velocity field approximates the solution of the Navier–Stokes equations. In the past 30 years, stochastic particle methods have been applied to a variety of systems, and in many instances, their convergence has been proved rigorously by probabilistic techniques (see Talay [14] for a review).

Since the 1990s Brownian simulation techniques have become popular in the context of non-Newtonian viscoelastic fluids. Many models of viscoelastic fluids are in the form of a PDE that governs the flow field (the *macroscopic* dynamics) coupled to a Fokker–Planck equation that governs the distribution of polymeric conformation (the *microscopic* dynamics). The coupling between these equations is bilateral: the flow field is forced by a term—the stress field—which is an average over the polymeric conformation. Reciprocally, the microscopic dynamics are affected by the macroscopic flow field. Such models are called *micro-macro* models; see Keunings [11] for a recent review.

Except for very simple realizations, the coupled system cannot be solved either analytically or numerically, due to its high dimensionality. Öttinger and coworkers introduced in the early 1990s a simulation technique to approximate such systems (the

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so-called CONNFFESSIT method [12, 6]). Their idea was to simulate the Fokker–Planck equation by a collection of randomly driven particles representing (in some coarse-grained sense) the polymers. The stress field is approximated by an empirical average over the state of those particles. In the CONNFFESSIT method each particle is driven by an independent Brownian noise, resulting in spatially noisy output.

An alternative method was proposed in 1997 by Hulsen, van Heel, and van den Brule, the Brownian configuration field (BCF) method [7]. Rather than simulating a collection of particles, the BCF method simulates a collection of random functions of space and time (random fields), each such field representing the local polymeric state. Each random field satisfies a SPDE, driven by a Brownian noise that is spatially constant. As a result BCF computations tend to generate solutions that are smooth compared to the output of CONNFFESSIT (for the same computational cost). This observation led in [13] to the speculation that BCF is a variance-reduced variant of CONNFFESSIT, a speculation that was later refuted. The reality, as found in [8], is that the use of spatially uniform Brownian motion reduces the variance of the velocity but significantly increases the variance of the stress.

From a fundamental point of view, BCF and CONNFFESSIT differ in two main aspects: (i) BCF is an "Eulerian" method, whereas CONNFFESSIT is a "Lagrangian" method, and (ii) BCF uses a spatially uniform noise, whereas CONNFFESSIT uses a spatially uncorrelated noise. In principle, one could design an Eulerian version of CONNFFESSIT by the use of configuration fields that are driven by Brownian noise that is spatially uncorrelated. This observation was made by Jourdain, Le Bris, and Lelievre [8], who generalized the two Brownian simulation techniques to arbitrary noise correlations. Furthermore, they formulated the choice of noise correlation as an optimization problem for error minimization. Their optimization problem was formulated in the context of specific discretization schemes and applied to particular situations, e.g., Hookean and FENE fluids in planar shear flow.

In this paper we study the problem of variance reduction by optimal noise correlation in a general context. We consider a class of systems in which a PDE is coupled to a Fokker–Planck equation with bilateral interaction, along with a Brownian simulation approximation that consists of a collection of N SPDEs driven by independent Brownian noises with arbitrary spatial correlation. The N fields are weakly coupled through their average. We then derive an expression for the mean error in the limit of large N; as expected, the error depends on the noise correlation. For a large class of such systems the minimization of the mean error forms a convex optimization problem that can be solved by standard methods. An important difference between [8] and the present work is that we operate on the level of the PDE/SPDE rather than on the level of a specific computational scheme. Thus we address the question of optimal noise correlation for a given problem independently from its method of approximation. Finally, we demonstrate our results by applying them to a number specific problems.

The structure of this paper is as follows: In section 2 we present the class of models under consideration and show that they can be reformulated in a stochastic setting, in a manner that is independent of the spatial correlation of the noise; the noise need only satisfy a local normalization property. The stochastic formulation leads naturally to an approximation scheme based on a Monte Carlo simulation of the Brownian trajectories. While BCF corresponds to a particular choice of Brownian processes, the CONNFFESSIT uncorrelated noise has to be interpreted as a limit of such processes. We conclude this section with a subclass of such systems that are closable and therefore amenable to rigorous analysis. In section 3 we analyze the error of the Brownian approximation in the limit of large N. The error is dominated by the

variance of the estimate, which scales like $1/N$. This analysis is continued in section 4, where we finally express the mean error in terms of the correlation operators of the Brownian noise and the initial data. In section 5 the variance reduction optimization problem is formulated. In particular, it becomes apparent that an optimizer does not necessarily exist, since the domain of suitable correlations is neither closed nor bounded. Since in most cases the optimization problem cannot be solved analytically, we present in section 6 an approximation theorem, whereby the infimum of the error can be attained as a limit of finite-dimensional optimization problems, each of which is solvable by standard methods of semidefinite programming. Specific examples are then presented in section 7, one of which is solvable analytically and another only numerically. A discussion follows in section 8.

2. Problem statement. Consider a general class of autonomous equations of the form

$$\eta \frac{\partial u}{\partial t} = f(u, c), \tag{2.1}$$

where $u = u(x,t)$ and $c = c(x,t)$; the parameter η is either one or zero, depending on whether (2.1) is an evolution equation for u, or a time-independent relation between the functions u and c. For notational convenience, we consider systems in one space dimension, $x \in D \subset \mathbb{R}$, where D is a bounded interval, and we assume that u and c are real-valued functions; our analysis applies with slight modifications to more general situations. The function $f = f(u(x,t), c(x,t))$ is a sufficiently regular function of its arguments and their spatial derivatives (e.g., a nonlinear differential operator). The function c is given by an integral

$$c(x,t) = \int_{\mathbb{R}} g(q)\psi(q,x,t)\,dq, \tag{2.2}$$

where $\psi(q,x,t)$ is a nonnegative integrable function, governed by a diffusion-transport equation of the form

$$\frac{\partial \psi}{\partial t} + a(u)\frac{\partial \psi}{\partial x} = -\frac{\partial}{\partial q}\left[b(q,u)\psi\right] + \frac{1}{2}\frac{\partial^2 \psi}{\partial q^2}. \tag{2.3}$$

The functions $a = a(u(x,t))$ and $b = b(q, u(x,t))$ are sufficiently regular functions of q, $u(x,t)$ and spatial derivatives of $u(x,t)$. The coupled system (2.1)–(2.3) is supplemented with initial conditions,

$$u(x,0) = u_0(x), \qquad \psi(q,x,0) = \psi_0(q,x), \tag{2.4}$$

and with suitable boundary conditions. Throughout this paper it is assumed that the coupled system (2.1)–(2.3) is well-posed (see Constantin [4] for a global-in-time existence theorem in a viscoelastic context).

In certain cases, an equation for $c(x,t)$ can be derived from (2.3), yielding a closed-form system of equations for u and c, without requiring the solution of $\psi(q,x,t)$. Two such examples are given below.

EXAMPLE 2.1. *Consider the system*

$$0 = -u(x,t) - c(x,t) + \int_0^1 c(y,t)\,dy,$$

$$c(x,t) = \int_{\mathbb{R}} q^2 \psi(q,x,t)\, dq,$$
$$\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial}{\partial q}[(s+u-1)q\,\psi] + \frac{1}{2}\frac{\partial^2 \psi}{\partial q^2},$$

where $x \in [0,1]$ and $s(x) = \sin(2\pi x)$; this system does not require boundary conditions. A closed system of equations for u and c can be derived by multiplying the diffusion-transport equation by q^2 and integrating over q. This yields an evolution equation for c,

$$\frac{\partial c}{\partial t} = (s+u-1)\, c + 1.$$

EXAMPLE 2.2. *The second example is inspired from the dumbbell model of viscoelastic fluids* [1]. *The equation for the "flow field" $u(x,t)$ is a viscous Burgers equation with forcing,*

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial c}{\partial x}, \tag{2.5}$$

where the "stress" $c(x,t)$ is given by

$$c(x,t) = \int_{\mathbb{R}} q^2 \psi(q,x,t)\, dq,$$

and the "polymer distribution" $\psi(q,x,t)$ is governed by the Smoluchowski equation

$$\frac{\partial \psi}{\partial t} + u\frac{\partial \psi}{\partial x} = \frac{\partial}{\partial q}(q\psi) + \frac{1}{2}\frac{\partial^2 \psi}{\partial q^2}.$$

Here again, multiplying the Smoluchowski equation by q^2 and integrating over q we obtain an evolution equation for c,

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = -2c + 1,$$

and together with (2.5) *this yields a closed-form system.*

In cases where closed-form equations can be derived, the resulting set of equations can often be solved by standard numerical methods (e.g., finite differences or finite elements). Otherwise, one has to solve the high-dimensional coupled system (2.1)–(2.3), a task which is often computationally prohibitive. A computational alternative is the use of Brownian simulation techniques, which we review next.

The idea, which is rigorously established in Proposition 2.1, is to first interpret the diffusion-transport equation (2.3) as a Fokker–Planck equation that governs the probability density function (PDF) of a random function $q_t(x)$; $\psi(q,x,t)$ is the probability density that $q_t(x) = q$. The random function $q_t(x)$, which is viewed as an H-valued stochastic process, where $H = L^2(D)$, is governed by the SPDE

$$dq_t + a(u)\frac{\partial q_t}{\partial x}\, dt = b(q_t,u)\, dt + dW_t, \tag{2.6}$$

with random initial conditions $q_0(x)$, distributed according to the initial density $\psi_0(q,x)$. Here $W_t = W_t(x)$ is a *standard H-valued Q-Wiener process*, where $Q : H \to H$ is the *autocorrelation* of W_t.

