



Adjoint-Based Calibration of Nonlinear Stochastic Differential Equations

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Abstract

To study the nonlinear properties of complex natural phenomena, the evolution of the quantity of interest can be often represented by systems of coupled nonlinear stochastic differential equations (SDEs). These SDEs typically contain several parameters which have to be chosen carefully to match the experimental data and to validate the effectiveness of the model. In the present paper the calibration of these parameters is described by nonlinear SDE-constrained optimization problems. In the optimize-before-discretize setting a rigorous analysis is carried out to ensure the existence of optimal solutions and to derive necessary first-order optimality conditions. For the numerical solution a Monte–Carlo method is applied using parallelization strategies to compensate for the high computational time. In the numerical examples an Ornstein–Uhlenbeck and a stochastic Prandtl–Tomlinson bath model are considered.

Keywords Optimization of SDEs · First-order optimality conditions · Monte Carlo methods · Stochastic gradient methods · Ornstein–Uhlenbeck model · Stochastic Prandtl–Tomlinson equations

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1 Introduction

Natural processes inherit noise and uncertainties and therefore are often modeled using stochastic differential equations (SDEs). Such equations consist of a deterministic part and a stochastic part, where the latter one is usually modeled by Brownian motions; see, e.g., [55, 56]. The application of SDEs ranges from physics and biology to finance;

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cf. [13, 28, 51], for instance. All these SDEs include parameters that need to be calibrated. For this calibration (also called parameter identification), usually real-world data is used and parameters are searched that lead to the best agreement of measured and predicted data. Therefore, parameter identification and optimal control of such processes are of interest to many communities and have been the subject of extensive research.

The main motivation for our work is the calibration of models that investigate the rheological properties of fluids using the microrheology technique. Specifically, the study of the behavior of fluids using a so-called tracer particle suspended in a fluid. Key tools to study properties of complex fluids are nonlinear bath models, for example, the Stochastic Prandtl–Tomlinson (SPT) model [29, 30, 43]. While linear models have been investigated in the Markovian framework [15, 52, 53], less is known for the nonlinear case together with memory effects in which the Markovian framework is no longer applicable. To study the properties of fluids, systems of coupled nonlinear SDEs representing the movement of particles are studied. The SDEs in this case typically possess the structure of (generalized) nonlinear Langevin equations [33, 35, 58].

In this paper, we express the calibration problems as SDE-constrained optimization problems of the form

$$\begin{cases} \min J(X, u) = j(X) + j_T(X(T)) + \frac{\kappa}{2} \|u\|_{\mathcal{U}}^2 \\ \text{subject to } X \text{ satisfies an SDE on } [0, T] \text{ for parameter or control } u \in \mathcal{U}_{\text{ad}} \subset \mathcal{U} \end{cases} \quad (1.1)$$

with $\kappa \geq 0$, a parameter or control space \mathcal{U} and with properly chosen functionals j , j_T which will be specified in Sects. 3 and 4, respectively. In particular, the tracking type functional

$$J(X, u) = \frac{1}{2} \left(\int_0^T \|\mathcal{C}(\mathbb{E}[X(t)]) - c^d(t)\|_{\mathbb{R}^\ell}^2 dt + \|\mathcal{C}(\mathbb{E}[X(T)]) - c_T^d\|_{\mathbb{R}^\ell}^2 + \kappa \|u\|_{\mathcal{U}}^2 \right) \quad (1.2)$$

is included. Notice that the objective defined in (1.2) differs from the one typically used in the stochastic optimal control setting (see, e.g., [19, 46]), but is present in literature for calibration problems; see, e.g., [17, 20, 22, 31, 36]).

To solve (1.1) let us mention three different approaches:

- One can lift the problem to the level of partial differential equations (PDEs). This lift can be viewed as taking the limit in several senses; see, e.g., [45] for a review in the deterministic setting. One way is to define a probability density function that contains information on the probability of the state of the model being in a certain configuration at a certain timestep. The PDE that governs the evolution of the probability density is given by the Fokker-Planck equation [1, 9]. In this setting, one can apply tools from PDE-constrained optimization; see, e.g., [27, 54]. If one wants to account for the structure of the space of probability measures, we refer to [4, 7, 14, 21]. However, one encounters certain challenges with this lift to the level of PDEs. One of them is the exponential growth of numerical complexity with the

dimension of the model since we encounter a high-dimensional PDE. This is also known as the *curse of dimensionality*.

- In another approach one stays on the microscopic level and directly characterizes the optimal control or calibration using SDEs [5, 6, 37]. Here, no probability density functions come into play and hence no PDEs have to be solved. However, their huge weakness is their quite slow convergence [24].
- Further, hybrid methods are utilized, where the models are solved on the microscopic level, but—to calculate the gradient—the density functions are assembled. These methods suffer from the time-consuming bottleneck of assembling probability density functions in hybrid methods [2, 3].

In the present paper we study (1.1) as an infinite dimensional optimization problem; see, e.g., [27, 38, 54]. The first objective is to derive sufficient conditions for the existence of optimal solutions and to carefully set up the correct framework in terms of solution spaces and control or parameter spaces. After we guarantee sufficient differentiability of the cost functional and the constraints, we derive first-order necessary optimality conditions by an adjoint calculus. This allows us to characterize an optimal control or optimal parameters; see, e.g., [27]. Up to the authors' knowledge, the rigorous derivation of the reduced gradient for the calibration problem using adjoint calculus is not present in the literature. Nevertheless, there are some works heading in a similar direction, in particular, [34] and very recently [11].

To solve (1.1) numerically, one possibility is to start with deriving first-order necessary optimality conditions for the optimal control problem on the continuous level. After this, the system is discretized and optimization schemes are applied. This approach is also known as *first-optimize-then-discretize*. Alternatively, in the *first-discretize-then-optimize* approach (1.1) is discretized first and then the first-order optimality system is derived for the discretized optimization problem. Utilizing the Lagrangian framework, we derive an optimality system consisting of the state equation, the adjoint equation and the optimality condition. Both approaches are compared. Moreover, convergence of the value of the discretized cost functional to the value of the continuous one is proved. Notice that the exploiting of adjoint-based models and staying on the microscopic level by using Monte–Carlo computations have several advantages, in particular, they are easy to implement and inherit huge flexibility [24].

The paper is structured as follows: In Sect. 2 we introduce the notation and recall some preliminaries when dealing with SDEs. In Sect. 3, a general state equation is introduced that governs the optimization problem that is defined in Sect. 4, where we prove the existence of solutions to the optimization problem. In Sect. 5 we introduce a discretization for (1.1) and derive the associated first-order necessary optimality system which is the basis for a gradient-based method utilized for our numerical tests. The Fréchet differentiability of the constraints and the objective as well as the first-order optimality system for (1.1) are proved in Sect. 6. The work is completed in Sect. 7, where we formulate our optimization strategy and validate it using two different examples. At first, we apply our method to the mean-reverting Ornstein–Uhlenbeck process where we try to find a time-dependent control function that drives the evolution of the SDE to follow a desired trajectory. Then, we solve the calibration model governed by the SPT model with one and two particles.

2 Notation and Preliminaries

In this section, we introduce our setting and a general model for calibration and stochastic control problems. We start by recalling some preliminaries. For more details, we refer the reader to [40, 57].

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space with a non-empty event set Ω , a σ -algebra \mathcal{F} and a probability measure $\mathbb{P} : \mathcal{F} \rightarrow [0, 1]$. For given $d \in \mathbb{N}$ let $\mathbf{X} = (X_1, \dots, X_d) : \Omega \rightarrow \mathbb{R}^d$ be \mathcal{F} -measurable. Then, \mathbf{X} is called a *d-dimensional random variable* and its *expected value* is defined as

$$\mathbb{E}[\mathbf{X}] := \int_{\Omega} \mathbf{X} \, d\mathbb{P} = \int_{\Omega} \mathbf{X}(\omega) \, d\mathbb{P}(\omega) \in \mathbb{R}^d.$$

A *d-dimensional stochastic process* is a family $\{\mathbf{X}(t)\}_{t \geq 0}$ of *d-dimensional random variables* $\mathbf{X}(t) : \Omega \rightarrow \mathbb{R}^d$. A *filtration* of the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is a family $\{\mathcal{F}(t)\}_{t \geq 0}$ of σ -algebras $\mathcal{F}(t) \subset \mathcal{F}$ with $\mathcal{F}(s) \subset \mathcal{F}(t)$ for all $s \in [0, t]$. A *d-dimensional stochastic process* $\{\mathbf{X}(t)\}_{t \geq 0}$ is called *adapted* with respect to the filtration $\{\mathcal{F}(t)\}_{t \geq 0}$ if each $\mathbf{X}(t)$ is $\mathcal{F}(t)$ -measurable. Furthermore, it is called *progressively measurable* if for every $t \geq 0$ the function $\mathbf{X}|_{[0,t]} : \Omega \times [0, t] \rightarrow \mathbb{R}^d, (\omega, t) \mapsto \mathbf{X}(\omega, t)$, is $\mathcal{F}(t) \otimes \mathcal{B}([0, t])$ -measurable, where $\mathcal{B}([0, t])$ is the σ -algebra of all Borel subsets of $[0, t]$ and \otimes denotes the product- σ -algebra. The stochastic Itô-integral will be considered in the L^2 -framework; cf., e.g., [18, Section 4.2]. For $T > 0$ we endow $L^2(0, T; \mathbb{R}^d)$ with the standard norm

$$\|\varphi\|_{L^2(0,T;\mathbb{R}^d)} := \left(\int_0^T \|\varphi(t)\|_{\mathbb{R}^d}^2 \, dt \right)^{1/2},$$

with the Euclidean norm $\|\cdot\|_{\mathbb{R}^d}$ in \mathbb{R}^d . In the same way, the space $L^2(\Omega; \mathbb{R}^d)$ of all equivalence classes of square-integrable random variables is endowed with the norm

$$\|\mathbf{X}_\circ\|_{L^2(\Omega;\mathbb{R}^d)} := \left(\mathbb{E} \left[\|\mathbf{X}_\circ\|_{\mathbb{R}^d}^2 \right] \right)^{1/2} = \left(\int_{\Omega} \|\mathbf{X}_\circ(\omega)\|_{\mathbb{R}^d}^2 \, d\mathbb{P}(\omega) \right)^{1/2}.$$

Finally, $L^2(\Omega \times (0, T); \mathbb{R}^d) \cong L^2(\Omega; L^2(0, T; \mathbb{R}^d))$ denotes the space of equivalence classes of \mathbb{R}^d -valued $\mathcal{F} \otimes \mathcal{B}([0, T])$ -measurable and square-integrable processes \mathbf{X} , with the norm

$$\|\mathbf{X}\|_{L^2(\Omega \times (0,T);\mathbb{R}^d)} := \left(\mathbb{E} \left[\int_0^T \|\mathbf{X}(t)\|_{\mathbb{R}^d}^2 \, dt \right] \right)^{1/2}.$$

We define

$$\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d) := \{ \mathbf{X} \in L^2(\Omega \times (0, T); \mathbb{R}^d) : \mathbf{X} \text{ progressively measurable} \}.$$

More precisely, $\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$ consists of all equivalence classes in $L^2(\Omega \times (0, T); \mathbb{R}^d)$ which contain at least one progressively measurable process. The space $\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$ will

be considered as a subspace of $L^2(\Omega \times (0, T); \mathbb{R}^d)$ supplied by the topology of $L^2(\Omega \times (0, T); \mathbb{R}^d)$, i.e., we set

$$\|X\|_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)} := \|X\|_{L^2(\Omega \times (0, T); \mathbb{R}^d)}.$$

In addition to the above Hilbert spaces, we will also consider processes with continuous paths, endowed with the sup-norm. For this, we define the norm

$$\|X\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))} := \sup_{t \in [0, T]} \|X(t)\|_{L^2(\Omega; \mathbb{R}^d)} = \sup_{t \in [0, T]} \left(\mathbb{E}[\|X(t)\|_{\mathbb{R}^d}^2] \right)^{1/2}$$

on the Banach space of all processes X which are continuous functions of t with values in the space $L^2(\Omega; \mathbb{R}^d)$.

Let now $m \in \mathbb{N}$ be given. By $\{\mathbf{B}(t) = (B_i(t))_{1 \leq i \leq m} \mid t \geq 0\}$ we denote an m -dimensional Brownian motion (or Wiener process); see, e.g., [40, Definition 4.1, Chapter 1]. We introduce the family of σ -algebras $\{\mathcal{F}^{\mathbf{B}}(t)\}_{t \geq 0}$, where $\mathcal{F}^{\mathbf{B}}(t)$ is generated by $\{\mathbf{B}(s) \mid 0 \leq s \leq t\}$ for any $t \geq 0$. Recall that $\{\mathcal{F}^{\mathbf{B}}(t)\}_{t \geq 0}$ is said to be the *natural filtration* generated by the Brownian motion $\{\mathbf{B}(t)\}_{t \geq 0}$. By $\{\mathcal{F}(t)\}_{t \geq 0}$ we introduce the filtration given by $\mathcal{F}(t) = \mathcal{F}^{\mathbf{B}}(t) \cup \mathcal{N}$, where the set \mathcal{N} is the set of all \mathbb{P} -null sets.

We fix a sub- σ -algebra $\mathcal{F}_\circ \subset \mathcal{F}$ which is independent of $\mathcal{F}(T)$, and define the extended filtration $\mathcal{F}_\circ(t) := \sigma(\mathcal{F}(t) \cup \mathcal{F}_\circ)$. Let \mathcal{X} denote the vector space of all $\{\mathcal{F}_\circ(t)\}_{t \in [0, T]}$ -adapted measurable processes of the form

$$Y(t) = \Phi(Y_\circ, \mathbf{a}, \mathbf{b}) := Y_\circ + \int_0^t \mathbf{a}(s) \, ds + \int_0^t \mathbf{b}(s) \, d\mathbf{B}(s) \quad \text{for every } t \in [0, T] \tag{2.1}$$

satisfying

$$\|Y\|_{\mathcal{X}} := \left(\mathbb{E}[\|Y_\circ\|_{\mathbb{R}^d}^2] + \mathbb{E} \left[\int_0^T \|\mathbf{a}(s)\|_{\mathbb{R}^d}^2 + \|\mathbf{b}(s)\|_{\mathbb{F}}^2 \, ds \right] \right)^{1/2} < \infty \tag{2.2}$$

with $Y_\circ \in L^2(\Omega; \mathbb{R}^d)$ being \mathcal{F}_\circ -measurable, $\mathbf{a} \in \mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)$ and $\mathbf{b} = [b_1 \mid \dots \mid b_m] \in \mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^{d \times m})$. In (2.2), we denote by $\|\cdot\|_{\mathbb{F}}$ the Frobenius (matrix) norm induced by the inner product

$$\langle \mathbf{b}, \tilde{\mathbf{b}} \rangle_{\mathbb{F}} = \sum_{j=1}^m \mathbf{b}_j^{\top} \tilde{\mathbf{b}}_j = \sum_{i=1}^d \sum_{j=1}^m b_{ij} \tilde{b}_{ij} \quad \text{for } \mathbf{b} = [b_1 | \dots | b_m], \tilde{\mathbf{b}} = [\tilde{b}_1 | \dots | \tilde{b}_m] \in \mathbb{R}^{d \times m}.$$

(2.3)

Then the stochastic process \mathbf{Y} in (2.1) is adapted with respect to the filtration $\{\mathcal{F}_\circ(t)\}_{t \in [0, T]}$, and for almost all $\omega \in \Omega$ the associated path $[0, T] \ni t \mapsto \mathbf{Y}(\omega, t) \in \mathbb{R}^d$ is continuous. In particular, \mathbf{Y} is progressively measurable; cf. [32, Proposition 1.13]. We consider on the space \mathcal{X} the inner product

$$\langle \mathbf{Y}, \mathbf{Z} \rangle_{\mathcal{X}} = \mathbb{E} \left[\mathbf{Y}_\circ^{\top} \mathbf{Z}_\circ \right] + \mathbb{E} \left[\int_0^T \mathbf{a}(s)^{\top} \tilde{\mathbf{a}}(s) \, ds + \int_0^T \langle \mathbf{b}(s), \tilde{\mathbf{b}}(s) \rangle_{\mathbb{F}} \, ds \right], \quad (2.4)$$

where $\mathbf{Z} := \Phi(\mathbf{Z}_\circ, \tilde{\mathbf{a}}, \tilde{\mathbf{b}})$ with $\mathbf{Z}_\circ \in L^2(\Omega; \mathbb{R}^d)$ being \mathcal{F}_\circ -measurable and with processes $\tilde{\mathbf{a}} \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$, $\tilde{\mathbf{b}} = [\tilde{b}_1 | \dots | \tilde{b}_m] \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m})$. Throughout this work, the symbol ‘ \top ’ stands for the transpose of vectors or matrices.

To show that \mathcal{X} is a Hilbert space, we consider the product space

$$\mathbb{X} = \{(\mathbf{Y}_\circ, \mathbf{a}, \mathbf{b}) \in L^2(\Omega; \mathbb{R}^d) \times \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d) \times \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m}) : \mathbf{Y}_\circ \text{ is } \mathcal{F}_0\text{-measurable}\}.$$

(2.5)

In Lemma 2.1 we show that the space \mathcal{X} is a Hilbert space with the inner product given by the right-hand side of (2.4), and the induced norm is given by the right-hand side of (2.2). In the proof of the lemma we utilize the notion of a martingale which is defined, e.g., in [18, Section 2.7].

Lemma 2.1 *The map $\Phi: \mathbb{X} \rightarrow \mathcal{X}$ is injective, i.e., the representation of $\mathbf{Y} \in \mathcal{X}$ of the form (2.1) is unique, and therefore the norm (2.2) is well defined in \mathcal{X} . With this norm in \mathcal{X} , Φ is an isometric isomorphism between \mathbb{X} and \mathcal{X} . In particular, \mathcal{X} is a Hilbert space.*

Proof Assume $\mathbf{Y} = \Phi(\mathbf{Y}_\circ, \mathbf{a}, \mathbf{b}) = 0$. Then $\mathbf{Y}_\circ = \mathbf{Y}(0) = 0$ (note that \mathbf{Y} has continuous paths), and

$$M_t := \int_0^t \mathbf{b}(s) \, d\mathbf{B}(s) = - \int_0^t \mathbf{a}(s) \, ds, \quad t \in [0, T],$$

is a continuous martingale with finite variation and therefore constant, see [49, Theorem III.12], and we obtain $M_t = M_0 = 0$ for all $t \in [0, T]$. As the integral representation of square integrable martingales with continuous paths is unique (see [32, Theorem 4.15]), this yields $\mathbf{b} = 0$ in $\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m})$. Moreover, we have $-M_t = \int_0^t \mathbf{a}(s) \, ds = 0$ for all $t \in [0, T]$ which implies $\mathbf{a} = 0$ in $\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$. Consequently, the map Φ is injective, which implies that the norm in (2.2) is well defined. By construction, Φ is an isometric isomorphism between \mathbb{X} and \mathcal{X} , which also yields that \mathcal{X} is a Hilbert space. □

As the following lemma shows, we obtain continuous embeddings of \mathcal{X} into standard spaces of processes. Part (2) of the lemma will be useful later in Sect. 6.3, when we derive backward equations.

Lemma 2.2 (1) For $C := \sqrt{3 \max\{T, 1\}}$ we have

$$\|Y\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))} \leq C \|Y\|_{\mathcal{X}} \text{ for every } Y \in \mathcal{X}.$$

In particular,

$$\mathcal{X} \subset C([0, T]; L^2(\Omega; \mathbb{R}^d)) \subset L^2(\Omega \times (0, T); \mathbb{R}^d) \tag{2.6}$$

holds with continuous embeddings, and we obtain $\mathcal{X} \subset \mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)$.

(2) Let $\Lambda := \Phi(\Lambda_0, \tilde{a}, \tilde{b}) \in \mathcal{X}$. Then the map

$$\ell_{\Lambda} : \mathcal{X} \rightarrow \mathbb{R}, \quad Y \mapsto \mathbb{E} \left[Y(T)^\top \Lambda(T) - \int_0^T Y(s)^\top \tilde{a}(s) \, ds \right] \tag{2.7}$$

defines a continuous linear functional on \mathcal{X} . Moreover, for $Y = \Phi(Y_0, a, b) \in \mathcal{X}$, we have

$$\ell_{\Lambda}(Y) = \langle (Y_0, a, b), (\Lambda_0, \Lambda, \tilde{b}) \rangle_{\mathbb{X}}, \tag{2.8}$$

where $\langle \cdot, \cdot \rangle_{\mathbb{X}}$ stands for the inner product in \mathbb{X} .

Proof (1) Let $Y \in \mathcal{X}$ be given. Then (2.1) holds with a random vector $X_0 \in L^2(\Omega; \mathbb{R}^d)$ and processes $a \in \mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)$ and $b \in \mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^{d \times m})$. From (2.1) and the inequality $(s_1 + s_2 + s_3)^2 \leq 3(s_1^2 + s_2^2 + s_3^2)$ for positive s_1, s_2, s_3 , we obtain for every $t \in [0, T]$

$$\mathbb{E} \left[\|Y(t)\|_{\mathbb{R}^d}^2 \right] \leq 3 \left(\mathbb{E} \left[\|Y_0\|_{\mathbb{R}^d}^2 \right] + \mathbb{E} \left[\left\| \int_0^t a(s) \, ds \right\|_{\mathbb{R}^d}^2 \right] + \mathbb{E} \left[\left\| \int_0^t b(s) \, d\mathbf{B}(s) \right\|_{\mathbb{R}^d}^2 \right] \right).$$

An application of the Cauchy-Schwarz inequality yields

$$\left\| \int_0^t a(s) \, ds \right\|_{\mathbb{R}^d}^2 \leq \left(\int_0^t \|a(s)\|_{\mathbb{R}^d} \, ds \right)^2 \leq T \int_0^t \|a(s)\|_{\mathbb{R}^d}^2 \, ds.$$

For the stochastic integral, we use the Itô-isometry (cf., e.g., [40, Chapter 1, Theorem 5.21])

$$\mathbb{E} \left[\left\| \int_0^t b(s) \, d\mathbf{B}(s) \right\|_{\mathbb{R}^d}^2 \right] = \mathbb{E} \left[\int_0^t \|b(s)\|_{\mathbb{F}}^2 \, ds \right] \leq \mathbb{E} \left[\int_0^t \|b(s)\|_{\mathbb{F}}^2 \, ds \right].$$

Therefore, recalling that Y has continuous paths, we obtain

$$\|Y\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))}^2 = \sup_{t \in [0, T]} \mathbb{E} \left[\|Y(t)\|_{\mathbb{R}^d}^2 \right] \leq 3 \max\{T, 1\} \|Y\|_{\mathcal{X}}^2$$

which shows the first embedding in (2.6). The second embedding follows from the obvious estimate

$$\|X\|_{L^2(\Omega \times (0, T); \mathbb{R}^d)} \leq \sqrt{T} \|X\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))}.$$

As every element of \mathcal{X} is progressively measurable, we obtain $\mathcal{X} \subset \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$.

(2) By the Cauchy-Schwarz inequality and the embeddings from (1), we can estimate

$$\begin{aligned} |\ell_{\Lambda}(Y)| &\leq \|Y\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))} \|\Lambda\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))} + \|Y\|_{\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)} \|\Lambda\|_{\mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)} \\ &\leq C' \|Y\|_{\mathcal{X}} \|\Lambda\|_{\mathcal{X}} \end{aligned}$$

for some constant $C' > 0$. Therefore, ℓ_{Λ} is a continuous linear functional on \mathcal{X} . The proof of (2.8) is based on the Itô lemma applied on $Y(T)^\top \Lambda(T)$, see [25, Lemma 2.2.16], which yields

$$\begin{aligned} Y(T)^\top \Lambda(T) &= Y(0)^\top \Lambda(0) + \int_0^T \left(Y(t)^\top \tilde{a}(t) + a(t)^\top \Lambda(t) + \langle b(t), \tilde{b}(t) \rangle_{\mathbb{F}} \right) dt \\ &\quad + \int_0^T \left(Y(t)^\top \tilde{b}(t) + \Lambda(t)^\top b(t) \right) d\mathbf{B}(t). \end{aligned}$$

Taking the expectation and noting that the expectation of the stochastic integral equals zero, we obtain

$$\ell_{\Lambda}(Y) = \mathbb{E} \left[Y_0^\top \Lambda_0 + \int_0^T \left(a(t)^\top \Lambda(t) + \langle b(t), \tilde{b}(t) \rangle_{\mathbb{F}} \right) dt \right],$$

which shows part (2). □

Remark 2.3 Let $Y \in \mathcal{X}$ hold. Then,

$$\sup_{t \in [0, T]} \|\mathbb{E}[Y(t)]\|_{\mathbb{R}^d} \leq \sup_{t \in [0, T]} \mathbb{E} [\|Y(t)\|_{\mathbb{R}^d}] \leq \sup_{t \in [0, T]} \left(\mathbb{E} [\|Y(t)\|_{\mathbb{R}^d}^2] \right)^{1/2} \leq C \|Y\|_{\mathcal{X}}$$

follows from Hölder’s inequality and Lemma 2.2.

3 The State Equation

For $r \in \mathbb{N}$ we introduce the Hilbert space $\mathcal{U} := L^2(0, T; \mathbb{R}^r)$ and the set of *admissible (deterministic) controls* which is given as

$$\mathcal{U}_{\text{ad}} := \{u \in \mathcal{U} \mid u(t) \in [u_a, u_b] \text{ for almost all (f.a.a.) } t \in [0, T]\} \tag{3.1}$$

with $u_a, u_b \in \mathbb{R}^r$ satisfying $u_a \leq u_b$ in \mathbb{R}^r (i.e., component by component) and $[u_a, u_b] := \{u \in \mathbb{R}^r \mid u_a \leq u \leq u_b \text{ in } \mathbb{R}^r\}$.

Remark 3.1 1) Notice that \mathcal{U}_{ad} defined in (3.1) is nonempty, convex and closed.
 2) In one numerical example carried out in Sect. 7.2, we consider calibration problems, where the unknowns are time-independent parameters. In that case we have $\mathcal{U}^c = \mathbb{R}^r$ and $\mathcal{U}_{\text{ad}}^c = [u_a, u_b] \subset \mathcal{U}^c$, i.e., the set $\mathcal{U}_{\text{ad}}^c$ is even compact.

Next let us start with the introduction of the coefficient functions that constitute the equation, where the following standard hypothesis on the coefficient functions is taken from [57, p. 44].