We remind the reader that the autocorrelation $\mathrm{Cor}(X)$ of an H-valued random variable X is defined by

$$\langle \mathrm{Cor}(X)\, a, b\rangle = \mathbb{E}\left[\langle X, a\rangle \langle X, b\rangle\right], \qquad a, b \in H,$$

where $\langle\cdot,\cdot\rangle$ is the inner product in H. A Q-valued Wiener process W_t satisfies

$$\frac{1}{t}\,\mathbb{E}\left[\langle W_t, a\rangle \langle W_t, b\rangle\right] = \langle Q\, a, b\rangle,$$

i.e., $\mathrm{Cor}(W_t) = Qt$. A Q-valued Wiener process is said to be *standard* if

$$\mathbb{E}[W_t(x) W_t(x)] = t$$

for every t and almost every $x \in D$. We refer the reader to Appendix B for a short review on Hilbert space-valued Wiener processes and the corresponding stochastic calculus.

The H-valued stochastic process $q_t(x)$ is then used to replace system (2.1)–(2.3) by the *conjugate stochastic system*

$$\begin{aligned} \eta \frac{\partial u}{\partial t} &= f(u, c), \\ c &= \mathbb{E}\left[g(q_t)\right], \\ dq_t + a(u)\frac{\partial q_t}{\partial x}\, dt &= b(q_t, u)\, dt + dW_t, \end{aligned} \tag{2.7}$$

where the expectation $\mathbb{E}$ is both with respect to the random initial data and the Brownian motion. The relation between the stochastic system (2.7) and the deterministic system (2.1)–(2.3) is established by the following proposition.

PROPOSITION 2.1. *Let (u, c, q_t) be a (strong) solution of the conjugate stochastic system* (2.7) *on some time interval $[0, T]$. Let $\psi(q, x, t)$ be the marginal PDF corresponding to $q_t(x)$. Then (u, c, ψ) is a solution for the coupled system* (2.1)–(2.3) *on* $[0, T]$.

Comment: The SPDE (2.7) induces an evolution on measures in function space. The function $\psi(q, x, t)$ is a marginal density of such a measure, namely,

$$\psi(q, x, t) = \frac{\partial}{\partial q}\Pr(q_t(\cdot) : q_t(x) \le q).$$

In particular, the initial distribution $\psi_0(q, x)$ does not uniquely determine the distribution of the random function $q_0(x)$. For example, $\psi_0(q, x)$ does not determine the correlation,

$$\mathrm{Cor}(q_0) = R.$$

Proof. By Itô's formula (B.3), for every twice-differentiable compactly supported function $G : \mathbb{R} \to \mathbb{R}$ and every $x \in D$,

$$dG(q_t(x)) = G'(q_t(x))\, dq_t(x) + \frac{1}{2} G''(q_t(x))\, dt. \tag{2.8}$$

Substituting the evolution equation of q_t into (2.8) and taking expectations we obtain

$$\frac{\partial}{\partial t}\mathbb{E}\left[G(q_t)\right] = -a(u)\frac{\partial}{\partial x}\mathbb{E}\left[G(q_t)\right] + \mathbb{E}\left[G'(q_t) b(q_t, u)\right] + \frac{1}{2}\mathbb{E}\left[G''(q_t)\right].$$

Writing the last equation in terms of $\psi(q,x,t)$,

$$\frac{\partial}{\partial t}\int G(q)\psi(q,x,t)\,dq = -a(u)\frac{\partial}{\partial x}\int G(q)\psi(q,x,t)\,dq + \int G'(q)b(q,u)\psi(q,x,t)\,dq + \frac{1}{2}\int G''(q)\psi(q,x,t)\,dq,$$

and upon integration by parts,

$$\frac{\partial}{\partial t}\int G(q)\left[\frac{\partial\psi}{\partial t} + a(u)\frac{\partial}{\partial x}\psi + \frac{\partial}{\partial q}[b(q,u)\psi] - \frac{1}{2}\frac{\partial^2\psi}{\partial q^2}\right]dq = 0.$$

Finally, the arbitrariness of G implies that ψ satisfies (2.3). ∎

The fact that the Brownian noise is standard was used in Itô's formula, resulting in a constant diffusion function. Note, however, that the equivalence between the deterministic and the stochastic systems is unaffected by the correlation of q_t, which is determined by the noise correlation operators Q and the correlation R of the initial data. Viewed that way, the coupled system (2.1)–(2.3) can be represented by a family of stochastic conjugate systems (2.7) which vary in the correlation operators Q and R.

The stochastic representation (2.7) is naturally approximated by the method of Brownian simulations. The SPDE (2.6) is simulated by a set of N realizations $Q_t^i(x)$, $i = 1, 2, \ldots, N$, of $q_t(x)$, and the expected value with respect to Brownian trajectories is approximated by an empirical mean over the N realizations. Denoting by $U_t(x)$ and $C_t(x)$ the (stochastic) numerical approximations to $u(x,t)$ and $c(x,t)$, the simulation scheme takes the form

$$\begin{aligned} \eta\frac{\partial U_t}{\partial t} &= f(U_t, C_t), \\ C_t &= \frac{1}{N}\sum_{i=1}^{N} g(Q_t^i), \\ dQ_t^i + a(U_t)\frac{\partial Q_t^i}{\partial x}\,dt &= b(Q_t^i, U_t)\,dt + dW_t^i, \qquad i = 1, \ldots, N, \end{aligned} \tag{2.9}$$

where W_t^i are N independent Q-Wiener processes and $Q_0^i(x)$ are N independent H-valued random variables with correlation R. Note that the realizations Q_t^i are weakly coupled, as they interact through their empirical mean. Although the spatial correlations of the noise and the initial data are immaterial for (2.7), they may influence the error of the approximation. Our ultimate goal is to find the correlation operators that minimize the error.

A class of semilinear problems. Examples 2.1 and 2.2 are amenable to closed-form PDEs for $u(x,t)$, $c(x,t)$. While Brownian simulations are prominently designed for systems that do not assume such closures, we will focus on closable systems, since the existence of closed-form equations facilitates the analysis of Brownian simulation methods. Specifically, we will examine the class of nonlinear systems for which

$$b(q,u) = b(u)q \qquad \text{and} \qquad g(q) = q^2, \tag{2.10}$$

where b is a function of u and its spatial derivatives. As above, the closure is derived by first using Itô's formula,

$$dq_t^2 = 2q_t\,dq_t + 1 = -a(u)\frac{\partial q_t^2}{\partial x}\,dt + 2b(u)q_t^2\,dt + 2q_t\,dW_t + dt,$$

and then averaging:

$$\frac{\partial}{\partial t}\mathbb{E}[q_t^2] = -a(u)\frac{\partial}{\partial x}\mathbb{E}[q_t^2] + 2b(u)\,\mathbb{E}[q_t^2] + 1.$$

The resulting PDEs that govern (u, c) are

$$\begin{aligned} \eta\frac{\partial u}{\partial t} &= f(u,c), \\ \frac{\partial c}{\partial t} + a(u)\frac{\partial c}{\partial x} &= 2b(u)c + 1. \end{aligned} \tag{2.11}$$

3. Error analysis. The Brownian simulation (2.9) provides approximations $U_t(x)$, $C_t(x)$ to the solutions $u(x,t)$, $c(x,t)$ of (2.7). We define the errors

$$\delta_t^u(x) = U_t(x) - u(x,t) \qquad \text{and} \qquad \delta_t^c(x) = C_t(x) - c(x,t).$$

In the semilinear case (2.10) the errors are governed by the system of equations

$$\begin{aligned} \eta\, d\delta_t^u &= [f(u+\delta_t^u, c+\delta_t^c) - f(u,c)]\,dt, \\ d\delta_t^c + \left[a(u+\delta_t^u)\frac{\partial(c+\delta_t^c)}{\partial x} - a(u)\frac{\partial c}{\partial x}\right]dt &= 2\left[(b(u+\delta_t^u) - b(u))c + b(u+\delta_t^u)\delta_t^c\right]dt \\ &\quad + \frac{2}{N}\sum_{i=1}^{N} Q_t^i\, dW_t^i. \end{aligned}$$

The error analysis is complicated by the fact that the processes Q_t^i are dependent. To bypass this difficulty we introduce a set of auxiliary stochastic processes q_t^i, which are independent realizations of the process q_t, driven by the same noise processes as the Q_t^i, namely,

$$dq_t^i + a(u)\frac{\partial q_t^i}{\partial x}\,dt = b(u)q_t^i\,dt + dW_t^i. \tag{3.1}$$

The deviations between the weakly dependent and the independent processes, $\delta_t^{q^i} = Q_t^i - q_t^i$, satisfy the system of equations

$$\begin{aligned} d\delta_t^{q^i} + \left[a(u+\delta_t^u)\frac{\partial \delta_t^{q^i}}{\partial x} + (a(u+\delta_t^u) - a(u))\,\frac{\partial q_t^i}{\partial x}\right]dt \\ = \left[b(u+\delta_t^u)\delta_t^{q^i} + (b(u+\delta_t^u) - b(u))\,q_t^i\right]dt. \end{aligned} \tag{3.2}$$

Substituting $Q_t^i = q_t^i + \delta_t^{q^i}$ into the equation for δ_t^c yields

$$\begin{aligned} d\delta_t^u &= [f(u+\delta_t^u, c+\delta_t^c) - f(u,c)]\,dt, \\ d\delta_t^c + \left[a(u+\delta_t^u)\frac{\partial(c+\delta_t^c)}{\partial x} - a(u)\frac{\partial c}{\partial x}\right]dt &= 2\left[(b(u+\delta_t^u) - b(u))c + b(u+\delta_t^u)\delta_t^c\right]dt \\ &\quad + \frac{2}{N}\sum_{i=1}^{N} q_t^i\, dW_t^i + \frac{2}{N}\sum_{i=1}^{N}\delta_t^{q^i}\, dW_t^i. \end{aligned} \tag{3.3}$$

Equations (3.1)–(3.3) govern the evolution of the errors. They do not form a closed system because they also depend on the exact solutions $u(x,t)$, $c(x,t)$.