Assumption 3.2 We are given measurable *drift* and *diffusion coefficient functions*

$$a : \mathbb{R}^d \times \mathbb{R}^r \times [0, T] \rightarrow \mathbb{R}^d \quad \text{and} \quad b : \mathbb{R}^d \times \mathbb{R}^r \times [0, T] \rightarrow \mathbb{R}^{d \times m},$$

respectively. Further, there exists a (Lipschitz) constant $L_U > 0$ such that for every $x, \tilde{x} \in \mathbb{R}^d, u, \tilde{u} \in [u_a, u_b]$ and f.a.a $t \in [0, T]$ there exists a constant $L_U > 0$ such that the *Lipschitz condition*

$$\begin{aligned} & \|a(x, u, t) - a(\tilde{x}, \tilde{u}, t)\|_{\mathbb{R}^d} + \|b(x, u, t) - b(\tilde{x}, \tilde{u}, t)\|_F \\ & \leq L_U (\|x - \tilde{x}\|_{\mathbb{R}^d} + \|u - \tilde{u}\|_{\mathbb{R}^r}) \end{aligned} \quad (3.2)$$

holds. Moreover,

$$\int_0^T \|a(0, u(t), t)\|_{\mathbb{R}^d}^2 + \|b(0, u(t), t)\|_F^2 dt \leq L_U^2 \quad (3.3)$$

is valid for all $u \in \mathcal{U}_{\text{ad}}$.

Suppose that $X_\circ \in L^2(\Omega; \mathbb{R}^d)$ is a fixed given initial condition being \mathcal{F}_\circ -measurable. For a given (deterministic) input function $u \in \mathcal{U}_{\text{ad}}$, the associated stochastic process X is an \mathbb{R}^d -valued solution to the stochastic differential equation (SDE):

$$\begin{cases} dX(t) = a(X(t), u(t), t) dt + b(X(t), u(t), t) d\mathbf{B}(t) & \text{for all } t \in (0, T], \\ X(0) = X_\circ. \end{cases} \quad (3.4)$$

The next definition specifies the concept of a solution and uniqueness in our context.

Definition 3.3 1) If X belongs to \mathcal{X} and satisfies

$$X(t) = X_\circ + \int_0^t a(X(s), u(s), s) ds + \int_0^t b(X(s), u(s), s) d\mathbf{B}(s) \quad \text{in } L^2(\Omega; \mathbb{R}^d)$$

for all $t \in [0, T]$, we call X a *solution* to (3.4).

2) We say that a solution $X \in \mathcal{X}$ to (3.4) is *unique* if for any other solution $\tilde{X} \in \mathcal{X}$ to (3.4) we have

$$\mathbb{P} \left(\{\omega \in \Omega \mid X(t) = \tilde{X}(t) \text{ for all } t \in [0, T]\} \right) = 1.$$

Remark 3.4 For the example introduced in Remark 3.1-2), the SDE (3.4) is given as

$$\begin{cases} d\mathbf{X}(t) = a(\mathbf{X}(t), u, t) dt + b(\mathbf{X}(t), u, t) d\mathbf{B}(t) & \text{for all } t \in (0, T], \\ \mathbf{X}(0) = \mathbf{X}_o \end{cases} \quad (3.5)$$

for a given (parameter) vector $u \in \mathcal{U}_{\text{ad}}^c$. In that case, its solution $\mathbf{X} \in \mathcal{X}$ satisfies

$$\begin{aligned} \mathbf{X}(t) &= \mathbf{X}_o + \int_0^t a(\mathbf{X}(s), u, s) ds \\ &\quad + \int_0^t b(\mathbf{X}(s), u, s) d\mathbf{B}(s) \quad \text{in } L^2(\Omega; \mathbb{R}^d) \text{ for all } t \in [0, T]. \end{aligned}$$

Now, we recall the existence result from [57, Corollary 1.6.4].

Theorem 3.5 *Let Assumption 3.2 hold and $\mathbf{X}_o \in L^2(\Omega; \mathbb{R}^d)$ be an \mathcal{F}_o -measurable random variable. Then for every $u \in \mathcal{U}_{\text{ad}}$ there exists a unique solution $\mathbf{X} \in \mathcal{X}$ of (3.4).*

Remark 3.6 To prove Theorem 3.5 we do not need the Lipschitz continuity of the coefficient functions a and b with respect to the control variable u . Moreover, for the unique solvability, the Lipschitz condition (with respect to x) can be weakened by a local one; cf. [40, Chapter 2, Theorem 3.4].

Let $\mathbf{X}_o \in L^2(\Omega; \mathbb{R}^d)$ be an \mathcal{F}_o -measurable random variable. Due to Theorem 3.5 we introduce the non-linear solution operator

$$\mathcal{S}: \mathcal{U}_{\text{ad}} \rightarrow \mathcal{X}, \quad \mathbf{X} = \mathcal{S}(u) \text{ is the unique solution to (3.4) for } u \in \mathcal{U}_{\text{ad}}. \quad (3.6)$$

Theorem 3.7 *Let Assumption 3.2 hold and $\mathbf{X}_o \in L^2(\Omega; \mathbb{R}^d)$ be an \mathcal{F}_o -measurable random variable. Then, for all $u, \tilde{u} \in \mathcal{U}_{\text{ad}}$, we have*

$$\|\mathcal{S}(u) - \mathcal{S}(\tilde{u})\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))} \leq C_1 \|u - \tilde{u}\|_{\mathcal{U}}, \quad (3.7)$$

$$\|\mathcal{S}(u)\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))} \leq C_2 \quad (3.8)$$

with non-negative constants $C_1 = C_1(L_U, T)$ and $C_2 = C_2(L_U, T, \mathbf{X}_o)$.

Proof To show the estimates (3.7) and (3.8), we follow a standard Gronwall approach (see [44, proof of Theorem 5.2.1]). For this, let $u, \tilde{u} \in \mathcal{U}_{\text{ad}}$ be given. We set $\mathbf{X} := \mathcal{S}(u)$ and $\tilde{\mathbf{X}} := \mathcal{S}(\tilde{u})$. In the same way as in the proof of Lemma 2.2, we obtain for fixed

$t \in [0, T]$

$$\begin{aligned}
 \mathbb{E} \left[\|X(t) - \tilde{X}(t)\|_{\mathbb{R}^d}^2 \right] &\leq 2 \mathbb{E} \left[\left\| \int_0^t a(X(s), u(s), s) - a(\tilde{X}(s), \tilde{u}(s), s) \, ds \right\|_{\mathbb{R}^d}^2 \right] \\
 &\quad + 2 \mathbb{E} \left[\left\| \int_0^t b(X(s), u(s), s) - b(\tilde{X}(s), \tilde{u}(s), s) \, d\mathbf{B}(s) \right\|_{\mathbb{R}^d}^2 \right] \\
 &\leq 2T \mathbb{E} \left[\int_0^t \|a(X(s), u(s), s) - a(\tilde{X}(s), \tilde{u}(s), s)\|_{\mathbb{R}^d}^2 \, ds \right] \\
 &\quad + 2 \mathbb{E} \left[\int_0^t \|b(X(s), u(s), s) - b(\tilde{X}(s), \tilde{u}(s), s)\|_{\mathbb{F}}^2 \, ds \right].
 \end{aligned}
 \tag{3.9}$$

Now the Lipschitz condition of Assumption 3.2 yields

$$\begin{aligned}
 &\int_0^t \|a(X(s), u(s), s) - a(\tilde{X}(s), \tilde{u}(s), s)\|_{\mathbb{R}^d}^2 \, ds \\
 &\quad \leq \int_0^t \left(L_U (\|X(s) - \tilde{X}(s)\|_{\mathbb{R}^d} + \|u(s) - \tilde{u}(s)\|_{\mathbb{R}^r}) \right)^2 \, ds \\
 &\quad \leq 2L_U^2 \int_0^t \|X(s) - \tilde{X}(s)\|_{\mathbb{R}^d}^2 + \|u(s) - \tilde{u}(s)\|_{\mathbb{R}^r}^2 \, ds
 \end{aligned}$$

for $t \in [0, T]$. We proceed analogously for the second term on the right-hand side of (3.9). Consequently, we obtain

$$\mathbb{E} \left[\|X(t) - \tilde{X}(t)\|_{\mathbb{R}^d}^2 \right] \leq c_1 \int_0^t \mathbb{E} \left[\|X(s) - \tilde{X}(s)\|_{\mathbb{R}^d}^2 + \|u(s) - \tilde{u}(s)\|_{\mathbb{R}^r}^2 \right] \, ds$$

for $t \in [0, T]$ and $c_1 = 4 \max\{T, 1\}L_U^2$. Now, an application of Gronwall’s inequality (cf., e.g., [18, p. 92]) gives

$$\mathbb{E} \left[\|X(t) - \tilde{X}(t)\|_{\mathbb{R}^d}^2 \right] \leq c_1 e^{\int_0^t c_1 \, ds} \int_0^t \|u(s) - \tilde{u}(s)\|_{\mathbb{R}^r}^2 \, ds \tag{3.10}$$

for $t \in [0, T]$, which yields (3.7) with $C_1(L_U, T) = \sqrt{c_1 e^{c_1 T}}$.

To show (3.8) we proceed similarly as in the proof of Lemma 2.2 and utilize again Assumption 3.2. Note that

$$\begin{aligned}
 \mathbb{E} \left[\|X(t)\|_{\mathbb{R}^d}^2 \right] &\leq 3 \left(\mathbb{E} \left[\|X_0\|_{\mathbb{R}^d}^2 \right] + T \mathbb{E} \left[\int_0^t \|a(X(s), u(s), s)\|_{\mathbb{R}^d}^2 \, ds \right] \right) \\
 &\quad + \mathbb{E} \left[\int_0^t \|b(X(s), u(s), s)\|_{\mathbb{F}}^2 \, ds \right]
 \end{aligned}$$

for $t \in [0, T]$. For brevity, we use the notation $\mathbf{a} = \|a(0, u(\cdot), \cdot)\|_{\mathbb{R}^d}$ and $\mathbf{b} = \|b(0, u(\cdot), \cdot)\|_{\mathbb{F}}$. Note that

$$\begin{aligned} & \mathbb{E} \left[\int_0^t \|a(\mathbf{X}(s), u(s), s)\|_{\mathbb{R}^d}^2 ds \right] \\ & \leq 2\mathbb{E} \left[\int_0^t \|a(\mathbf{X}(s), u(s), s) - a(0, u(s), s)\|_{\mathbb{R}^d}^2 + \|a(0, u(s), s)\|_{\mathbb{R}^d}^2 ds \right] \\ & \leq 2\mathbb{E} \left[\int_0^t L_U^2 \|\mathbf{X}(s)\|_{\mathbb{R}^d}^2 + |\mathbf{a}(s)|^2 ds \right] = 2 \int_0^t L_U^2 \mathbb{E}[\|\mathbf{X}(s)\|_{\mathbb{R}^d}^2] + |\mathbf{a}(s)|^2 ds. \end{aligned} \tag{3.11}$$

Similarly, we infer that

$$\mathbb{E} \left[\int_0^t \|b(\mathbf{X}(s), u(s), s)\|_{\mathbb{F}}^2 ds \right] \leq 2 \int_0^t L_U^2 \mathbb{E}[\|\mathbf{X}(s)\|_{\mathbb{R}^d}^2] + |\mathbf{b}(s)|^2 ds. \tag{3.12}$$

By Assumption 3.2, we obtain

$$\begin{aligned} \mathbb{E}[\|\mathbf{X}(t)\|_{\mathbb{R}^d}^2] & \leq 3 \left(\mathbb{E}[\|\mathbf{X}_o\|_{\mathbb{R}^d}^2] + 2 \max\{T, 1\} \int_0^T |\mathbf{a}(s)|^2 + |\mathbf{b}(s)|^2 ds \right. \\ & \quad \left. + 2(T + 1)L_U^2 \int_0^t \mathbb{E}[\|\mathbf{X}(s)\|_{\mathbb{R}^d}^2] ds \right) \\ & \leq 3\mathbb{E}[\|\mathbf{X}_o\|_{\mathbb{R}^d}^2] + 6 \max\{T, 1\}L_U^2 + \hat{c}_2 \int_0^t \mathbb{E}[\|\mathbf{X}(s)\|_{\mathbb{R}^d}^2] ds \\ & \leq \tilde{c}_2 + \hat{c}_2 \int_0^t \mathbb{E}[\|\mathbf{X}(s)\|_{\mathbb{R}^d}^2] ds \end{aligned}$$

for $t \in [0, T]$ with $\hat{c}_2 = 6(T + 1)L_U^2$ and $\tilde{c}_2 = 3\mathbb{E}[\|\mathbf{X}_o\|_{\mathbb{R}^d}^2] + 6 \max\{T, 1\}L_U^2$. By Gronwall’s inequality and Assumption 3.2, this implies

$$\mathbb{E}[\|\mathbf{X}(t)\|_{\mathbb{R}^d}^2] \leq \tilde{c}_2 \exp \left(\int_0^t \hat{c}_2 d\tau \right) \leq \tilde{c}_2 \exp(\hat{c}_2 T) =: c_2$$

where c_2 depends on L_U, T and \mathbf{X}_o . Therefore, (3.8) holds with $C_2(L_U, T, \mathbf{X}_o) = c_2^{1/2}$. □

Corollary 3.8 *In the situation of Theorem 3.5, we have for all $u, \tilde{u} \in \mathcal{U}_{ad}$*

$$\|\mathcal{S}(u) - \mathcal{S}(\tilde{u})\|_{\mathcal{X}} \leq C'_1 \|u - \tilde{u}\|_{\mathcal{U}}, \tag{3.13}$$

$$\|\mathcal{S}(u)\|_{\mathcal{X}} \leq C'_2 \tag{3.14}$$

with constants $C'_1 = C'_1(L_U, T)$ and $C'_2 = C'_2(L_U, T, \mathbf{X}_o)$. Therefore, $\mathcal{S}: \mathcal{U}_{ad} \rightarrow \mathcal{X}$ is Lipschitz continuous and has bounded range.

Proof Again we set $\mathbf{a} = \|a(0, u(\cdot), \cdot)\|_{\mathbb{R}^d}$ and $\mathbf{b} = \|b(0, u(\cdot), \cdot)\|_{\mathbb{F}}$. Utilizing the definition of the norm in \mathcal{X} , (3.11), (3.12) and Assumption 3.2, we find that

$$\begin{aligned} \|X\|_{\mathcal{X}}^2 &= \mathbb{E}[\|X_0\|_{\mathbb{R}^d}^2] + \mathbb{E}\left[\int_0^T \|a(X(s), u(s), s)\|_{\mathbb{R}^d}^2 ds\right] \\ &\quad + \mathbb{E}\left[\int_0^T \|b(X(s), u(s), s)\|_{\mathbb{F}}^2 ds\right] \\ &\leq \mathbb{E}[\|X_0\|_{\mathbb{R}^d}^2] + \int_0^T 4L_U^2 \mathbb{E}[\|X(s)\|_{\mathbb{R}^d}^2] + |a(s)|^2 + |b(s)|^2 ds \\ &\leq \max\{1, 4L_U^2\} \|X\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))}^2 + L_U^2. \end{aligned}$$

Now (3.14) follows directly from (3.8) in Theorem 3.7. To show (3.13), let $u, \tilde{u} \in \mathcal{U}_{ad}$ and set $X := \mathcal{S}(u)$ and $\tilde{X} := \mathcal{S}(\tilde{u})$. In the same way as above, the Lipschitz continuity condition in Assumption 3.2 leads to

$$\|X - \tilde{X}\|_{\mathcal{X}}^2 \leq 4L_U^2 (\|X - \tilde{X}\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))}^2 + \|u - \tilde{u}\|_{\mathcal{U}}^2).$$

Therefore, (3.13) follows from (3.7) in Theorem 3.7. □

4 The Optimization Problem

Next, we focus on the optimization problem itself. We start by introducing the cost functional

$$J(X, u) := j(X) + j_T(X(T)) + \frac{\kappa}{2} \|u\|_{\mathcal{U}}^2, \tag{4.1}$$

where j and j_T fulfill the following hypothesis:

Assumption 4.1 The functionals $j : \mathcal{X} \rightarrow \mathbb{R}$ and $j_T : L^2(\Omega; \mathbb{R}^d) \rightarrow \mathbb{R}$ are convex, lower semicontinuous and bounded from below.

Notice that j and j_T take random variables and map them to deterministic outputs.

Example 4.2 For example, we may consider the following non-negative functional of tracking type for which Assumption 4.1 holds:

$$J(X, u) = \frac{1}{2} \left(\int_0^T \|C(\mathbb{E}[X(t)]) - c^d(t)\|_{\mathbb{R}^\ell}^2 dt + \|C(\mathbb{E}[X(T)]) - c_T^d\|_{\mathbb{R}^\ell}^2 + \kappa \|u\|_{\mathcal{U}}^2 \right) \tag{4.2}$$

for $(X, u) \in \mathcal{X} \times \mathcal{U}$. In (4.2) and $\kappa > 0$ is the control weight. We suppose that the (non-linear) mapping $C : \mathbb{R}^d \rightarrow \mathbb{R}^\ell$ is given in such a way that J is convex and lower semicontinuous. Notice that the objective defined in (4.2) differs from the one typically used in the stochastic optimal control setting (see, e.g., [19, 46]), but is present in literature for calibration problems; see, e.g., [17, 20, 22, 31, 36]).

Now we can formulate our stochastic optimization problem:

$$\min J(\mathbf{X}, u) \quad \text{subject to (s.t.) } (\mathbf{X}, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}} \text{ satisfies (3.4).} \quad (4.3)$$

Utilizing the solution operator \mathcal{S} (introduced in (3.6)), we define the reduced cost functional

$$\hat{J}(u) := J(\mathcal{S}(u), u) \quad \text{for } u \in \mathcal{U}_{\text{ad}}. \quad (4.4)$$

The associated reduced problem reads

$$\min \hat{J}(u) \quad \text{s.t. } u \in \mathcal{U}_{\text{ad}}. \quad (4.5)$$

In Theorem 4.5, we deal with the question of the existence of optimal solutions to (4.5). In view of our numerical example later on, we restrict ourselves to the case of a linear SDE in the case of $\mathcal{U} = L^2(0, T; \mathbb{R}^r)$; see also the discussion after the proof of Theorem 4.5.

Assumption 4.3 Suppose that (3.4) is a linear SDE. More precisely, the coefficients a and b are of the following form

$$\begin{aligned} a(x, u, t) &= \mathfrak{a}(t) + \mathfrak{A}_1(t)x + \mathfrak{A}_2(t)u \quad \text{for } (x, u, t) \in \mathbb{R}^d \times \mathbb{R}^r \times [0, T], \\ b(x, u, t) &= \mathfrak{b}(t) + \mathfrak{B}_1(t)x + \mathfrak{B}_2(t)u \quad \text{for } (x, u, t) \in \mathbb{R}^d \times \mathbb{R}^r \times [0, T] \end{aligned} \quad (4.6)$$

with (deterministic) functions

$$\begin{aligned} \mathfrak{a} &\in L^2(0, T; \mathbb{R}^d), & \mathfrak{A}_1 &\in L^\infty(0, T; \mathbb{R}^{d \times d}), & \mathfrak{A}_2 &\in L^\infty(0, T; \mathbb{R}^{d \times r}), \\ \mathfrak{b} &\in L^2(0, T; \mathbb{R}^{d \times m}), & \mathfrak{B}_1 &\in L^\infty(0, T; \mathbb{R}^{d \times m \times d}), & \mathfrak{B}_2 &\in L^\infty(0, T; \mathbb{R}^{d \times m \times r}) \end{aligned}$$

and

$$\left. \begin{aligned} (\mathfrak{B}_1(t)x)_{ij} &= \sum_{l=1}^d \mathfrak{B}_{1,ijl}(t)x_l, \\ (\mathfrak{B}_2(t)u)_{ij} &= \sum_{l=1}^r \mathfrak{B}_{2,ijl}(t)u_l \end{aligned} \right\} \quad \text{for } 1 \leq i \leq d \text{ and } 1 \leq j \leq m.$$

Remark 4.4 (1) It follows from Assumption 4.3 that

$$\left\{ \begin{aligned} d\mathbf{X}(t) &= (\mathfrak{a}(t) + \mathfrak{A}_1(t)\mathbf{X}(t) + \mathfrak{A}_2(t)u(t)) dt \\ &\quad + (\mathfrak{b}(t) + \mathfrak{B}_1(t)\mathbf{X}(t) + \mathfrak{B}_2(t)u(t)) d\mathbf{B}(t) \quad \text{for all } t \in (0, T], \\ \mathbf{X}(0) &= \mathbf{X}_\circ \end{aligned} \right. \quad (4.7)$$

possesses a unique solution $\mathbf{X} \in \mathcal{X}$ for every $u \in \mathcal{U}$ and every \mathcal{F}_\circ -measurable $\mathbf{X}_\circ \in L^2(\Omega; \mathbb{R}^d)$; cf. [57, Theorem 6.14].

- (2) Notice that Assumption 4.3 implies Assumption 3.2. Thus, the estimates of Theorem 3.7 and Lemma 3.8 are satisfied also in the linear setting.
- (3) Suppose that Assumptions 3.2 and 4.3 hold. For given initial condition $X_o : \Omega \rightarrow \mathbb{R}^d$ let $\hat{X} \in \mathcal{X}$ be the unique solution to the linear SDE

$$d\hat{X}(t) = a(t) dt + b(t) d\mathbf{B}(t) \text{ for all } t \in (0, T], \quad \hat{X}(0) = X_o. \tag{4.8}$$

Moreover, for given control $u \in \mathcal{U}_{ad}$ we denote by $X_h \in \mathcal{X}_o$ the unique solution to

$$\begin{cases} dX_h(t) = (\mathfrak{A}_1(t)X_h(t) + \mathfrak{A}_2(t)u(t)) dt \\ \quad + (\mathfrak{B}_1(t)X_h(t) + \mathfrak{B}_2(t)u(t)) d\mathbf{B}(t) \text{ for all } t \in (0, T], \\ X_h(0) = 0, \end{cases} \tag{4.9}$$

where we set $\mathcal{X}_o = \{Y \in \mathcal{X} \mid Y(0) = 0 \text{ in } L^2(\Omega; \mathbb{R}^d)\}$. Then the solution operator $\mathcal{S}_h : \mathcal{U}_{ad} \rightarrow \mathcal{X}_o$, where $X_h = \mathcal{S}_h(u)$ solves (4.9), is well defined, linear and bounded. Moreover, $\mathcal{S}(u) = \hat{X} + \mathcal{S}_h(u)$ solves (3.4) with the setting (4.6).

Theorem 4.5 *Let Assumptions 3.2, 4.1 and 4.3 hold. Then there exists a (global) optimal solution $\bar{u} \in \mathcal{U}_{ad}$ to (4.5).*

Proof We follow the main ideas of the proofs in [57, Theorem 5.2, Chapter 2]. First, we observe that the reduced cost \hat{J} is bounded from below. Thus, there exists a minimizing sequence $\{u^k\}_{k \in \mathbb{N}} \subset \mathcal{U}_{ad}$ such that

$$-\infty < \bar{J} = \inf \{ \hat{J}(u) \mid u \in \mathcal{U}_{ad} \} = \lim_{k \rightarrow \infty} \hat{J}(u^k) < \infty. \tag{4.10}$$

We set $X^k = \mathcal{S}(u^k)$ for $k \in \mathbb{N}$. Due to Remark 4.4-(1), the sequence $\{X^k\}_{k \in \mathbb{N}} \subset \mathcal{X}$ is well defined. Since \mathcal{U}_{ad} is bounded, the sequence $\{u^k\}_{k \in \mathbb{N}}$ is bounded as well. Hence, there exists a subsequence (which is still labeled by u^k) $\{u^k\}_{k \in \mathbb{N}} \subset \mathcal{U}_{ad}$ and an element $\bar{u} \in \mathcal{U}_{ad}$ such that $u^k \rightarrow \bar{u}$ in \mathcal{U} as $k \rightarrow \infty$. We set $\bar{X} = \mathcal{S}(\bar{u})$. By Mazur’s theorem [50, Lemma 10.19], we get the existence of a function $N : \mathbb{N} \rightarrow \mathbb{N}$ and a sequence of sets of real numbers $\{\alpha_{ik}\}_{i=k}^{N(k)}$ such that the sequence of convex combinations

$$\tilde{u}^k := \sum_{i=k}^{N(k)} \alpha_{ik} u^i \in \mathcal{U}_{ad} \quad \text{with } \alpha_{ik} \geq 0 \text{ and } \sum_{i=k}^{N(k)} \alpha_{ik} = 1 \tag{4.11}$$

converges strongly to \bar{u} in \mathcal{U} , i.e.

$$\tilde{u}^k \rightarrow \bar{u} \text{ in } \mathcal{U}. \tag{4.12}$$

Since the set \mathcal{U}_{ad} is convex and closed, we have $\bar{u} \in \mathcal{U}_{ad}$. Furthermore, if \tilde{X}^k is the state corresponding to the control \tilde{u}^k , then we have the strong convergence (see

Theorem 3.5 and Lemma 3.8)

$$\tilde{\mathbf{X}}^k \rightarrow \bar{\mathbf{X}} \quad \text{in } \mathcal{X}. \quad (4.13)$$

Using Remark 4.4-(3), we find that

$$\begin{aligned} \tilde{\mathbf{X}}^k &= \mathcal{S}(\tilde{u}^k) = \hat{\mathbf{X}} + \mathcal{S}_h(\tilde{u}^k) = \hat{\mathbf{X}} + \mathcal{S}_h\left(\sum_{i=k}^{N(k)} \alpha_{ik} u^i\right) = \sum_{i=k}^{N(k)} \alpha_{ik} (\hat{\mathbf{X}} + \mathcal{S}_h(u^i)) \\ &= \sum_{i=k}^{N(k)} \alpha_{ik} \mathbf{X}^i. \end{aligned} \quad (4.14)$$

Due to Assumption 4.1 both j and j_T are lower semicontinuous and convex. Thus, we infer from (4.11), (4.13) and (4.14) that

$$\begin{aligned} j(\bar{\mathbf{X}}) + j_T(\bar{\mathbf{X}}) &\leq \lim_{k \rightarrow \infty} j(\tilde{\mathbf{X}}^k) + \lim_{k \rightarrow \infty} j_T(\tilde{\mathbf{X}}^k) \\ &= \lim_{k \rightarrow \infty} j\left(\sum_{i=k}^{N(k)} \alpha_{ik} \mathbf{X}^i\right) + \lim_{k \rightarrow \infty} j_T\left(\sum_{i=k}^{N(k)} \alpha_{ik} \mathbf{X}^i(T)\right) \\ &\leq \lim_{k \rightarrow \infty} \sum_{i=k}^{N(k)} \alpha_{ik} \left(j(\mathbf{X}^i) + j_T(\mathbf{X}^i(T))\right). \end{aligned} \quad (4.15)$$

Since $u \mapsto \|u\|_{\mathcal{U}}^2$ is continuous and convex in \mathcal{U} , we infer from (4.12)

$$\|\bar{u}\|_{\mathcal{U}}^2 = \lim_{k \rightarrow \infty} \|\tilde{u}^k\|_{\mathcal{U}}^2 = \lim_{k \rightarrow \infty} \left\| \sum_{i=k}^{N(k)} \alpha_{ik} u^i \right\|_{\mathcal{U}}^2 \leq \lim_{k \rightarrow \infty} \sum_{i=k}^{N(k)} \alpha_{ik} \|u^i\|_{\mathcal{U}}^2. \quad (4.16)$$