Since we expect (mean) errors to scale like $N^{-1/2}$ for large N, we introduce the *normalized errors*,

$$\Delta_t^u = \sqrt{N}\,\delta_t^u, \qquad \Delta_t^c = \sqrt{N}\,\delta_t^c, \quad \text{and} \quad \Delta_t^{q^i} = \sqrt{N}\,\delta_t^{q^i}.$$

We then Taylor expand the functions f, a, and b about u, c, and q_t^i and reorganize the equations for the normalized errors in powers of $1/\sqrt{N}$,

$$\begin{aligned}
d\Delta_t^u &= \left[\frac{\partial f}{\partial u}(u,c)\Delta_t^u + \frac{\partial f}{\partial c}(u,c)\Delta_t^c + \frac{1}{\sqrt{N}}R_y\right]dt,\\
d\Delta_t^c &+ \left[\frac{\partial c}{\partial x}a'(u)\Delta_t^u + a(u)\frac{\partial \Delta_t^c}{\partial x}\right]dt = 2\left(b(u)\Delta_t^c + cb'(u)\Delta_t^u\right)dt\\
&\quad + \frac{2}{\sqrt{N}}\sum_{i=1}^{N} q_t^i\,dW_t^i + \frac{1}{\sqrt{N}}dR_c\\
d\Delta_t^{q^i} &+ \left[\frac{\partial q_t^i}{\partial x}a'(u)\Delta_t^u + a(u)\frac{\partial \Delta_t^{q^i}}{\partial x}\right]dt = \left[q_t^i b'(u)\Delta_t^u + b(u)\Delta_t^{q^i}\right]dt + \frac{1}{\sqrt{N}}R_q\,dt,
\end{aligned}$$

where the residuals R_y, R_c, and R_q are quadratic expressions of Δ_t^u, Δ_t^c, and their spatial derivatives; the first-order derivatives of f, a, and b are linear differential operators acting on Δ_t^u, Δ_t^c, and $\Delta_t^{q^i}$.

To leading order in powers of $1/\sqrt{N}$ the errors satisfy the linearized stochastic system

(3.4)
$$\begin{aligned}
d\Delta_t^u &= \left[\frac{\partial f}{\partial u}(u,c)\Delta_t^u + \frac{\partial f}{\partial c}(u,c)\Delta_t^c\right]dt,\\
d\Delta_t^c &+ \left[a'(u)\frac{\partial c}{\partial x}\Delta_t^u + a(u)\frac{\partial \Delta_t^c}{\partial x}\right]dt = 2\left(b(u)\Delta_t^c + cb'(u)\Delta_t^u\right)dt + \frac{2}{\sqrt{N}}\sum_{i=1}^{N} q_t^i\,dW_t^i,
\end{aligned}$$

with q_t^i defined by (3.1). The omission of the higher-order terms as $N \gg 1$ can be justified by a formal asymptotic analysis for the corresponding Fokker–Planck equation.

System (3.4) is a nonautonomous linear stochastic system for the normalized errors Δ_t^u and Δ_t^c. The explicit time dependence stems from the dependence on the (deterministic) solutions $u(x,t)$ and $c(x,t)$. Henceforth we restrict ourselves to stationary situations, assuming that u and c are initialized at steady state $u_\infty(x)$, $c_\infty(x)$ (assuming that such a steady state exists and that it is stable). Such an analysis is also relevant to situations in which one is interested in long time behavior. The treatment of fully time-dependent cases is, in principle, not much harder.

A natural quantifier of the error is the mean-square deviation, $e(t)$, defined by

$$e^2(t) = \mathbb{E}\int_D \left[(\Delta_t^u(x))^2 + (\Delta_t^c(x))^2\right]dx.$$

Our goal is to minimize $e(t)$ with respect to the choice of noise correlation operator Q and initial data correlation R. In general, the optimal correlation operators depend on the target time.

4. Abstraction. To simplify notation, we consider an abstract version of the linear stochastic system (3.1), (3.4) at steady state,

$$\begin{aligned} d\xi_t &= A(\xi_t)\,dt + \frac{1}{\sqrt{N}}\sum_{i=1}^{N} q_t^i\,dW_t^i, \\ dq_t^i &= B(q_t^i)\,dt + dW_t^i, \qquad i = 1,\dots,n, \end{aligned} \tag{4.1}$$

where $\xi_t = \xi_t(x)$ represents the vector of errors $(\Delta_t^u(x), \Delta_t^c(x))$ and A, B are linear differential operators. This system is supplemented with initial conditions

$$\xi_0 = 0, \qquad q_0^i = q_0,$$

where q_0 is an H-valued random variable with correlation operator R, satisfying $\mathbb{E}[q_0^2] = c_\infty$. The "error" ξ_t is given by the Itô integral

$$\xi_t = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\int_0^t e^{A(t-s)} q_s^i\,dW_s^i.$$

The mean error is thus given by

$$\begin{aligned} e(t) &= \mathbb{E}\int_D \xi_t^2(x)\,dx \\ &= \frac{1}{N}\sum_{i,j=1}^{N}\int_0^t\int_0^t \mathbb{E}\left\langle e^{A(t-s)}\left(q_s^i dW_s^i\right), e^{A(t-s')}\left(q_{s'}^j dW_{s'}^j\right)\right\rangle \\ &= \frac{1}{N}\sum_{i=1}^{N}\int_0^t\int_0^t \mathbb{E}\left\langle e^{A(t-s)}\left(q_s^i dW_s^i\right), e^{A(t-s')}\left(q_{s'}^i dW_{s'}^i\right)\right\rangle \\ &= \int_0^t\int_0^t \mathbb{E}\left\langle e^{A(t-s)}\left(q_s dW_s\right), e^{A(t-s')}\left(q_{s'} dW_{s'}\right)\right\rangle dx, \end{aligned} \tag{4.2}$$

where in the passage from the second to the third line we used the fact that the W_t^i's (and correspondingly the q_t^i's) are independent, and in the passage to the fourth line we used the fact that they are identically distributed, setting $q_t = q_t^1$ and $W_t = W_t^1$.

As a first step toward the minimization of the error, we express the error in terms of the correlation operators Q and R. We denote by $\tilde{H}$ the Hilbert space of H-valued stochastic processes (see Appendix B). Let (e_k) be an orthonormal basis in H; then

$$dW_s = \sum_{k=1}^{\infty}\langle dW_s, e_k\rangle\, e_k,$$

where the series converges in $\tilde{H}$. Substituting this expansion into (4.2) gives

$$\begin{aligned} e(t) &= \sum_{i,j}\int_0^t\int_0^t \mathbb{E}\left\langle e^{A(t-s)}\left(q_s e_i\right), e^{A(t-s')}\left(q_{s'} e_j\right)\right\rangle \mathbb{E}\left[\langle dW_s, e_i\rangle\langle dW_{s'}, e_j\rangle\right] \\ &= \sum_{i,j}\int_0^t \mathbb{E}\left\langle e^{A(t-s)}\left(q_s e_i\right), e^{A(t-s)}\left(q_s e_j\right)\right\rangle Q_{ij}\,ds, \end{aligned}$$

where for every operator $T : H \to H$ we denote $T_{ij} = \langle e_i, T\, e_j \rangle$. Expanding $q_s e_i$ and $q_s e_j$ in the orthonormal basis we obtain

$$\begin{aligned} e(t) &= \sum_{i,j,k,l} \int_0^t \left\langle e^{A(t-s)} e_k, e^{A(t-s)} e_l \right\rangle \mathbb{E}\left[\langle q_s e_i, e_k \rangle \langle q_s e_j, e_l \rangle \right] Q_{ij}\, ds \\ &= \sum_{i,j,k,l} \int_0^t K_{kl}(t-s)\, \mathbb{E}\left[\langle q_s, e_i e_k \rangle \langle q_s, e_j e_l \rangle \right] Q_{ij}\, ds, \end{aligned}$$

where

$$K(t) = e^{A^* t} e^{At}.$$

Next, expanding the products $e_i e_k$ and $e_j e_l$ in the orthonormal basis,

$$e(t) = \sum_{i,j,k,l,m,n} \int_0^t K_{kl}(t-s) \left(\mathrm{Cor}(q_s)\right)_{mn} \langle e_m, e_i e_k \rangle \langle e_n, e_j e_l \rangle\, Q_{ij}\, ds.$$

We further simplify this expression by defining for every function $f \in H$ the corresponding linear pointwise multiplication operator $\hat{f}$, defined by

$$\hat{f}(g)(x) = f(x) g(x).$$

Then

$$e(t) = \sum_{i,j,k,l} \int_0^t \left[\hat{e}_i K(t-s) \hat{e}_j \right]_{kl} \left(\mathrm{Cor}(q_s)\right)_{kl} Q_{ij}\, ds.$$

Finally, since

$$q_s = e^{Bs} q_0 + \int_0^s e^{B(s-r)}\, dW_r,$$

it follows that (see Lemma B.1)

$$\mathrm{Cor}(q_s) = e^{Bs} R e^{B^* s} + \int_0^s e^{B(s-r)} Q e^{B^*(s-r)}\, dr.$$

Substituting into the expression for $e(t)$ we get, after straightforward manipulations,

$$e(t) = e_1(t) + e_2(t),$$

where

$$\begin{aligned} e_1(t) &= \sum_{i,j,k,l} \left[\int_0^t \left(e^{B^* s} \hat{e}_i K(t-s) \hat{e}_j e^{Bs} \right)_{kl} ds \right] R_{kl} Q_{ij}, \\ e_2(t) &= \sum_{i,j,k,l} \left[\int_0^t \int_0^s \left(e^{B^*(s-r)} \hat{e}_i K(t-s) \hat{e}_j e^{B(s-r)} \right)_{kl} dr\, ds \right] Q_{kl} Q_{ij}. \end{aligned}$$

It follows that we can express the total mean error in the following compact form:

$$e(t) = \mathrm{Tr}\left[M_1(t) \left(R \otimes Q \right) \right] + \mathrm{Tr}\left[M_2(t) \left(Q \otimes Q \right) \right],$$

where the operators $M_1(t)$ and $M_2(t)$ are (formally) defined by

$$
\begin{aligned}
(M_1(t))_{kl}^{ij} &= \int_0^t \left(e^{B^* s}\hat{e}_i K(t-s)\hat{e}_j e^{Bs}\right)_{kl} ds, \\
(M_2(t))_{kl}^{ij} &= \int_0^t \int_0^s \left(e^{B^*(s-r)}\hat{e}_i K(t-s)\hat{e}_j e^{B(s-r)}\right)_{kl} dr\, ds.
\end{aligned} \tag{4.3}
$$