Combining (4.10), (4.15) and (4.16), we obtain

$$\begin{aligned} \hat{J}(\bar{u}) &= j(\bar{\mathbf{X}}) + j_T(\bar{\mathbf{X}}(T)) + \frac{\kappa}{2} \|\bar{u}\|_{\mathcal{U}}^2 \\ &\leq \lim_{k \rightarrow \infty} \sum_{i=k}^{N(k)} \alpha_{ik} \left(j(\mathbf{X}^i) + j_T(\mathbf{X}^i(T))\right) + \frac{\kappa}{2} \|u^i\|_{\mathcal{U}}^2 = \lim_{k \rightarrow \infty} \sum_{i=k}^{N(k)} \alpha_{ik} \hat{J}(u^i). \end{aligned} \quad (4.17)$$

To pass to the limit in the last equality in (4.17), we perform the following estimates. Due to (4.10) we have $\lim_{k \rightarrow \infty} \hat{J}(u^k) = \bar{J}$. Thus, for every $\varepsilon > 0$ there exists a $K = K(\varepsilon) \in \mathbb{N}$ such that $|\hat{J}(u^k) - \bar{J}| < \varepsilon$ for all $k \geq K$. Moreover, it holds that

$\sum_{i=k}^{N(k)} \alpha_{ik} = 1$ and $0 \leq \alpha_{ik} \leq 1$ for $i = k, \dots, N(k)$ and for any k . Consequently,

$$\begin{aligned} \sum_{i=k}^{N(k)} \alpha_{ik} \hat{J}(u^i) &= \sum_{i=k}^{N(k)} \alpha_{ik} \bar{J} + \sum_{i=k}^{N(k)} \alpha_{ik} (\hat{J}(u^i) - \bar{J}) \\ &\leq \bar{J} \sum_{i=k}^{N(k)} \alpha_{ik} + \sum_{i=k}^{N(k)} \alpha_{ik} |\hat{J}(u^i) - \bar{J}| \leq \bar{J} + \varepsilon \quad \text{for all } k \geq K \end{aligned}$$

and analogously

$$\sum_{i=k}^{N(k)} \alpha_{ik} \hat{J}(u^i) \geq \bar{J} \sum_{i=k}^{N(k)} \alpha_{ik} - \sum_{i=k}^{N(k)} \alpha_{ik} |\hat{J}(u^i) - \bar{J}| \geq \bar{J} - \varepsilon \quad \text{for all } k \geq K.$$

Since $\varepsilon > 0$ is chosen arbitrarily, we conclude that $\lim_{k \rightarrow \infty} \sum_{i=k}^{N(k)} \alpha_{ik} \hat{J}(u^i) = \bar{J}$ holds true. Thus, it follows from (4.17) that \bar{u} solves (4.5). □

Remark 4.6 Notice that the assumption of the linearity of the SDE is quite restrictive. However, it is in general not possible to prove existence of optimal controls for general SDE in the strong sense. On the contrary, one has to consider so-called *relaxed controls* for which the probability space can not be fixed a-priori [10, 57]. In [16], the authors deal with the question of existence of optimal stochastic control for a quite general form of stochastic optimal controls problems with a state equation of the form (3.4).

Let us come back to the case when the control is time-independent and just a vector in $\mathcal{U}^c = \mathbb{R}^k$; see Remarks 3.1 and 3.4. In this case, the proof of the existence of optimal parameters can also be executed for a non-linear SDE.

Theorem 4.7 *Let Assumptions 3.2 and 4.1 hold for $\mathcal{U} = \mathcal{U}^c$ and $\mathcal{U}_{ad} = \mathcal{U}_{ad}^c$. Then there exists a (global) optimal solution $\bar{u} \in \mathcal{U}_{ad}^c$ to (4.5).*

Proof First, notice as in the proof of Theorem 4.5 that the reduced cost \hat{J} is non-negative and the existence of a minimizing minimizing sequence $\{u^k\}_{k \in \mathbb{N}} \subset \mathcal{U}_{ad}^c$. We use again the notation $X^k = \mathcal{S}(u^k)$ for $k \in \mathbb{N}$. Due to Theorem 3.5, the sequence $\{X^k\}_{k \in \mathbb{N}} \subset \mathcal{X}$ is well defined. Since \mathcal{U}_{ad}^c is compact, there exists a subsequence of the minimizing sequence (which is still labeled by u^k) $\{u^k\}_{k \in \mathbb{N}} \subset \mathcal{U}_{ad}^c$ and an element $\bar{u} \in \mathcal{U}_{ad}^c$ such that we have the strong convergence $u^k \rightarrow \bar{u}$ in \mathcal{U} as $k \rightarrow \infty$. We set $\bar{X} = \mathcal{S}(\bar{u}) \in \mathcal{X}$. It follows from Theorem 3.7 that $X^k(T) \rightarrow \bar{X}(T)$ in $L^2(\Omega, \mathbb{R}^d)$ as $k \rightarrow \infty$. Due to Lemma 3.8 we have $X^k \rightarrow \bar{X}$ in \mathcal{X} as $k \rightarrow \infty$. Now, with the notation of (4.10) and Assumption 4.1, it holds that

$$\begin{aligned} \hat{J}(\bar{u}) &= j(\bar{X}) + j_T(\bar{X}(T)) + \frac{\kappa}{2} \|\bar{u}\|_{\mathcal{U}}^2 \leq \lim_{k \rightarrow \infty} (j(X^k) + j_T(X^k(T))) + \frac{\kappa}{2} \|u^k\|_{\mathcal{U}}^2 \\ &= \inf \{ \hat{J}(u) \mid u \in \mathcal{U}_{ad}^c \}. \end{aligned}$$

□

5 Discretization of the Optimization Problem

In this section, we introduce a discretization for (4.3) and derive the associated first-order necessary optimality system which is the basis for a gradient-based method utilized for our numerical tests in Sect. 7. For that reason, the following hypotheses are required.

Assumption 5.1 1) The mapping $\mathcal{C} : \mathbb{R}^d \rightarrow \mathbb{R}^\ell$ is continuously differentiable and the function $c^d : [0, T] \rightarrow \mathbb{R}^\ell$ is continuous.
2) The functions $a : \mathbb{R}^d \times \mathbb{R}^r \times [0, T] \rightarrow \mathbb{R}^d$ and $b : \mathbb{R}^d \times \mathbb{R}^r \times [0, T] \rightarrow \mathbb{R}^{d \times m}$ are continuous and satisfy Assumption 3.2. Moreover,

$$\begin{aligned} \mathbb{R}^d \ni x \mapsto a(x, u(t), t) \in \mathbb{R}^d, \quad \mathbb{R}^d \ni x \mapsto b(x, u(t), t) \in \mathbb{R}^{d \times m} & \quad (\text{for any } u \in \mathcal{U}_{\text{ad}}), \\ \mathbb{R}^r \ni u \mapsto a(x, u, t) \in \mathbb{R}^d, \quad \mathbb{R}^r \ni u \mapsto b(x, u, t) \in \mathbb{R}^{d \times m} & \quad (\text{for any } x \in \mathbb{R}^d) \end{aligned}$$

are continuously differentiable for all $t \in [0, T]$.

We remark that if Assumption 5.1-2) holds, then (3.2) holds for all $t \in [0, T]$, by continuity of a and b . In a first discretization step, we consider a semidiscrete version of the calibration problem and prove a convergence result. For the numerical implementation, we then follow [31] and apply a Monte–Carlo discretization for (3.4) to get a discretized and high-dimensional, but now deterministic constrained optimization problem. Then, we can apply a Lagrangian framework to get optimality conditions.

5.1 The Semidiscrete Calibration Problem

In this section, we study the calibration problem (cf. Remark 3.1-2)), where the control space $\mathcal{U}^c = \mathbb{R}^r$ is already finite-dimensional and needs not to be discretized:

$$\min \hat{J}(u) = J(\mathcal{S}(u), u) \quad \text{s.t.} \quad u \in \mathcal{U}_{\text{ad}}^c = [u_a, u_b] \subset \mathcal{U}^c, \quad (5.1)$$

where $X = \mathcal{S}(u) \in \mathcal{X}$ is the solution to (3.5). In order to keep the presentation clear and concise, we restrict ourselves in this section to the form of the functional given in (4.2). However, all results can be extended to functionals that satisfy Assumption 4.1 and Assumption 5.1.

For the semidiscrete approximation of (3.5), we split the time interval $[0, T]$ in N intervals of equal length $\Delta t = T/N$. We set

$$t_\nu := \nu \Delta t \quad \text{for } \nu = 0, \dots, N$$

and define an elementary time interval as

$$\mathcal{J}_\nu := [t_\nu, t_{\nu+1}] = [t_\nu, t_\nu + \Delta t] \subset [0, T] \quad \text{for } \nu = 0, \dots, N-1.$$

We will approximate continuous functions $f : [0, T] \rightarrow \mathbb{R}^d$ by step functions of the form

$$\sum_{v=0}^{N-1} f(t_v) \chi_{\mathcal{I}^v}(t),$$

where $\chi_{\mathfrak{S}}$ denotes the indicator function for the set \mathfrak{S} , i.e.

$$\chi_{\mathfrak{S}}(\mathfrak{s}) := \begin{cases} 1 & \text{if } \mathfrak{s} \in \mathfrak{S}, \\ 0 & \text{otherwise.} \end{cases} \tag{5.2}$$

Following, e.g., [26], we discretize (3.5) with respect to time and obtain an explicit semidiscrete scheme of Euler–Maruyama type. For $u \in \mathcal{U}_{\text{ad}}^c$, we define $\mathbf{X}^N = \{\mathbf{X}_v^N\}_{v=0}^N \subset L^2(\Omega; \mathbb{R}^d)$ as the solution of

$$\begin{aligned} \mathbf{X}_{v+1}^N &= \mathbf{X}_v^N + a(\mathbf{X}_v^N, u, t_v) \Delta t + b(\mathbf{X}_v^N, u, t_v) \Delta \mathbf{B}_v \quad \text{for } v = 0, \dots, N-1, \\ \mathbf{X}_0^N &= \mathbf{X}_\circ, \end{aligned} \tag{5.3}$$

where $\Delta \mathbf{B}_v := \mathbf{B}(t_{v+1}) - \mathbf{B}(t_v) \in L^2(\Omega; \mathbb{R}^m)$. Note that $(\Delta \mathbf{B}_v)_i \sim \mathcal{N}(0, \Delta t)$ for $1 \leq i \leq m$. Here, $\mathcal{N}(0, \Delta t)$ defines a normal distribution with mean 0 and standard deviation $\Delta t^{1/2}$. For the explicit realization of sampling Brownian motion increments, we refer to Sect. 5.2. As the scheme (5.3) is explicit, there exists a unique solution \mathbf{X}^N , and \mathbf{X}_v^N is $\mathcal{F}_\circ(t_v)$ -measurable for $v = 0, \dots, N$. We introduce the discrete solution space

$$\mathcal{X}^N := \{\mathbf{Y}^N = \{\mathbf{Y}_v^N\}_{v=0}^N \mid \mathbf{Y}_v^N \in L^2(\Omega; \mathbb{R}^d)\} = (L^2(\Omega; \mathbb{R}^d))^{N+1}$$

with norm

$$\|\mathbf{Y}^N\|_{\mathcal{X}^N} := \max_{v=0, \dots, N} \|\mathbf{Y}_v^N\|_{L^2(\Omega, \mathbb{R}^d)}$$

and the discrete solution operator

$$\mathcal{S}^N : \mathcal{U}_{\text{ad}}^c \rightarrow \mathcal{X}^N, \quad u \mapsto \mathcal{S}^N(u) := \mathbf{X}^N,$$

where \mathbf{X}^N denotes the solution of (5.3).

The following result is the time-discrete analogon of Theorem 3.7.

Lemma 5.2 *Let Assumption 5.1-2). hold, and let $\mathbf{X}_\circ \in L^2(\Omega; \mathbb{R}^d)$ be an \mathcal{F}_\circ -measurable random variable. Then, for all $u, \tilde{u} \in \mathcal{U}_{\text{ad}}^c$, we have*

$$\|\mathcal{S}^N(u) - \mathcal{S}^N(\tilde{u})\|_{\mathcal{X}^N} \leq C_1 \|u - \tilde{u}\|_{\mathcal{U}^c}, \tag{5.4}$$

$$\|\mathcal{S}^N(u)\|_{\mathcal{X}^N} \leq C_2 \tag{5.5}$$

with non-negative constants $C_1 = C_1(L_U, T)$ and $C_2 = C_2(L_U, T, \mathbf{X}_o)$ independent of N .

Proof Let $u, \tilde{u} \in \mathcal{U}_{\text{ad}}^c$, and set $\mathbf{X}^N := \mathcal{S}^N(u)$ and $\tilde{\mathbf{X}}^N := \mathcal{S}^N(\tilde{u})$. We consider the differences $\Delta_\nu^N := \mathbf{X}_\nu^N - \tilde{\mathbf{X}}_\nu^N \in L^2(\Omega; \mathbb{R}^d)$, $0 \leq \nu \leq N$. Obviously, we have $\Delta_0^N = 0$. Iteratively, we obtain

$$\begin{aligned} \Delta_{\nu+1}^N &= \Delta_\nu^N + (a(\mathbf{X}_\nu^N, u, t_\nu) - a(\tilde{\mathbf{X}}_\nu^N, \tilde{u}, t_\nu)) \Delta t + (b(\tilde{\mathbf{X}}_\nu^N, u, t_\nu) - b(\tilde{\mathbf{X}}_\nu^N, \tilde{u}, t_\nu)) \Delta \mathbf{B}_\nu \\ &= \sum_{l=0}^\nu \left((a(\mathbf{X}_l^N, u, t_l) - a(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l)) \Delta t + (b(\mathbf{X}_l^N, u, t_l) - b(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l)) \Delta \mathbf{B}_l \right) \end{aligned}$$

for $\nu = 0, \dots, N - 1$. From this, we see that

$$\begin{aligned} \mathbb{E}[\|\Delta_{\nu+1}^N\|_{\mathbb{R}^d}^2] &\leq 2 \mathbb{E}\left[\left\| \sum_{l=0}^\nu (a(\mathbf{X}_l^N, u, t_l) - a(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l)) \Delta t \right\|_{\mathbb{R}^d}^2\right] \\ &\quad + 2 \mathbb{E}\left[\left\| \sum_{l=0}^\nu (b(\mathbf{X}_l^N, u, t_l) - b(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l)) \Delta \mathbf{B}_l \right\|_{\mathbb{R}^d}^2\right] \end{aligned} \tag{5.6}$$

for $\nu = 0, \dots, N - 1$. With Assumption 5.1-2), $\Delta t = T/N$ and $\sum_{l=0}^\nu 1 \leq N$, we get

$$\begin{aligned} &\mathbb{E}\left[\left\| \sum_{l=0}^\nu (a(\mathbf{X}_l^N, u, t_l) - a(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l)) \Delta t \right\|_{\mathbb{R}^d}^2\right] \\ &\leq (\Delta t)^2 \mathbb{E}\left[\left(\sum_{l=0}^\nu \|a(\mathbf{X}_l^N, u, t_l) - a(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l)\|_{\mathbb{R}^d}\right)^2\right] \\ &\leq (\Delta t)^2 L_U^2 \mathbb{E}\left[\left(\sum_{l=0}^\nu (\|\Delta_l^N\|_{\mathbb{R}^d} + \|u - \tilde{u}\|_{\mathcal{U}^c})\right)^2\right] \\ &\leq \Delta t L_U^2 T \mathbb{E}\left[\sum_{l=0}^\nu (\|\Delta_l^N\|_{\mathbb{R}^d} + \|u - \tilde{u}\|_{\mathcal{U}^c})^2\right] \\ &\leq 2L_U^2 T \left(\Delta t \sum_{l=0}^\nu \mathbb{E}[\|\Delta_l^N\|_{\mathbb{R}^d}^2] + \|u - \tilde{u}\|_{\mathcal{U}^c}^2\right). \end{aligned}$$

For the second expectation on the right-hand side of (5.6), we set

$$G_l = (G_l^{ji})_{j=1, \dots, d, i=1, \dots, m} := b(\mathbf{X}_l^N, u, t_l) - b(\tilde{\mathbf{X}}_l^N, \tilde{u}, t_l) \quad \text{for } l = 0, \dots, \nu$$

and get (cf. also [18, Subsection 4.2.2])

$$\begin{aligned} \mathbb{E} \left[\left\| \sum_{l=0}^{\nu} G_l \Delta \mathbf{B}_l \right\|_{\mathbb{R}^d}^2 \right] &= \mathbb{E} \left[\sum_{l,\ell=0}^{\nu} \left(G_l \Delta \mathbf{B}_l \right)^\top \left(G_\ell \Delta \mathbf{B}_\ell \right) \right] \\ &= \sum_{l,\ell=0}^{\nu} \mathbb{E} \left[\Delta \mathbf{B}_l^\top G_l^\top G_\ell \Delta \mathbf{B}_\ell \right] \\ &= \sum_{l,\ell=0}^{\nu} \sum_{i=1}^m \sum_{j=1}^d \sum_{k=1}^m \mathbb{E} \left[\Delta B_{li} G_l^{ji} G_\ell^{jk} \Delta B_{\ell k} \right]. \end{aligned}$$

If $\ell > l$, then $\Delta B_{\ell k}$ is independent of $\Delta B_{li} G_l^{ji} G_\ell^{jk}$, and we get

$$\mathbb{E} \left[\Delta B_{li} G_l^{ji} G_\ell^{jk} \Delta B_{\ell k} \right] = \mathbb{E} \left[\Delta B_{li} G_l^{ji} G_\ell^{jk} \right] \mathbb{E} \left[\Delta B_{\ell k} \right] = 0.$$

In the same way, the expectation vanishes for $\ell < l$ and for $i \neq k$. With this and $\mathbb{E}[(\Delta B_{li})^2] = t_{i+1} - t_i = \Delta t$, we obtain

$$\begin{aligned} \mathbb{E} \left[\left\| \sum_{l=0}^{\nu} G_l \Delta \mathbf{B}_l \right\|_{\mathbb{R}^d}^2 \right] &= \sum_{l=0}^{\nu} \sum_{i=1}^m \sum_{j=1}^d \mathbb{E}[(G_l^{ji})^2] \mathbb{E}[(\Delta B_{li})^2] \\ &= \Delta t \sum_{l=0}^{\nu} \mathbb{E} \left[\sum_{i=1}^m \sum_{j=1}^d (G_l^{ji})^2 \right] \\ &= \Delta t \sum_{l=0}^{\nu} \mathbb{E}[\|G_l\|_{\mathbb{F}}^2]. \end{aligned}$$

From the definition of G_l and the Lipschitz continuity of b (see Assumption 5.1-2)) it follows that

$$\mathbb{E} \left[\left\| \sum_{l=0}^{\nu} (b(X_l^N, u, t_l) - b(\tilde{X}_l^N, \tilde{u}, t_l)) \Delta \mathbf{B}_l \right\|_{\mathbb{R}^d}^2 \right] \leq 2L_U^2 \left(\Delta t \sum_{l=0}^{\nu} \mathbb{E}[\|\Delta_l^N\|_{\mathbb{R}^d}^2] + \|u - \tilde{u}\|_{\mathcal{U}C}^2 \right).$$

Inserting this into (5.6) yields

$$\mathbb{E}[\|\Delta_{\nu+1}^N\|_{\mathbb{R}^d}^2] \leq c_1 \Delta t \sum_{l=0}^{\nu} \mathbb{E}[\|\Delta_l^N\|_{\mathbb{R}^d}^2] + c_1 \|u - \tilde{u}\|_{\mathcal{U}C}^2 \quad \text{for } \nu = 0, \dots, N - 1$$

with $c_1 := 4(T + 1)L_U^2$. Now an application of the discrete Gronwall inequality (see [12, Theorem 3.2]) gives the desired estimate

$$\max_{\nu=0, \dots, N} \mathbb{E}[\|X_\nu^N - \tilde{X}_\nu^N\|_{\mathbb{R}^d}^2] \leq C_1 \|u - \tilde{u}\|_{\mathcal{U}C}^2$$

with a constant $C_1 = C_1(T, L_U)$, which shows (5.4). The proof of (5.5) follows the same lines, writing

$$a(\mathbf{X}_l^N, u, t_l) = \left(a(\mathbf{X}_l^N, u, t_l) - a(0, u, t_l) \right) + a(0, u, t_l)$$

(see the proof of Theorem 3.7). We obtain

$$\mathbb{E}[\|\mathbf{X}_\nu^N\|^2] \leq c_2 \Delta t \sum_{l=0}^{\nu} \mathbb{E}[\|\mathbf{X}_l^N\|^2] + c_2 + c_2 \sum_{l=0}^{N-1} \Delta t \left(\|a(0, u, t_l)\|_{\mathbb{R}^d}^2 + \|b(0, u, t_l)\|_{\mathbb{F}}^2 \right),$$

with a constant $c_2 = c_2(L_U, T, \mathbf{X}_o)$. By Assumption 5.1-2), the (deterministic) coefficient $a(0, u, \cdot)$ is continuous and therefore uniformly continuous in the interval $[0, T]$. Therefore, $\sum_{\nu=0}^{N-1} \|a(0, u, t_l)\|_{\mathbb{R}^d}^2 \chi_{\mathcal{J}^\nu}(\cdot)$ converges uniformly to $\|a(0, u, \cdot)\|_{\mathbb{R}^d}^2$ for $N \rightarrow \infty$. Integration with respect to $t \in [0, T]$ shows that

$$\sum_{l=0}^{N-1} \Delta t \|a(0, u, t_l)\|_{\mathbb{R}^d}^2 \rightarrow \int_0^T \|a(0, u, \cdot)\|_{\mathbb{R}^d}^2 dt \leq L_U^2,$$

and, in particular, this sum is bounded by a constant for all $N \in \mathbb{N}$. Treating the coefficient b in the same way, we get

$$\mathbb{E}[\|\mathbf{X}_{\nu+1}^N\|^2] \leq c_2 \Delta t \sum_{l=0}^{\nu} \mathbb{E}[\|\mathbf{X}_l^N\|^2] + c'_2 \quad \text{for } \nu = 0, \dots, N - 1$$

for some constant $c'_2 = c'_2(L_U, T, \mathbf{X}_o)$. Now the discrete Gronwall inequality yields (5.5). □

We set $c_v^d := c^d(t_v)$ for $\nu = 0, \dots, N$ and introduce the discrete cost functional

$$J^N(\mathbf{X}^N, u) := \frac{\Delta t}{2} \sum_{\nu=0}^{N-1} \left\| \mathcal{C}(\mathbb{E}[\mathbf{X}_\nu^N]) - c_\nu^d \right\|_{\mathbb{R}^\ell}^2 + \frac{1}{2} \left\| \mathcal{C}(\mathbb{E}[\mathbf{X}_N^N]) - c_N^d \right\|_{\mathbb{R}^\ell}^2 + \frac{\kappa}{2} \|u\|_{\mathcal{U}^c}^2$$

for $\mathbf{X}^N \in \mathcal{X}^N$ and $u \in \mathcal{U}_{ad}^c$ as well as the discrete reduced cost functional

$$\hat{J}^N(u) := J^N(\mathcal{S}^N(u), u) \quad \text{for } u \in \mathcal{U}_{ad}^c.$$

The following is the main result on convergence of the semidiscrete approximation.

Theorem 5.3 *Let Assumption 5.1 hold.*

- (1) *The map $\hat{J}^N : \mathcal{U}_{ad}^c \rightarrow \mathbb{R}$ is Lipschitz continuous with Lipschitz constant independent of N , i.e., there exists a constant $L_d > 0$ such that for all $N \in \mathbb{N}$ and all $u, \tilde{u} \in \mathcal{U}_{ad}^c$ we have*

$$|\hat{J}^N(u) - \hat{J}^N(\tilde{u})| \leq L_d \|u - \tilde{u}\|_{\mathcal{U}^c}.$$

- (2) For any $u \in \mathcal{U}_{\text{ad}}^c$, we have $\hat{J}^N(u) \rightarrow \hat{J}(u)$ for $N \rightarrow \infty$.
- (3) Let $\{u^k\}_{k \in \mathbb{N}} \subset \mathcal{U}_{\text{ad}}^c$ be a sequence with $u^k \rightarrow u \in \mathcal{U}_{\text{ad}}^c$ for $k \rightarrow \infty$, and let $\{N_k\}_{k \in \mathbb{N}} \subset \mathbb{N}$ be a sequence with $N_k \rightarrow \infty$ for $k \rightarrow \infty$. Then

$$\hat{J}^{N_k}(u^k) \rightarrow \hat{J}(u) \text{ for } k \rightarrow \infty.$$

Proof (1) For $v = 0, \dots, N$ and $\mathbf{X}^N, \tilde{\mathbf{X}}^N \in \mathcal{X}^N$, we have

$$\begin{aligned} \|\mathbb{E}[\mathbf{X}_v^N] - \mathbb{E}[\tilde{\mathbf{X}}_v^N]\|_{\mathbb{R}^d} &= \|\mathbb{E}[\mathbf{X}_v^N - \tilde{\mathbf{X}}_v^N]\|_{\mathbb{R}^d} \leq \|\mathbf{X}_v^N - \tilde{\mathbf{X}}_v^N\|_{L^1(\Omega; \mathbb{R}^d)} \\ &\leq \sqrt{T} \|\mathbf{X}_v^N - \tilde{\mathbf{X}}_v^N\|_{L^2(\Omega; \mathbb{R}^d)}, \end{aligned}$$

which shows that the map $\mathcal{X}^N \rightarrow \mathbb{R}^d, \mathbf{X}^N \mapsto \mathbb{E}[\mathbf{X}_v^N]$ is Lipschitz continuous. Since Assumption 5.1-2) holds, we can apply Lemma 5.2. We conclude that $\mathcal{S}^N : \mathcal{U}_{\text{ad}}^c \rightarrow \mathcal{X}^N$ is Lipschitz continuous with constant independent of N and that $\mathcal{S}^N(\mathcal{U}_{\text{ad}}^c)$ is bounded by virtue of (5.5). Therefore, the same holds for the map

$$\phi_v : \mathcal{U}_{\text{ad}}^c \rightarrow \mathbb{R}^d \quad u \mapsto \mathbb{E}[\mathbf{X}_v^N] \quad \text{with } \mathbf{X}^N := \mathcal{S}^N(u).$$

By Assumption 5.1-1),

$$\mathbb{R}^d \rightarrow \mathbb{R}, \quad x \mapsto \|\mathcal{C}(x) - c_v^d\|_{\mathbb{R}^\ell}^2 \tag{5.7}$$

is continuously differentiable and therefore Lipschitz on the bounded range of ϕ_v . As the composition of Lipschitz functions is again a Lipschitz function, we see that

$$\mathcal{U}_{\text{ad}}^c \rightarrow \mathbb{R}, \quad u \mapsto \|\mathcal{C}(\mathbb{E}[\mathbf{X}_v^N]) - c_v^d\|_{\mathbb{R}^\ell}^2 \quad \text{with } \mathbf{X}^N := \mathcal{S}^N(u)$$

is Lipschitz continuous with a Lipschitz constant $L > 0$ independent of N . As $u \mapsto \|u\|_{\mathcal{U}^c}^2$ is continuously differentiable and therefore Lipschitz with some constant $L' > 0$ on the compact set $\mathcal{U}_{\text{ad}}^c$, we obtain for $u, \tilde{u} \in \mathcal{U}_{\text{ad}}^c$ and for every $N \in \mathbb{N}$

$$\begin{aligned} |\hat{J}^N(u) - \hat{J}^N(\tilde{u})| &\leq \frac{\Delta t}{2} \sum_{v=0}^{N-1} L \|u - \tilde{u}\|_{\mathcal{U}^c} + \frac{1}{2} L \|u - \tilde{u}\|_{\mathcal{U}^c} + \frac{\kappa}{2} L' \|u - \tilde{u}\|_{\mathcal{U}^c} \\ &\leq L_d \|u - \tilde{u}\|_{\mathcal{U}^c} \end{aligned}$$

for $L_d := ((T + 1)L + \kappa L')/2$, where we used $\Delta t = T/N$, which gives part 1).