A comment on notation: the tensorial operator $R \otimes Q$ is defined on the Hilbert space $H \otimes H$, which consists of formal linear combinations of the form

$$\sum_{i,j=1}^{\infty} \alpha_{ij} e_i \otimes e_j,$$

and the inner product is dictated by the requirement that the set $e_i \otimes e_j$ is an orthonormal set. For any element $e_i \otimes e_j \in H \otimes H$, $(R \otimes Q)(e_i \otimes e_j)$ is defined by

$$(R \otimes Q)(e_i \otimes e_j) = R(e_i) \otimes Q(e_j) = \sum_{k,l=1}^{\infty} R_{ik} Q_{jl} e_k \otimes e_l.$$

The operators $M_1(t)$ and $M_2(t)$ are operators on $H \otimes H$, defined via

$$M_{1,2}(t)(e_i \otimes e_k) = \sum_{j,l=1}^{\infty} (M_{1,2}(t))_{kl}^{ij}\, e_j \otimes e_l.$$

Finally, the trace of the linear operator $M_{1,2}$ on $H \otimes H$ is defined by

$$\operatorname{Tr} M_{1,2} = \sum_{i,k=1}^{\infty} (M_{1,2})_{kk}^{ii}.$$

To conclude, the mean error at time t is given by the following expression:

$$\operatorname{Tr}\left[M_1(t)\,(R \otimes Q)\right] + \operatorname{Tr}\left[M_2(t)\,(Q \otimes Q)\right] \equiv F(t, R, Q).$$

We have thus explicitly expressed the error in terms of the correlation operators.

5. The optimization problem. To rigorously define an optimization problem that minimizes the error $F(t, R, Q)$ we need to specify the sets in which the correlation operators R and Q take values.

The correlation of the Brownian process. We denote by $\mathscr{Q}$ the set of all correlation operators Q corresponding to standard Wiener processes, i.e.,

$$\mathscr{Q} = \{Q : \text{ there exists an } H\text{-valued standard } Q\text{-Wiener process}\}. \tag{5.1}$$

The set of correlation operators of H-valued Wiener processes coincides with the cone $C(H)$ of symmetric, self-adjoint nuclear operators (see Appendices A and B). The requirement that the process be standard implies that

$$\mathscr{Q} = \{Q \in C(H) : \; k_Q(x,x) = 1 \quad \text{a.e.}\}, \tag{5.2}$$

where k_Q is the kernel of Q,

$$\langle Qf, g\rangle = \iint_D k_Q(z,y) f(y) g(z)\, dy\, dz.$$

The correlation of the initial data. Similarly, we denote by $\mathscr{R}$ the set of all correlation operators R compatible with the initial state of the H-valued random variable q_0, i.e.,

$$\mathscr{R} = \{R \in C(H) : \ k_R(x,x) = c_\infty(x) \quad \text{a.e.}\}. \tag{5.3}$$

Optimization. We are looking for the correlation operators $Q \in \mathscr{Q}$ and $R \in \mathscr{R}$ that minimize the error $F(t,R,Q)$. There is no guarantee, however, that such a minimum exists, as the domains $\mathscr{Q}$ and $\mathscr{R}$ are not compact (in all natural topologies). Thus, there may be no optimal choices of correlations, and one has to modify the optimization problem as follows: find sequences of operators $(Q_n) \subset \mathscr{Q}$ and $(R_n) \subset \mathscr{R}$ such that

$$\lim_{n\to\infty} F(t,R_n,Q_n) = \inf\{F(t,R,Q) : \ R \in \mathscr{R},\, Q \in \mathscr{Q}\}. \tag{5.4}$$

EXAMPLE 5.1. *In this context, the noise correlation associated with* CONNFFESSIT [12] *does not correspond to a Q-Wiener process but rather to a sequence of such processes. Consider the sequence of finite rank operators*

$$Q_n = \frac{1}{n} I_n, \tag{5.5}$$

where I_n is the identity on the linear span of $e_1, \dots, e_n$; a Brownian simulation driven by a Q_n-Wiener process can be viewed as an approximation to CONNFFESSIT. *Although each of the Q_n belongs to the set of admissible correlations $\mathscr{Q}$, we have $Q_n \to 0 \notin \mathscr{Q}$ in the Hilbert–Schmidt topology, and Q_n does not converge at all in the space of nuclear operators. Hence the domain of the optimization problem is not closed.*

EXAMPLE 5.2. *Consider the sequence of finite-dimensional "alternating" operators, defined by*

$$Q_n = \frac{1}{n} \sum_{i,j=1}^{n} (-1)^{i+j} \langle \cdot, e_j \rangle \, e_i.$$

While $Q_n \in \mathscr{Q}$ for every n, this sequence is unbounded in the norm topology, i.e., $\|Q_n\| \to \infty$. This demonstrates that the domain of optimization $\mathscr{Q}$ is also unbounded.

6. Finite-dimensional approximation. Except for very simple situations, the optimization problem (5.4) cannot be solved analytically. In this section, the infinite-dimensional optimization problem is approximated by a finite-dimensional optimization problem, which is shown to be solvable by standard methods. See Appendix A for relevant background on operators in Hilbert spaces.

The approximation is based on the following steps:

1. The target function

   $$F(t,R,Q) = \mathrm{Tr}[M_1(t)(R \otimes Q)] + \mathrm{Tr}[M_2(t)(Q \otimes Q)], \tag{6.1}$$

   with fixed t, is shown to be continuous in the $L_2(H) \times L_2(H)$ topology.
2. Sequences of sets of finite-dimensional operators $\mathscr{R}_n \subset \mathscr{R}$, $\mathscr{Q}_n \subset \mathscr{Q}$ are introduced such that

   $$\overline{\cup_{n=1}^{\infty} \mathscr{Q}_n} = \mathscr{Q} \qquad \text{and} \qquad \overline{\cup_{n=1}^{\infty} \mathscr{R}_n} = \mathscr{R}, \tag{6.2}$$

   where the closure is with respect to the $L_2(H)$ topology.

3. For every n, the optimization problem (5.4) is altered with $\mathscr{R}$ and $\mathscr{Q}$ replaced by $\mathscr{R}_n$, $\mathscr{Q}_n$. The optimal error obtained from the n-dimensional optimization problem is

$$e_n = \inf\{F(t,R,Q) : R \in \mathscr{R}_n,\, Q \in \mathscr{Q}_n\}.$$

It is shown that

$$\lim_{n\to\infty} e_n = e_{opt} = \inf\{F(t,R,Q) : R \in \mathscr{R},\, Q \in \mathscr{Q}\}.$$

4. It is shown that each n-dimensional optimization problem can be solved by a standard algorithm.

1. *Continuity of F.* The target function $F(t,R,Q)$ can be reorganized as follows: for a nuclear operator $T \in L_1(H)$, we consider the family of operators $P_T(t)$, (formally) defined by

$$(P_T(s,t))_{ij} = \operatorname{Tr}\left[Te^{B*s}\hat{e}_i K(t)\hat{e_j}e^{Bs}\right],$$

where, as before, $K(t) = e^{A^*t}e^{At}$. Substituting the expressions for $M_1(t)$ and $M_2(t)$ and reorganizing summations we obtain that

$$F(t,R,Q) = \int_0^t \operatorname{Tr}[P_R(s,t-s)Q]\,ds + \int_0^t\int_0^s \operatorname{Tr}[P_Q(t-r,t-s)Q]\,dr\,ds.$$

Since the mapping $T \to P_T$ is linear, then for $Q_1, Q_2 \in \mathscr{Q}$ and $R_1, R_2 \in \mathscr{R}$,

$$\begin{aligned} F(t,R_2,Q_2) - F(t,R_1,Q_1) = &\int_0^t \operatorname{Tr}[P_{\Delta R}(s,t-s)Q_2]\,ds \\ &+ \int_0^t \operatorname{Tr}[P_{R_1}(s,t-s)\Delta Q]\,ds \\ &+ \int_0^t\int_0^s \operatorname{Tr}[P_{\Delta Q}(s-r,t-s)Q_2]\,dr\,ds \\ &+ \int_0^t\int_0^s \operatorname{Tr}[P_{Q_1}(s-r,t-s)\Delta Q]\,dr\,ds, \end{aligned}$$

where $\Delta Q = Q_2 - Q_1$ and $\Delta R = R_2 - R_1$. By (A.2) the trace of a product is bounded by the product of the $L_2(H)$-norms, and by (A.1) $L_2(H)$ is a two-sided ideal in $L(H)$. Hence

$$\begin{aligned} |F(t,R_2,Q_2) - F(t,R_1,Q_1)| \le &\int_0^t \|P_{\Delta R}(s,t-s)\|_2\|Q_2\|_2\,ds \\ &+ \int_0^t \|P_{R_1}(s,t-s)\|_2\|\Delta Q\|_2\,ds \\ &+ \int_0^t\int_0^s \|P_{\Delta Q}(s-r,t-s)\|_2\|Q_2\|_2\,dr\,ds \\ &+ \int_0^t\int_0^s \|P_{Q_1}(s-r,t-s)\|_2\|\Delta Q\|_2\,dr ds. \end{aligned}$$

Our goal is to show that this can be bounded by an expression of the form

$$|F(t,R_2,Q_2) - F(t,R_1,Q_1)| \le m\,(\|\Delta R\|_2 + \|\Delta Q\|_2),$$

where the constant m may depend on t, R_1, Q_1, and Q_2, as well as on the operators A, B. To complete the proof of this assertion, it is sufficient to show that for every $S \in L_2(H)$,

$$\sup_{0\le s,t\le T} \|P_S(s,t)\|_2 \le m_1 \|S\|_2.$$

This requires mild assumptions on the operators $K(t)$ as shown in the following lemma.