(2) Let $u \in \mathcal{U}_{\text{ad}}^c$ and set $\mathbf{X} := \mathcal{S}(u)$ and $\mathbf{X}^N := \mathcal{S}^N(u)$ for $N \in \mathbb{N}$. By Theorem 3.7, we have $\mathbf{X} \in C([0, T]; L^2(\Omega; \mathbb{R}^d))$ which implies that $\mathbb{E}[\mathbf{X}(\cdot)] \in C([0, T]; \mathbb{R}^d)$. From this and the continuity of \mathcal{C} and c^d , we see that the integrand in the cost functional $J(\mathbf{X}, u)$ (see (4.2)), which is given as $\|\mathcal{C}(\mathbb{E}[\mathbf{X}(\cdot)]) - c^d(\cdot)\|_{\mathbb{R}^\ell}^2$, is a continuous function

on $[0, T]$ and can be approximated uniformly by the step function

$$t \mapsto \sum_{\nu=0}^{N-1} \left\| \mathcal{C}(\mathbb{E}[\mathbf{X}(t_\nu)]) - c_\nu^d \right\|_{\mathbb{R}^\ell}^2 \chi_{\mathcal{J}^\nu}(t).$$

Integrating this with respect to $t \in [0, T]$, we obtain

$$J^N((\mathbf{X}(t_\nu))_{\nu=0, \dots, N}, u) \rightarrow J(\mathbf{X}, u) \quad \text{for } N \rightarrow \infty. \quad (5.8)$$

Now we use the fact that \mathbf{X}^N is computed with the Euler-Murayama scheme (5.3) which is known to be of convergence order $1/2$ (see [42, Section 1.1.5]). Therefore, we can apply the convergence result from [42, Theorem 1.1.1] which tells us that

$$\sup_{\nu=0, \dots, N} \mathbb{E} \left[\left\| \mathbf{X}_\nu^N - \mathbf{X}(t_\nu) \right\|_{\mathbb{R}^d}^2 \right] \rightarrow 0 \quad \text{for } N \rightarrow \infty.$$

This implies $\mathbb{E}[\mathbf{X}_\nu^N] \rightarrow \mathbb{E}[\mathbf{X}(t_\nu)]$ for $N \rightarrow \infty$ and, by uniform continuity of the function (5.7) on bounded subsets,

$$\sup_{\nu=0, \dots, N} \left| \left\| \mathcal{C}(\mathbb{E}[\mathbf{X}_\nu^N]) - c_\nu^d \right\|_{\mathbb{R}^\ell}^2 - \left\| \mathcal{C}(\mathbb{E}[\mathbf{X}(t_\nu)]) - c_\nu^d \right\|_{\mathbb{R}^\ell}^2 \right| \rightarrow 0 \quad \text{for } N \rightarrow \infty.$$

Summing up over ν and using $\Delta t = T/N$ again, we get

$$\left| J^N(\mathbf{X}^N, u) - J^N((\mathbf{X}(t_\nu))_{\nu=0, \dots, N}, u) \right| \rightarrow 0 \quad \text{for } N \rightarrow \infty. \quad (5.9)$$

As $J^N(\mathbf{X}^N, u) = \hat{J}^N(u)$ and $J(\mathbf{X}, u) = \hat{J}(u)$, the statement in (2) now follows from (5.8) and (5.9).

(3) This is an immediate consequence of parts (1) and (2). In fact, for $\varepsilon > 0$ we first choose $k_0 \in \mathbb{N}$ such that for all $k \geq k_0$, we have $\|u^k - u\|_{\mathcal{U}^c} \leq \varepsilon/(2L_d)$ with L_d from 1). Then $|\hat{J}^N(u^k) - \hat{J}^N(u)| \leq \varepsilon/2$ holds by 1) for all $N \in \mathbb{N}$. Now we apply (2) and $N_k \rightarrow \infty$ to see that there exists $k_1 \geq k_0$ such that for all $k \geq k_1$ we obtain $|\hat{J}^{N_k}(u) - \hat{J}(u)| \leq \varepsilon/2$. This yields $|\hat{J}^{N_k}(u^k) - \hat{J}(u)| \leq \varepsilon$ for $k \geq k_1$, which shows (3). \square

5.2 The Fully Discretized Problem

In this section, we explain how we solve (5.1) numerically. In Sect. 5.1, we already described the discretization with respect to time and formulated a semi-discrete scheme (5.3). In order to obtain a fully discrete scheme, we use a Monte Carlo approximation. More specifically, we consider $M \gg 1$ realizations of the SDE and for every realization and every time instant $t_\nu \in [0, T]$, we precompute samples of the Brownian motion. We denote these samples by

$$\Delta \mathbf{B}^\mu = [\Delta \mathbf{B}_1^\mu \dots \Delta \mathbf{B}_N^\mu] \in \mathbb{R}^{m \times N} \quad \text{with } \Delta \mathbf{B}_\nu^\mu = (\Delta B_{\nu,j}^\mu)_{j=1}^m \text{ and } \Delta B_{\nu,j}^\mu \sim \mathcal{N}(0, \Delta t)$$

for $\mu = 1, \dots, M$. In order to simplify the notation, we set $h = (M, N)$.

We can now introduce the discretization of the state equation (3.4) as follows: For any given control $u \in \mathcal{U}_{ad}^c$ find

$$\mathbf{X}^h \in \mathcal{X}^h := \{ \tilde{\mathbf{X}}_v^\mu \in \mathbb{R}^d \mid v = 0, \dots, N \text{ and } \mu = 1, \dots, M \}$$

satisfying

$$\begin{aligned} \mathbf{X}_{v+1}^\mu &= \mathbf{X}_v^\mu + a(\mathbf{X}_v^\mu, u, t_v)\Delta t + b(\mathbf{X}_v^\mu, u, t_v)\Delta \mathbf{B}_v^\mu, \quad \mu = 1, \dots, M, v = 0, \dots, N - 1, \\ \mathbf{X}_0^\mu &= \mathbf{X}_o, \quad \mu = 1, \dots, M. \end{aligned} \tag{5.10}$$

Notice that the solution in (5.10) depends on the pre-computed samples of the Brownian motion. For the discrete \mathbf{X}^h , we define the discrete expectation value as the arithmetic mean, i.e., for $v \in \{0, \dots, N\}$

$$\mathbb{E}^M \left[\mathbf{X}_v^h \right] := \frac{1}{M} \sum_{\mu=1}^M \mathbf{X}_v^\mu. \tag{5.11}$$

The finite-dimensional (Hilbert) space \mathcal{X}^h is isomorphic to $\mathbb{R}^{(N+1)M}$ and is supplied by the weighted inner product

$$\langle \mathbf{X}^h, \tilde{\mathbf{X}}^h \rangle_{\mathcal{X}^h} = \frac{\Delta t}{M} \sum_{\mu=1}^M \sum_{v=0}^N (\mathbf{X}_v^\mu)^\top \tilde{\mathbf{X}}_v^\mu = \mathbb{E}^M \left[\Delta t \sum_{v=0}^N (\mathbf{X}_v^h)^\top \tilde{\mathbf{X}}_v^h \right] \text{ for } \mathbf{X}^h, \tilde{\mathbf{X}}^h \in \mathcal{X}^h,$$

where we set $\mathbf{X}_v^h = \{ \mathbf{X}_v^\mu \}_{\mu=1}^M$ and $\tilde{\mathbf{X}}_v^h = \{ \tilde{\mathbf{X}}_v^\mu \}_{\mu=1}^M$ for $v \in \{0, \dots, N\}$. Notice that (5.10) is an explicit difference scheme. Thus, the existence of the sequence \mathbf{X}^h satisfying (5.10) is clear. In that case the discrete non-linear solution operator

$$\mathcal{S}^h : \mathcal{U}_{ad}^c \rightarrow \mathcal{X}^h, \quad \mathbf{X}^h = \mathcal{S}^h(u) \text{ is the unique solution to (5.10) for } u \in \mathcal{U}_{ad}^c \text{ given the } M \text{ pre-computed Brownian increments}$$

is well defined. We formulate a discrete version of (5.1) as follows:

$$\min \hat{J}^h(u) \quad \text{s.t. } u \in \mathcal{U}_{ad}^c, \tag{5.12}$$

where the discrete reduced cost functional is defined as

$$\hat{J}^h(u) := J^h(\mathbf{X}^h, u) \quad \text{for } u \in \mathcal{U}_{ad}^c \text{ and } \mathbf{X}^h = \mathcal{S}^h(u)$$

with

$$\begin{aligned}
 J^h(\mathbf{X}^h, u) &:= \frac{1}{2} \left(\Delta t \sum_{v=0}^{N-1} \left\| \mathcal{C}(\mathbb{E}^M[\mathbf{X}_v^h]) - c_v^d \right\|_{\mathbb{R}^\ell}^2 + \left\| \mathcal{C}(\mathbb{E}^M[\mathbf{X}_N^h]) - c_N^d \right\|_{\mathbb{R}^\ell}^2 + \kappa \|u\|_{\mathcal{U}}^2 \right) \\
 &= \frac{\Delta t}{2} \sum_{v=0}^{N-1} \left\| \mathcal{C}\left(\frac{1}{M} \sum_{\mu=1}^M \mathbf{X}_v^\mu\right) - c_v^d \right\|_{\mathbb{R}^\ell}^2 + \frac{1}{2} \left\| \mathcal{C}\left(\frac{1}{M} \sum_{\mu=1}^M \mathbf{X}_N^\mu\right) - c_N^d \right\|_{\mathbb{R}^\ell}^2 + \frac{\kappa}{2} \sum_{i=1}^r |u_i|^2.
 \end{aligned}$$

The next step is to introduce the associated Lagrange functional for the discretized problem (5.12). It is given by

$$\begin{aligned}
 \mathcal{L}(\mathbf{X}^h, u, \mathbf{\Lambda}^h) &:= \\
 &\frac{1}{2} \left(\Delta t \sum_{v=0}^{N-1} \left\| \mathcal{C}(\mathbb{E}^M[\mathbf{X}_v^h]) - c_v^d \right\|_{\mathbb{R}^\ell}^2 + \left\| \mathcal{C}(\mathbb{E}^M[\mathbf{X}_N^h]) - c_N^d \right\|_{\mathbb{R}^\ell}^2 + \kappa \|u\|_{\mathcal{U}}^2 \right) \\
 &+ \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\mathbf{X}_{v+1}^\mu - \mathbf{X}_v^\mu - a(\mathbf{X}_v^\mu, u, t_v) \Delta t - b(\mathbf{X}_v^\mu, u, t_v) \Delta \mathbf{B}_v^\mu \right]^\top \mathbf{\Lambda}_{v+1}^\mu \\
 &+ \frac{1}{M} \sum_{\mu=1}^M \left[\mathbf{X}_0^\mu - \mathbf{X}_\circ^\mu \right]^\top \mathbf{\Lambda}_0^\mu
 \end{aligned} \tag{5.13}$$

for $\mathbf{X}^h = \{\mathbf{X}_v^\mu\} \in \mathcal{X}^h$, and where we have introduced the Lagrange multiplier

$$\mathbf{\Lambda}^h = \{\mathbf{\Lambda}_v^\mu \in \mathbb{R}^d \mid v = 0, \dots, N \text{ and } \mu = 1, \dots, M\} \in \mathcal{X}^h.$$

In particular, $\mathbf{\Lambda}_0^\mu$ is the Lagrange multiplier associated with the initial condition. Note that

$$\underbrace{b(\mathbf{X}_v^\mu, u, t_v)}_{\in \mathbb{R}^{d \times m}} \underbrace{\Delta \mathbf{B}_v^\mu}_{\in \mathbb{R}^m} = \sum_{j=1}^m \Delta B_{v,j}^\mu \underbrace{b_j(\mathbf{X}_v^\mu, u, t_v)}_{\in \mathbb{R}^d} \quad \text{for } \mu = 1, \dots, M, \quad v = 0, \dots, N-1.$$