LEMMA 6.1. *Suppose that $K(t)$ is of the form*

$$K(t)f = \int_D k_K(\cdot, y, t) f(y)\, dy,$$

and $k_K(x, y, t)$ is a continuous function of its arguments. Then for every operator $S \in L_2(H)$,

$$\|P_S\|_2 \le m_1 \|S\|_2,$$

where $m_1 = \sup_{D^2\times[0,T]} |k_K(x, y, t)| \cdot \max_{[0,T]} \|e^{Bs}\|^2$.

Proof. Since $L_2(H)$ is a two-sided ideal in $L(H)$, then $e^{Bs}Se^{B^*s} \in L_2(H)$ and

$$\|e^{Bs}Se^{B^*s}\|_2 \le \|e^{Bs}\|^2 \|S\|_2.$$

Moreover, the operator $e^{Bs}Se^{B^*s}$ can be represented as an integral operator with kernel $k_S \in L^2(D^2)$ with $\|e^{Bs}Se^{B^*s}\|_2 = \|k_S\|_{L^2(D^2)}$ (see Proposition A.2). Substituting this representation,

$$\begin{aligned}
(P_S(s,t))_{ij} &= \mathrm{Tr}[e^{Bs}Se^{B^*s}\hat{e}_i K(t)\hat{e_j}] \\
&= \sum_{k=1}^{\infty} \left\langle e^{Bs}Se^{B^*s}\hat{e}_i K(t)\hat{e}_j e_k, e_k \right\rangle \\
&= \sum_{k=1}^{\infty} \iiint_D k_S(x,y) e_i(y) k_K(y,z) e_j(z) e_k(z) e_k(x)\, dz\, dy\, dx \\
&= \iint_D k_S(x,y) k_K(y,x) e_j(x) e_i(y)\, dx,
\end{aligned} \tag{6.3}$$

where in the last equality we used the identity

$$\sum_{k=1}^{\infty} e_k(x) e_k(y) = \delta(x-y).$$

It follows that the operator P_S has the explicit representation

$$P_S(t)\, f = \int_D k_S(y,\cdot) k_K(\cdot, y, t) f(y)\, dy.$$

Finally, as k_K is continuous, P_S is a Hilbert–Schmidt operator with

$$\|P_S\|_2 \le m_1 \|k_S\|_{L^2(D^2)} \le m_1 \|S\|_2. \qquad \square$$

To conclude we have shown the following.

PROPOSITION 6.2. *If $K(t)$ is a Hilbert–Schmidt operator with a continuous kernel, then there exists a constant m that depends on t, A, B, R_1, Q_1, Q_2 such that*

$$|F(t, R_2, Q_2) - F(t, R_1, Q_1)| \le m\,(\|\Delta R\|_2 + \|\Delta Q\|_2),$$

which implies that $F(t, \cdot, \cdot)$ is continuous in the $L_2(H) \times L_2(H)$ topology.

2. *Construction of the approximating sets.* We next construct the sequences of sets $\mathscr{Q}_n, \mathscr{R}_n$. We first start with $\mathscr{Q}_n$: Consider a uniform partition of D into n intervals of size $|D|/n$; we denote the jth interval by I_j and the corresponding indicator function by χ_j. We define

$$\mathscr{Q}_n = \left\{ Q \in \mathscr{Q} : k_Q(x, y) = \sum_{i,j=1}^{n} a_{ij} \chi_i(x) \chi_j(y) \right\},$$

that is, operators $Q \in \mathscr{Q}$ that have a correlation function k_Q that is piecewise constant with respect to the partitions.

PROPOSITION 6.3. $\overline{\cup_{n=1}^{\infty} \mathscr{Q}_n} = \mathscr{Q}$, *where the closure is in $L_2(H)$.*

Proof. We show that for every $Q \in \mathscr{Q}$ there exists a sequence of operators $Q_n \in \mathscr{Q}_n$ that converges to Q in the Hilbert–Schmidt topology. Let $x_j \in I_j$, $j = 1, \ldots, n$, be n points for which $k_Q(x_i, x_j)$ is well defined for any $1 \le i, j \le n$. (See Proposition A.3 for the existence of such set.) Let Q_n be the n-dimensional operator defined by

$$Q_n f(\cdot) = \int_D k_{Q_n}(\cdot, y) f(y)\, dy,$$

where

$$k_{Q_n}(x, y) = \sum_{i,j=1}^{n} k_Q(x_i, x_j) \chi_i(x) \chi_j(y);$$

i.e., k_{Q_n} is a simple function formed by a sampling of k_Q at the points (x_i, x_j). We now show that for every n, $Q_n \in \mathscr{Q}_n$, and that $Q_n \to Q$ in the Hilbert–Schmidt topology. Note that k_{Q_n} is a piecewise constant function, and

$$k_{Q_n}(x, x) = \sum_{i,j=1}^{n} k_Q(x_i, x_j) \chi_i(x) \chi_j(x) = k_Q(x_s, x_s) \chi_s^2(x) = 1,$$

where I_s is the unique interval for which $x \in I_s$. By Proposition A.3, there is a representation

$$k_Q(x, y) = \int_D l(x, z) l(y, z)\, dz,$$

where l is in $L^2(D^2)$. It follows that

$$k_{Q_n}(x, y) = \int_D l_n(x, z) l_n(y, z)\, dz,$$

where $l_n(x, y) = \sum_{i=1}^{n} l(x_i, y) \chi_i(x)$. Consequently, Q_n is nonnegative and self-adjoint. The convergence of Q_n to Q in the Hilbert–Schmidt topology

follows immediately from the convergence of k_{Q_n} to k_Q in $L^2(D^2)$ and from Proposition A.2. ∎

To define the sequence $\mathscr{R}_n$, we introduce an invertible mapping $g : \mathscr{Q} \to \mathscr{R}$ defined by its action on kernels,

$$g : k_Q(x,y) \mapsto c_\infty^{1/2}(x) k_Q(x,y) c_\infty^{1/2}(y).$$

We now define

$$\mathscr{R}_n = \{g(Q) : Q \in \mathscr{Q}_n\},$$

which is indeed a subset of $\mathscr{R}$ consisting of n-dimensional operators. Given $R \in \mathscr{R}$, we set $R_n = g(Q_n)$, where $Q_n \in \mathscr{Q}_n$ converges to $Q = g^{-1}(R)$. The convergence of R_n to R follows from the fact that the mapping g is continuous with respect to the Hilbert–Schmidt topology, as long as $\|c_\infty\|_\infty < \infty$. This proves the second part of (6.2).

3. *Convergence.* Given n, we consider the following finite-dimensional optimization problem:

(6.4) Find $Q_n \in \mathscr{Q}_n$ and $R_n \in \mathscr{R}_n$ that minimize $F(t, R, Q)$.

The minimum always exists since F is continuous with respect to R, Q and $\mathscr{R}_n, \mathscr{Q}_n$ are compact. The optimal error with respect to the finite-dimensional optimization problem is

$$e_n = \min\{F(t,R,Q) : R \in \mathscr{R}_n,\, Q \in \mathscr{Q}_n\}.$$

PROPOSITION 6.4. *e_n converges to e_{opt}.*

Proof. The proof follows immediately from (6.2) and the continuity of F. ∎

4. *The finite-dimensional optimization problem.* We reformulate the finite-dimensional optimization problem (6.4) in matrix language; every operator S with $\operatorname{Im} S \subseteq L_n = \operatorname{Span}\{\chi_1, \dots, \chi_n\}$ corresponds to an n-by-n matrix $[S]$ defined by

$$[S]_{ij} = n \langle \chi_i, S\, \chi_j \rangle.$$

The mapping $S \mapsto [S]$ is an isometry between the linear space of operators $T : L_n \to L_n$ with the Hilbert–Schmidt topology, and $M_n(R)$, endowed with the Frobenius norm,

$$\|A\|_2^2 = \sum_{i,j=1}^n A_{ij}^2.$$

Under this isometry, the set of operators $\mathscr{Q}_n$ corresponds to a set of matrices $\mathscr{Q}^n = \{[Q] : Q \in \mathscr{Q}_n\}$, which coincides with the set of all nonnegative, symmetric n-by-n matrices $[Q]$, such that $[Q]_{ii} = 1/n$ for $1 \le i \le n$. Since every operator $R \in \mathscr{R}_n$ is of the form $R = g(Q)$, where $Q \in \mathscr{Q}_n$, the corresponding matrix is therefore defined by

$$[R]_{ij} = \sum_{k,l=1}^n [Q]_{kl} \left\langle \hat{c}_\infty^{1/2} \chi_i, \chi_k \right\rangle \left\langle \hat{c}_\infty^{1/2} \chi_j, \chi_l \right\rangle = [\hat{c}_\infty^{1/2} Q \hat{c}_\infty^{1/2}], \qquad i,j = 1, \dots, n,$$

where as before $\hat{c}_\infty^{1/2}$ is a multiplication operator. The finite-dimensional optimization problem can be formulated alternatively in matrix form.

PROPOSITION 6.5. *Let $R \in \mathscr{R}_n$ and $Q \in \mathscr{Q}_n$. Then*

$$F(t,R,Q) = \operatorname{Tr}\left[[\Pi_n M_1(t)\Pi_n][R]\otimes[Q]\right] + \operatorname{Tr}\left[[\Pi_n M_2(t)\Pi_n][Q]\otimes[Q]\right], \tag{6.5}$$

where Π_n is the orthonormal projection from $H\otimes H$ into $L_n\otimes L_n$.

Proof. We complete the orthonormal set $\sqrt{n}\chi_1,\dots,\sqrt{n}\chi_n$ into an orthonormal basis (e_k) in H. It follows that for every $1\le i,j\le n$,

$$Q_{ij} = \langle Q\, e_j, e_i\rangle = n\,\langle Q\chi_i,\chi_j\rangle = [Q]_{ij}.$$

Consequently, $R_{ij} = [R]_{ij}$ for $1\le i,j\le n$ and $R_{ij}=0$ otherwise. As $\operatorname{Im} R, \operatorname{Im} Q \subseteq L_n$, the first term on the right-hand side of (6.1) is

$$\begin{aligned}
\sum_{i,j,k,l=1}^{\infty} \langle M_1(t)\, e_i\otimes e_j, e_k\otimes e_l\rangle\, R_{ij}Q_{kl} &= \sum_{i,j,k,l=1}^{n} \langle M_1(t)\, e_i\otimes e_j, e_k\otimes e_l\rangle\, R_{ij}Q_{kl}\\
&= \sum_{i,j,k,l=1}^{n} \langle M_1(t)\, e_i\otimes e_j, e_k\otimes e_l\rangle\, [R]_{ij}[Q]_{kl}\\
&= \sum_{i,j,k,l=1} (M_1(t))_{kl}^{ij}\, [R]_{ij}[Q]_{kl}\\
&= \operatorname{Tr}\left[[\Pi_n M_1(t)\Pi_n][R]\otimes[Q]\right].
\end{aligned}$$

The second term is treated similarly. ∎

Consequently, the finite-dimensional optimization problem is equivalent to solving the following problem: find $[Q]\in\mathscr{Q}^n$ and $[R]\in\mathscr{R}^n$ that minimize the function

$$F(t,[R],[Q]) = \operatorname{Tr}\left([\Pi_n M_1(t)\Pi_n][R]\otimes[Q]\right) + \operatorname{Tr}\left([\Pi_n M_2(t)\Pi_n][Q]\otimes[Q]\right). \tag{6.6}$$

The optimization problem (6.6) can be identified with a convex optimization problem in $\mathbb{R}^{n^4}$ of the following general form:

$$\text{Minimize } f(x,y) = y^T A x + y^T B y,$$

where A, B are matrices $M_n(R^{n^4})$, subject to the nonlinear constraints

$$x\in\mathscr{R}^n, \qquad y\in\mathscr{Q}^n.$$

This problem is solvable via standard algorithmic methods (see Appendix C).

7. Examples. In this section we examine two model problems. The goal of these examples is to demonstrate how our formalism applies in specific situations, as well as to get more insight into the relation between differential operators and noise minimizers.

7.1. A linear advection equation. Consider a function $c(x,t)$, $x\in[0,1]$, governed by the linear first-order PDE

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = -2c + 1,$$

with periodic boundary conditions and initial condition $c(x,0) = c_0(x)$. While the use of Brownian simulations for this problem is senseless, we provide this example as a toy model for our formalism, since it is fully solvable by analytical means.

In the stochastic setting, $c(x,t)$ can be expressed as

$$c(x,t) = \mathbb{E}[q_t^2],$$

where q_t is governed by the SPDE

$$dq_t + \frac{\partial q_t}{\partial x}\,dt = -q_t\,dt + dW_t,$$

with initial conditions that are consistent with the initial data $c_0 = 1/2$ and periodic boundary conditions. The Brownian simulation scheme takes the form

$$\begin{aligned} C_t &= \frac{1}{N}\sum_{i=1}^{N} (Q_t^i)^2, \\ dQ_t^i &= -\left(\frac{\partial Q_t^i}{\partial x} + Q_t^i\right) dt + dW_t^i, \qquad i = 1,\dots,N. \end{aligned}$$

Unlike in the general case, the Q_t^i are independent. Since no linearization is required, the normalized error, $\Delta_t^c(x,t) = \sqrt{n}(C_t(x) - c(x,t))$, is governed by the system

$$\begin{aligned} d\Delta_t^c &= -\left(\frac{\partial \Delta_t^c}{\partial x} + 2\Delta_t^c\right) dt + \frac{2}{\sqrt{N}}\sum_{i=1}^{N} Q_t^i\,dW_t^i, \\ dQ_t^i &= -\left(\frac{\partial Q_t^i}{\partial x} + Q_t^i\right) dt + dW_t^i, \qquad i = 1,\dots,N. \end{aligned}$$

In the notation of (4.1), the operators A and B are given by

$$A = -2I - \frac{\partial}{\partial x}, \qquad B = -I - \frac{\partial}{\partial x},$$

where I is the identity operator.

Take, for example, $M_1(t)$, which is given by (4.3). In the present case,

$$(M_1(t))_{kl}^{ij} = e^{-4t}\int_0^t e^{2s}\int_0^1 e_i(x+s)e_j(x+s)e_k(x)e_l(x)\,dx\,ds,$$

where $x+s$ is to be taken modulo one, and (e_j) is an arbitrary basis in H. Thus, the first term of the mean error reduces to

$$\begin{aligned} \mathrm{Tr}[M_1(t)(R\otimes Q)] &= e^{-4t}\int_0^t e^{2s}\int_0^1 k_R(x+s,x+s)k_Q(x,x)\,dx\,ds \\ &= e^{-4t}\left(\frac{e^{2t}-1}{4}\right), \end{aligned}$$

where we have used the fact that $k_Q(x,x) = 1$ and $k_R(x,x) = 1/2$.

Similarly,

$$\mathrm{Tr}[M_2(t)(Q\otimes Q)] = e^{-4t}\left(\frac{e^{2t}-1}{2}\right)^2.$$

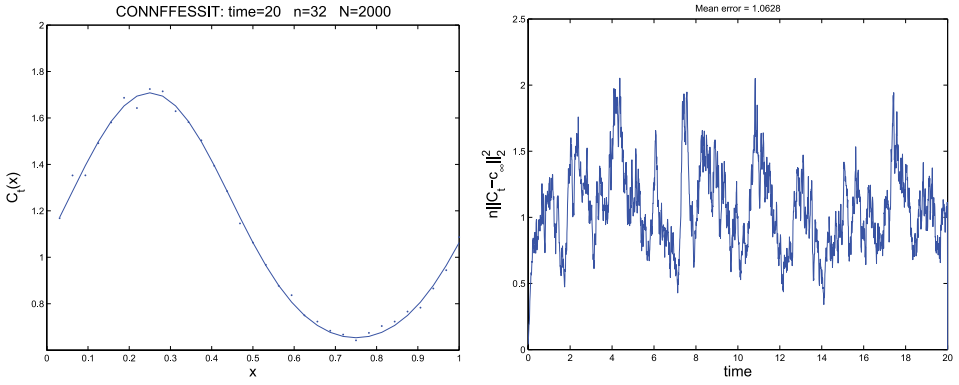

FIG. 7.1. *Numerical solution of system* (7.1) *discretized on an* $n = 32$*-point mesh and using* $N = 2000$ *random fields. The correlation operator is of* CONNFFESSIT *type, represented by an* n*-by-*n *correlation matrix with entries* $[Q]_{ij} = n^{-1}\delta_{ij}$*. The graph on the left shows the exact solution* $c(x,t)$ *at time* $t = 20$ *(solid line) along with the approximate solution* $C_t(x)$ *(dots). The graph on the right shows the time evolution of the normalized error* (7.3).

It follows that the error is independent of the correlations of the noise and the initial data. This is not surprising, since the dynamics can be represented as uncoupled SDEs along characteristics, and hence the evolution on a given characteristic is unaffected by the noise of another characteristic. Therefore the error is affected only by the diagonal elements $k_Q(x,x)$, $k_R(x,x)$ of the correlation functions, which are fixed by the constraints.

7.2. An integral equation. The next example is the integral system given in Example 2.1. The corresponding Brownian simulation is

$$\begin{aligned} U_t(x) &= -C_t(x) + \overline{C_t}, \\ C_t(x) &= \frac{1}{N}\sum_{i=1}^{N} (Q_t^i(x))^2, \\ dQ_t^i(x) &= \frac{1}{2}\left(s(x) + U_t(x) - 1\right) Q_t^i\, dt + dW_t^i, \end{aligned} \tag{7.1}$$

where $x \in [0,1]$ and for every function f, $\bar{f} = \int_0^1 f(x)\,dx$. As $t \to \infty$, the deterministic solution (u,c) converges to the attracting steady-state solution (u_∞, c_∞), given by

$$\begin{aligned} u_\infty &= -c_\infty + \overline{c_\infty}, \\ c_\infty &= -k_\infty + \sqrt{k_\infty^2 + 1}, \end{aligned} \tag{7.2}$$

with $k_\infty = \frac{1}{2}(1 - s - \overline{c_\infty})$.

Figures 7.1 and 7.2 show simulation results of this system discretized on an $n = 32$-point mesh and using $N = 2000$ random fields. The initial conditions are taken to be deterministic: $Q_0^i(x) = 1$. Figure 7.1 corresponds to a CONNFFESSIT simulation, where the (finite) correlation matrix has entries $[Q]_{ij} = n^{-1}\delta_{ij}$. The figure on the left compares the exact solution $c(x,t)$ (solid line) and the approximate solution $C_t(x)$ (dots) at time $t = 20$. Note how the use of a spatially uncorrelated noise gives rise to a rough solution. The figure on the right shows the time evolution of the normalized

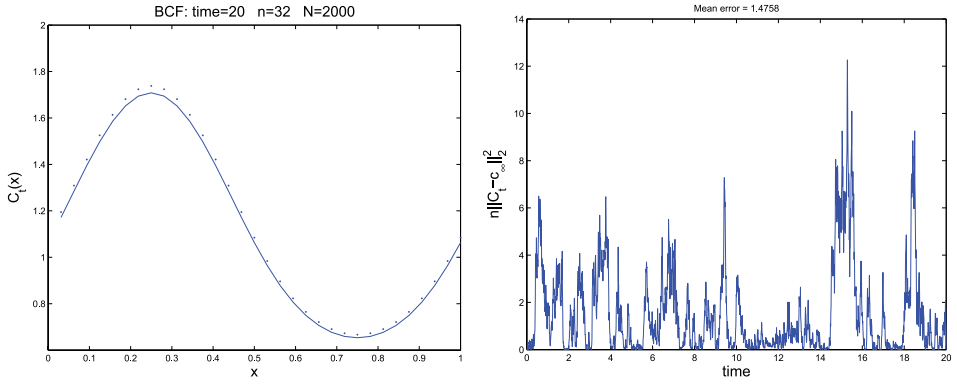

FIG. 7.2. *Same as Figure* 7.1 *for a* BCF*-type correlation operator, represented by an* n*-by-*n *correlation matrix with entries* $[Q]_{ij} = n^{-1}$.

error,

$$N \int_0^1 (c(x,t) - C_t(x))^2 \, dx. \tag{7.3}$$

The mean error oscillates in time at an average value of about 1.06.

In contrast, we display in Figure 7.2 the corresponding graphs for a spatially uniform noise (BCF); i.e., the correlation matrix has entries $[Q]_{ij} = n^{-1}$. As expected, the approximate solution remains smooth. The notable difference is the behavior of the mean error, which assumes a much broader range of values, occasionally becoming very small but also attaining values as large as 12. The time averaged mean error in this particular realization is 1.47, i.e., larger than for the spatially uncorrelated noise. Such a behavior is consistent with earlier studies of the BCF method, where solutions were observed to strongly oscillate around the exact solution. The events where the errors are vanishingly small correspond to the approximate solution "crossing" the exact solution in the course of such oscillations.

We now turn to the error analysis. To linear approximation, the error Δ_t^c satisfies the SPDE

$$d\Delta_t^c = (s + u_\infty - 1 - c_\infty)\Delta_t^c + c_\infty \overline{\Delta_t^c} + \frac{2}{\sqrt{N}} \sum_{i=1}^N q_t^i \, dW_t^i,$$

$$dq_t^i = \frac{1}{2} (s + u_\infty - 1) \, q_t^i \, dt + dW_t^i,$$

so that in terms of the formalism (4.1), the operators A and B are given by

$$Af = (s + u_\infty - 1 - c_\infty) \, f + c_\infty \overline{f},$$

$$Bf = \frac{1}{2}(s + u_\infty - 1) f.$$

Note the factor 2 in front of the noise term, which implies that the error $e(t)$ should be multiplied by a factor of 4.

Our first observation is that both operators A and B are dissipative, which implies that the entries $(M_1(t))_{kl}^{ij}$ decay exponentially in time. Hence, for large enough times

TABLE 7.1
Normalized error for various mesh sizes: comparison between the (optimal) spatially uncorrelated noise and spatially uniform noise.

n	CONNFFESSIT	BCF
8	1.197	2.188
16	1.121	2.188
32	1.083	2.188

the error is dominated by the quadratic term $e_2(t)$. This is of no surprise, as (ergodic) dissipative systems are insensitive to initial data at long times. The leading error contribution is thus given by

$$e_2(t) = 4 \sum_{i,j,k,l=1}^{\infty} (M_2(t))_{kl}^{ij} Q_{ij} Q_{kl},$$

where

$$(M_2(t))_{kl}^{ij} = \int_0^t \int_0^s \left(e^{B^*(s-r)} \hat{e}_i e^{A^*(t-s)} e^{A(t-s)} \hat{e}_j e^{B(s-r)} \right)_{kl} dr\, ds.$$

Using the fact that the operator B and $\hat{e}_i$ commute, this can be brought to the following simpler form:

$$e_2(t) = 4 \sum_{i,j,k,l=1}^{\infty} Q_{ij} Q_{kl} \left\langle e_i e_k, G(t) e_j e_l \right\rangle,$$

where

$$G(t) = \int_0^t \int_0^s e^{B^*(s-r)} e^{A^*(t-s)} e^{A(t-s)} e^{B(s-r)}\, dr\, ds;$$

unlike $M_2(t)$, $G(t)$ is an operator on H. The error can be estimated in the limit of large t. First note that

$$B^* G(t) + G(t) B = \int_0^t e^{B^* s} e^{A^*(t-s)} e^{A(t-s)} e^{Bs}\, ds - \int_0^t e^{A^*(t-s)} e^{A(t-s)}\, ds.$$

Since both A and B are dissipative, the first integral on the right-hand side vanishes in the limit of large t. Multiplying the left-hand side by A^* and A, respectively, we end up with the following system of Lyapunov equations:

$$\begin{aligned} &B^* G(t) + G(t) B = F(t), \\ &A^* F(t) + F(t) A = I, \qquad t \gg 1. \end{aligned} \tag{7.4}$$

We have discretized the system (7.4) as described in section 6 and computed the optimal correlation Q_n for various values of the mesh size. The optimal correlation was found to be the CONNFFESSIT correlation, $[Q]_{ij} = n^{-1} \delta_{ij}$. In Table 7.1 we display the computed values of the normalized error for various mesh sizes and for both spatially uncorrelated and spatially uniform noise. The computed errors are in agreement with the simulation results.

An insight into why is CONNFFESSIT optimal is obtained by noting that $e_2(t)$ can be represented in terms of the correlation functions,

$$e_2(t) = 4 \iint_D k_Q^2(x,y) k_G(x,y)\, dx\, dy,$$

where k_G is the kernel of $G(t)$, which is a distribution rather than a function. Specifically, k_G is singular along the diagonal and a smooth, positive function off the diagonal. It follows that the minimizer k_Q must vanish outside the diagonal.

8. Discussion. We derived an expression for the mean-square error in Brownian simulations as a function of the spatial correlation of the noise. We formulated an optimization problem for the variance minimizing correlation, and showed that it can be approximated by finite-dimensional convex optimization problems, solvable by standard methods. At this point, our analysis is restricted to a class of systems that are closable and to steady-state situations. Our analysis can easily be extended to time-dependent situations, with relatively minor technical complications. The extension to nonclosable systems seems to be more complicated and remains to be done.

This paper exposes a theoretical framework for variance reduction in spatially dependent Brownian simulations. In practice, one needs to solve a nontrivial optimization problem for each given realization. Our belief is that the optimal correlation does not depend on the fine details of the problem, but on coarser properties, such as the type of equations. Understanding the relation between the type of equations and the optimizer remains an open problem of much interest.

Appendix A. Operators on Hilbert spaces. In this section we review some basic facts about operators on Hilbert spaces. In particular, we focus on two classes of operators, namely, *nuclear* and *Hilbert–Schmidt* operators. While all of the contents of this section can be found in [10], we summarize the facts that are essential to our analysis.

For a Hilbert space H, the space of all bounded linear operators from H to itself is denoted by $L(H)$; it is a Banach space with respect to the norm topology. The subspace $K(H) \subset L(H)$ of *compact operators* consists of the closure of the finite-dimensional operators in the norm topology.

Nuclear operators. An operator $T \in L(H)$ is called *nuclear* if there exist sequences $(x_n), (y_n) \subset H$ such that

$$T = \sum_{j=1}^{\infty} \langle \cdot, y_j \rangle\, x_j$$

and

$$\sum_{j=1}^{\infty} \|x_j\| \|y_j\| < \infty.$$

The space $L_1(H)$ of nuclear operators is a Banach space with respect to the norm

$$\|T\|_1 = \inf \left\{ \sum_{j=1}^{\infty} \|x_j\| \|y_j\| :\ T = \sum_{j=1}^{\infty} \langle \cdot, y_j \rangle\, x_j \right\}.$$

It is a two-sided ideal in $L(H)$, and for $T \in L_1(H)$ and $S \in L(H)$,

$$\|TS\|_1 \le \|T\|_1 \|S\| \qquad \text{and} \qquad \|ST\|_1 \le \|T\|_1 \|S\|.$$

The *trace* of a nuclear operator $T \in L_1(H)$ is defined by

$$\operatorname{Tr} T = \sum_{j=1}^{\infty} \langle Te_j, e_j \rangle ,$$

where (e_j) is an orthonormal basis in H. For every nuclear operator, this sum converges and is independent of the choice of orthonormal basis.

A subset of the nuclear operators that is of particular importance is the cone $C(H)$ of nonnegative, self-adjoint nuclear operators. For every $T \in C(H)$ the $L_1(H)$-norm and the trace are in fact equivalent, namely,

$$\operatorname{Tr} T = \|T\|_1.$$

Hilbert–Schmidt operators. An operator $T \in L(H)$ is called *Hilbert–Schmidt* if, for some orthonormal basis (e_j),

$$\sum_{j=1}^{\infty} \|Te_j\|^2 < \infty.$$

The space $L_2(H)$ of Hilbert–Schmidt operators is a Hilbert space with the inner product

$$\langle T, S \rangle_2 = \operatorname{Tr}(T^* S).$$

The corresponding norm is denoted by $\|\cdot\|_2$. The space of Hilbert–Schmidt operators is a two-sided ideal in $L(H)$, and for $T \in L_2(H)$ and $S \in L(H)$,

$$\|TS\|_2 \le \|T\|_2 \, \|S\| \qquad \text{and} \qquad \|ST\|_2 \le \|T\|_2 \, \|S\|. \tag{A.1}$$

Nuclear operators can be characterized by the following statement.

PROPOSITION A.1. *An operator $T \in L(H)$ is nuclear if and only if there exist operators $T_1, T_2 \in L_2(H)$ such that*

$$T = T_1 T_2$$

and

$$\|T\|_1 \le \|T_1\|_2 \|T_2\|_2. \tag{A.2}$$

Moreover, a nonnegative, self-adjoint operator $T \in L(H)$ is nuclear if and only if $T^{1/2}$ is Hilbert–Schmidt and

$$\|T\|_1 = \|T^{1/2}\|_2^2.$$

In particular, every nuclear operator is a Hilbert–Schmidt operator. In fact,

$$L_1(H) \subset L_2(H) \subset K(H),$$

and $L_1(H)$, $L_2(H)$ are dense subsets of $K(H)$ with respect to the norm topology.

Now consider the particular case which is considered in this paper, where $H = L^2(D)$ with $D \subset \mathbb{R}$ a bounded interval. Then Hilbert–Schmidt operators can be characterized by the following statement.

PROPOSITION A.2. *An operator $T \in L(H)$ is Hilbert–Schmidt if and only if there exists a kernel $k_T \in L^2(D^2)$ such that*

$$Tf = \int_D k_T(\cdot, y) f(y)\, dy, \qquad f \in H.$$

Moreover, the mapping $T \mapsto k_T$ is an isometry, that is, $\|T\|_2 = \|k_T\|_{L^2(D^2)}$.

The characterization of nuclear operators stated in Proposition A.1 can be reformulated in terms of kernels.

PROPOSITION A.3. *An operator $T \in L_2(H)$ is nuclear if and only if there exist kernels $k_1, k_2 \in L^2(D^2)$ such that, for almost every $x, y \in D$,*

$$k_T(x, y) = \int_D k_1(x, z) k_2(y, z)\, dz.$$

Moreover, if $T \in C(H)$, then one can take $k_1 = k_2$.

In particular, the kernel of an operator $T \in L_1(H)$ is defined almost everywhere on its diagonal by

$$k_T(x, x) = \int_D k_1(x, z) k_2(x, z)\, dz.$$

Moreover, it is integrable on the diagonal, and

$$\operatorname{Tr} T = \int_D k_T(x, x)\, dx.$$

Appendix B. Hilbert space-valued stochastic processes. The notion of a Hilbert space-valued stochastic process is a generalization of a stochastic process in $\mathbb{R}^n$ and plays a fundamental role in the theory of SPDEs. Its correlation, rather than being a matrix, is a linear operator in H. In this section we briefly review the definitions and properties of Hilbert space-valued stochastic processes, and, in particular, Hilbert space-valued Wiener processes, together with the associated stochastic calculus. We focus on $H = L^2(D)$, where D is a finite interval in $\mathbb{R}$.

An *H-valued random variable* is a measurable function $X(\omega) : \Omega \to H$. For a given pair of H-valued random variables X and Y, the *correlation operator*, $\operatorname{Cor}(X, Y)$, is defined by

$$\operatorname{Cor}(X, Y)(f) = \mathbb{E}[\langle X, f \rangle\, Y], \qquad f \in H.$$

The *autocorrelation* operator of X is $\operatorname{Cor}(X, X)$; it is a nonnegative, symmetric nuclear operator (see Appendix A).

An *H-valued stochastic process* is a measurable function $X_t(\omega) : [0, T] \times \Omega \to H$ such that, for every $t \in [0, T]$,

$$\mathbb{E} \int_0^t \|X_s\|^2\, ds < \infty.$$

We denote by $\tilde{H}$ the Hilbert space of all H-valued stochastic processes, endowed with the inner product

$$\langle X, Y \rangle_{\tilde{H}} = \mathbb{E} \int_0^T \langle X_s, Y_s \rangle\, ds.$$

We will often abuse notation, denoting by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ the norms and inner products of both spaces H and $\tilde{H}$, as long as it remains clear from the context.

Now let Q be a bounded operator in H. An H-valued stochastic process W_t is a *Q-Wiener process* if the following hold:

1. $W_0 = 0$.
2. W_t has continuous trajectories.
3. W_t has independent increments.
4. For every $t \geq s \geq 0$, $W_t - W_s$ is a zero mean Gaussian H-valued random variable with autocorrelation $(t-s)Q$.

As tQ is the autocorrelation of W_t, it follows that

$$\mathbb{E}[\langle W_t, f\rangle \langle W_t, g\rangle] = t\langle Qf, g\rangle, \qquad f, g \in H,$$

and

$$\mathbb{E}\|W_t\|^2 = \operatorname{Tr} Q\, t,$$

which implies that $Q \in C(H)$.

Given an operator $Q \in C(H)$, a Q-Wiener process can be constructed by taking a sequence of mutually independent real-valued Wiener processes, (W_t^k), and an orthonormal basis (e_k) in H, and by setting

$$W_t = \sum_{k=1}^{\infty} W_t^k Q^{1/2}(e_k). \tag{B.1}$$

For a detailed proof of the above statement, we refer the reader to [5].

In the case of $H = L^2(D)$, it is often more convenient to associate a *correlation function* with a Q-Wiener process, rather than an operator: for almost every $x, y \in D$, define $k_Q(x,y)$ by

$$k_Q(x,y) = \frac{1}{t}\mathbb{E}[W_t(x)W_t(y)].$$

One can easily verify that the correlation function k_Q is a symmetric function with a nonnegative diagonal such that

$$\int_{D^2} k_Q^2(x,y)\,dx\,dy < \infty,$$

and that it is the kernel corresponding to the correlation operator,

$$Qf(x) = \int_D k_Q(x,y)f(y)\,dy.$$

An H-valued Q-Wiener process $W(t)$ is said to be *standard* if, for almost every $x \in D$,

$$k_Q(x,x) = 1.$$

The stochastic integral. The H-valued Itô integral can easily be constructed using the representation (B.1) of the Q-Wiener process as a series of real-valued Wiener processes. In general, the stochastic Itô integral takes values in another Hilbert space H'.

Let $L(H,H')$ denote the space of all bounded operators from H to H'. A stochastic process $g : [0,T) \times \Omega \to L(H,H')$ is said to be *adapted* to an H-valued Q-Wiener

process W_t if, for every t, $g(t)$ is measurable with respect to the Brownian filtration up to time t. Let e_k be an orthonormal basis of eigenfunctions of Q, and let λ_k be the corresponding eigenvalues. We then define the Itô integral of g with respect to W_t by

$$\int_0^t g(s)\,dW_s = \sum_{k=1}^{\infty} \int_0^t g(s)\left(\sqrt{\lambda_k} e_k\right) dW_s^k, \tag{B.2}$$

where the series is convergent in $\tilde{H}'$. For a detailed proof of the above statement, see, e.g., [9].

Stochastic calculus in Hilbert spaces can be based on the series representation of the Q-Wiener process combined with the stochastic calculus for real-valued Wiener processes. A straightforward application is the following proposition.

PROPOSITION B.1. *Let W_t be an H-valued Q-Wiener process, and let X_t^1, X_t^2 be two stochastic processes of the form*

$$X_t^i = \int_0^t g_i(s)\,dW_s, \qquad i = 1, 2,$$

where g_i are adaptable processes in $L(H)$. Then the correlation function of X_t^1, X_t^2 is given by

$$\mathbb{E}\left\langle X_{t_1}^2, X_{t_2}^2 \right\rangle = \mathbb{E}\int_0^{\min(t_1,t_2)} \mathrm{Tr}[g_1(s) Q g_2^*(s)]\,ds.$$

We proceed by stating the Hilbert space versions of Itô's isometry and Itô's formula, which play a fundamental role in stochastic analysis. See [5] for detailed proofs of these statements.

THEOREM B.2. *Itô's isometry. For any adapted process $g : [0, \infty) \to L(H)$,*

$$\mathbb{E}\left\| \int_0^t g(s)\,dW_s \right\|^2 = \mathbb{E}\int_0^t \mathrm{Tr}\left[g(s) Q g^*(s)\right] ds.$$

Note that the left-hand side is a square of a norm in H, whereas the right-hand side is a square of a trace norm in H.

THEOREM B.3. *Itô's formula. Let $F : H \to R$ be a differentiable function such that its partial derivatives ∇F and $\nabla^2 F$ are uniformly continuous on bounded subsets of H. Consider the H-valued stochastic process $X(t)$ defined by the SDE*

$$dX_t = a(X_t, t)\,dt + dW_t,$$

which is a shorthand notation for

$$X_t = X_0 + \int_0^t a(X_s, s)\,ds + W_t.$$

Then

$$dF(X_t) = \left\langle \nabla F\left(X_t\right), dX_t \right\rangle + \frac{1}{2}\,\mathrm{Tr}\left[\nabla^2 F\left(X_t\right) Q\right] dt.$$

As an application, consider the case where $H = L^2(D)$ and $F : \mathbb{R} \to \mathbb{R}$. Then

$$dF(X_t) = F'(X_t)\,dX_t + \frac{1}{2}\operatorname{Tr}\left[F''(X_t)Q\right]dt$$
$$= F'(X_t)\,dX_t + \frac{1}{2}F''(X_t)\operatorname{Tr}Q\,dt.$$

Appendix C. Semidefinite programming. Semidefinite programming is a class of convex optimization problems, which consist of minimizing a real-valued linear function F, defined on S_d, the cone of nonnegative, semidefinite d-by-d matrices, and subject to some additional affine constraints. A canonical formulation for semidefinite programming (SDP) optimization problems is the following:

$$\begin{aligned} &\text{Minimize } F(X) = \operatorname{Tr}[RX] \\ &\text{subject to } AX = B, \qquad X \in S_d, \end{aligned} \tag{C.1}$$

where R, A, and B are given matrices.

The nonlinearity of the optimization problem (C.1) arises from the nonlinear geometric structure of S_d. This nonlinear constraint $X \in S_d$ can be represented alternatively by a collection of d algebraic inequalities,

$$\det X^i \geq 0, \qquad i = 1, \ldots, d, \tag{C.2}$$

where X^i denotes the ith principal submatrix of X, together with the linear constraint of symmetry,

$$X = X^T.$$

The standard algorithm for solving (C.1) can also be applied to convex functions $F(X)$. It consists of constructing a sequence of feasible (i.e., compatible with the constraints) points X_n that converge to an optimal solution X_{opt}. To impose the nonlinear constraints (C.2), one minimizes $F + \Phi^\epsilon$, rather than F itself, where $\Phi^\epsilon(X)$ is a one-parameter family of *barrier functions*, each of which diverges as X tends to the boundary of S_d. More explicitly, Φ^ϵ is a logarithmic barrier function, defined by

$$\Phi^\epsilon(X) = -\epsilon \sum \log\det(X^i), \qquad t > 0.$$

When ϵ is small, an optimal solution of (C.1) is close to an optimal solution of (C.3), with F replaced by $F + \Phi^\epsilon$. Formally, every $\epsilon > 0$ results in an optimal solution X^ϵ_{opt}, called a central path solution, and X_{opt} arises as a limit of the central path solutions as $\epsilon \to 0$. The optimization problem (C.1) is therefore reduced to an optimization problem depending on a parameter ϵ:

$$\begin{aligned} &\text{Minimize } F(X) + \Phi^\epsilon(X) \\ &\text{subject to } AX = B, \qquad X = X^T. \end{aligned} \tag{C.3}$$

The optimization problem (C.3) can be solved with a standard Newton method. For further reading about SDP algorithms, see [2].

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