Next, we derive the adjoint equation by computing the partial derivative \mathcal{L}_X of \mathcal{L} with respect to \mathbf{X}^h . Let us refer to [31] for a similar approach, but in our case, we consider data that is given over the whole time interval $[0, T]$. Notice that in the discretize-before-optimize approach, the solution of the adjoint problem is only the variable $\mathbf{\Lambda}^h$. This is a crucial difference to the optimize-before-discretize approach, where the solution of the adjoint problem is in fact a tuple of stochastic processes (cf. Section 6.3 and [57]). For any direction $\tilde{\mathbf{X}}^h = \{\tilde{\mathbf{X}}_v^\mu\} \in \mathcal{X}^h$, we obtain the following expression

$$\begin{aligned}
 \mathcal{L}_X(\mathbf{X}^h, u, \mathbf{\Lambda}^h) \tilde{\mathbf{X}}^h &= \Delta t \sum_{v=0}^{N-1} \left[\mathcal{C}(\mathbb{E}^M[\mathbf{X}_v^h]) - c_v^d \right]^\top \mathcal{C}'(\mathbb{E}^M[\mathbf{X}_v^h]) \mathbb{E}^M[\tilde{\mathbf{X}}_v^h] \\
 &+ \left[\mathcal{C}(\mathbb{E}^M[\mathbf{X}_N^h]) - c_N^d \right]^\top \mathcal{C}'(\mathbb{E}^M[\mathbf{X}_N^h]) \mathbb{E}^M[\tilde{\mathbf{X}}_N^h]
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\tilde{X}_{v+1}^\mu - \tilde{X}_v^\mu - (a_x(X_v^\mu, u, t_v) \tilde{X}_v^\mu) \Delta t \right]^\top \Lambda_{v+1}^\mu \\
 & - \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\sum_{j=1}^m \Delta B_{v,j}^\mu (b_{jx}(X_v^\mu, u, t_v) \tilde{X}_v^\mu) \right]^\top \Lambda_{v+1}^\mu \\
 & + \frac{1}{M} \sum_{\mu=1}^M [\tilde{X}_0^\mu]^\top \Lambda_0^\mu
 \end{aligned} \tag{5.14}$$

with $b_{jx}(X_v^\mu, u, t_v) \in \mathbb{R}^{d \times d}$. Using an index shift, we can write

$$\begin{aligned}
 & \sum_{\mu=1}^M \sum_{v=0}^{N-1} [\tilde{X}_{v+1}^\mu - \tilde{X}_v^\mu]^\top \Lambda_{v+1}^\mu + \sum_{\mu=1}^M [\tilde{X}_0^\mu]^\top \Lambda_0^\mu \\
 & = \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left([\tilde{X}_{v+1}^\mu]^\top \Lambda_{v+1}^\mu - [\tilde{X}_v^\mu]^\top \Lambda_{v+1}^\mu \right) + \sum_{\mu=1}^M [\tilde{X}_0^\mu]^\top \Lambda_0^\mu \\
 & = \sum_{\mu=1}^M \sum_{v=0}^N [\tilde{X}_v^\mu]^\top \Lambda_v^\mu - \sum_{\mu=1}^M \sum_{v=0}^{N-1} [\tilde{X}_v^\mu]^\top \Lambda_{v+1}^\mu \\
 & = \sum_{\mu=1}^M \sum_{v=0}^{N-1} [\Lambda_v^\mu - \Lambda_{v+1}^\mu]^\top \tilde{X}_v^\mu + \sum_{\mu=1}^M [\Lambda_N^\mu]^\top \tilde{X}_N^\mu.
 \end{aligned} \tag{5.15}$$

Furthermore, we can calculate

$$\sum_{\mu=1}^M \sum_{v=0}^{N-1} [(a_x(X_v^\mu, u, t_v) \tilde{X}_v^\mu) \Delta t]^\top \Lambda_{v+1}^\mu = \sum_{\mu=1}^M \sum_{v=0}^{N-1} [(a_x(X_v^\mu, u, t_v)^\top \Lambda_{v+1}^\mu) \Delta t]^\top \tilde{X}_v^\mu \tag{5.16}$$

and

$$\begin{aligned}
 & \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\sum_{j=1}^m \Delta B_{v,j}^\mu (b_{jx}(X_v^\mu, u, t_v) \tilde{X}_v^\mu) \right]^\top \Lambda_{v+1}^\mu \\
 & = \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\sum_{j=1}^m \Delta B_{v,j}^\mu (b_{jx}(X_v^\mu, u, t_v)^\top \Lambda_{v+1}^\mu) \right]^\top \tilde{X}_v^\mu.
 \end{aligned} \tag{5.17}$$

Using (5.11), inserting (5.15)-(5.17) into (5.14) and setting $\mathcal{L}_X(X, u, \Lambda) \tilde{X} = 0$, we derive

$$\begin{aligned}
 & \frac{\Delta t}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\mathcal{C}(\mathbb{E}^M[\mathbf{X}_v^h]) - c_v^d \right]^\top \mathcal{C}'(\mathbb{E}^M[\mathbf{X}_v^h]) \tilde{\mathbf{X}}_v^\mu \\
 & + \frac{1}{M} \sum_{\mu=1}^M \left[\mathcal{C}(\mathbb{E}^M[\mathbf{X}_N^h]) - c_N^d \right]^\top \mathcal{C}'(\mathbb{E}^M[\mathbf{X}_N^h]) \tilde{\mathbf{X}}_N^\mu \\
 & + \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\mathbf{\Lambda}_v^\mu - \mathbf{\Lambda}_{v+1}^\mu - (a_x(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu) \Delta t \right]^\top \tilde{\mathbf{X}}_v^\mu + \frac{1}{M} \sum_{\mu=1}^M [\mathbf{\Lambda}_N^\mu]^\top \tilde{\mathbf{X}}_N^\mu \\
 & - \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left[\sum_{j=1}^m \Delta B_{v,j}^\mu (b_{jx}(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu) \right]^\top \tilde{\mathbf{X}}_v^\mu = 0 \tag{5.18}
 \end{aligned}$$

for any direction $\tilde{\mathbf{X}}^h = \{\tilde{\mathbf{X}}_v^\mu\} \in \mathcal{X}^h$. If we choose $\tilde{\mathbf{X}}^h$ with $\tilde{\mathbf{X}}_N^\mu = 0$, we deduce from (5.18)

$$\begin{aligned}
 & \mathbf{\Lambda}_{v+1}^\mu - \mathbf{\Lambda}_v^\mu + a_x(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu \Delta t + \sum_{j=1}^m \Delta B_{v,j}^\mu (b_{jx}(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu) \\
 & = \Delta t \mathcal{C}'(\mathbb{E}^M[\mathbf{X}_v^h])^\top (\mathcal{C}(\mathbb{E}^M[\mathbf{X}_v^h]) - c_v^d) \quad \text{for } \mu = 1, \dots, M, v = 0, \dots, N - 1. \tag{5.19a}
 \end{aligned}$$

Inserting (5.19a) into (5.18) we obtain the terminal condition

$$\mathbf{\Lambda}_N^\mu = \mathcal{C}'(\mathbb{E}^M[\mathbf{X}_N^h])^\top (c_N^d - \mathcal{C}(\mathbb{E}^M[\mathbf{X}_N^h])) \tag{5.19b}$$

for $\mu = 1, \dots, M$. Next, we compute the partial derivative with respect to u and derive for $u \in \text{int } \mathcal{U}_{\text{ad}}^c$ and for any direction $\tilde{u} \in \mathcal{U}^c$ such that $u + \tilde{u} \in \mathcal{U}_{\text{ad}}^c$

$$\begin{aligned}
 & \mathcal{L}_u(\mathbf{X}^h, u, \mathbf{\Lambda}^h) \tilde{u} \\
 & = \kappa u^\top \tilde{u} - \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left((a_u(\mathbf{X}_v^\mu, u, t_v) \Delta t) \tilde{u} + \left(\sum_{j=1}^m \Delta B_{v,j}^\mu b_{ju}(\mathbf{X}_v^\mu, u, t_v) \right) \tilde{u} \right)^\top \mathbf{\Lambda}_{v+1}^\mu \\
 & = \left(\kappa u - \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} (a_u(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu) \Delta t + \left(\sum_{j=1}^m \Delta B_{v,j}^\mu b_{ju}(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu \right) \right)^\top \tilde{u}.
 \end{aligned}$$

Suppose that for given $u \in \mathcal{U}_{\text{ad}}^c$ the state $\mathbf{X}^h = \mathbf{X}_u^h$ solves (3.5). Moreover, $\mathbf{\Lambda}^h = \mathbf{\Lambda}_u^h$ is the solution to (5.19) with $\mathbf{X}^h = \mathbf{X}_u^h$. Then, it follows that (cf., e.g., [27, Section 1.6.4])

$$\begin{aligned}
 & \nabla \hat{J}^h(u) = \mathcal{L}_u(\mathbf{X}_u^h, u, \mathbf{\Lambda}_u^h) \\
 & = \kappa u - \frac{1}{M} \sum_{\mu=1}^M \sum_{v=0}^{N-1} \left(a_u(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu \Delta t + \sum_{j=1}^m \Delta B_{v,j}^\mu b_{ju}(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu \right)
 \end{aligned}$$

$$= \kappa u - \mathbb{E}^M \left[\sum_{v=0}^{N-1} a_u(\mathbf{X}_v^\mu, u, t_v)^\top \boldsymbol{\Lambda}_{v+1}^\mu \Delta t + \sum_{j=1}^m \Delta B_{v,j}^\mu b_{ju}(\mathbf{X}_v^\mu, u, t_v)^\top \boldsymbol{\Lambda}_{v+1}^\mu \right]. \tag{5.20}$$

All together, we can formulate first-order necessary optimality conditions for (5.1) in Theorem 5.4.

Theorem 5.4 *Suppose that (5.10) and (5.19) are uniquely solvable and moreover that $\bar{u} \in \mathcal{U}_{\text{ad}}^c$ is a local solution to (5.1). Then, it follows*

$$\begin{aligned} & \left\langle \kappa \bar{u} - \mathbb{E}^M \left[\sum_{v=0}^{N-1} a_u(\mathbf{X}_v^\mu, u, t_v)^\top \boldsymbol{\Lambda}_{v+1}^\mu \Delta t \right], u - \bar{u} \right\rangle_{\mathcal{U}} \\ & - \left\langle \mathbb{E}^M \left[\sum_{v=0}^{N-1} \sum_{j=1}^m \Delta B_{v,j}^\mu b_{ju}(\mathbf{X}_v^\mu, u, t_v)^\top \boldsymbol{\Lambda}_{v+1}^\mu \right], u - \bar{u} \right\rangle_{\mathcal{U}} \geq 0 \text{ for all } u \in \mathcal{U}_{\text{ad}}^c, \end{aligned} \tag{5.21}$$

where $\mathbf{X}^h \in \mathcal{X}^h$ solves (5.10) for $u = \bar{u}$ and $\boldsymbol{\Lambda}^h \in \mathcal{X}^h$ is the solution to (5.19) with $u = \bar{u}$.

In Remark 6.9, we compare the discrete gradient (5.20) with the continuous one that will be derived in Sect. 6.3.

5.3 Continuous Control Inputs

Let us just explain briefly how we derive a discretization of the general optimization problem (4.3). Again, we set $h = (M, N)$ to simplify the notation. We approximate a time-dependent control $u \in \mathcal{U}$ by the piecewise constant function

$$u^h(t) = \sum_{v=0}^{N-1} u_v \chi_{\mathcal{J}_v}(t) \in \mathbb{R}^r \text{ for } t \in [0, T]$$

with $u_0, \dots, u_{N-1} \in \mathbb{R}^r$ and characteristic functions $\chi_{\mathcal{J}_v} : [0, T] \rightarrow \{0, 1\}$ defined in (5.2). Thus, each control u^h is characterized by a coefficient matrix $\mathbf{U}^h = [u_0 | \dots | u_{N-1}] \in \mathbb{R}^{r \times N}$. We set $\mathcal{U}^h = \mathbb{R}^{r \times N}$ which is a Hilbert space endowed with the (weighted) inner product

$$\langle \mathbf{U}^h, \tilde{\mathbf{U}}^h \rangle_{\mathcal{U}^h} = \Delta t \sum_{i=1}^r \sum_{v=0}^{N-1} U_{iv}^h \tilde{U}_{iv}^h = \Delta t \sum_{v=0}^{N-1} u_v^\top \tilde{u}_v$$

for $\mathbf{U}^h = [u_0 | \dots | u_{N-1}]$ and $\tilde{\mathbf{U}}^h = [\tilde{u}_0 | \dots | \tilde{u}_{N-1}]$. The associated induced norm is given as $\|\mathbf{U}^h\|_{\mathcal{U}^h} = \sqrt{\Delta t} \|\mathbf{U}^h\|_F$.

Clearly, $u^h \in \mathcal{U}_{\text{ad}}$ holds true provided $u_\nu \in [u_a, u_b]$ for $\nu = 0, \dots, N - 1$. Thus, we define the set of admissible control coefficient matrices as

$$\mathcal{U}_{\text{ad}}^h = \{U^h = [u_0 | \dots | u_{N-1}] \in \mathcal{U}^h \mid u_\nu \in [u_a, u_b] \text{ for } \nu = 0, \dots, N - 1\}.$$

Next we introduce a discretization of the state equation (3.4) as follows: For any given control matrix $U^h = [u_0 | \dots | u_{N-1}] \in \mathcal{U}_{\text{ad}}^h$ find $X^h \in \mathcal{X}^h$ satisfying

$$\begin{aligned} X_{\nu+1}^\mu &= X_\nu^\mu + a(X_\nu^\mu, u_\nu, t_\nu) \Delta t + b(X_\nu^\mu, u_\nu, t_\nu) \Delta B_\nu^\mu \\ &\text{for } \mu = 1, \dots, M \text{ and } \nu = 0, \dots, N - 1, \\ X_0^\mu &= X_\circ \quad \text{for } \mu = 1, \dots, M. \end{aligned} \tag{5.22}$$

For any $U^h \in \mathcal{U}_{\text{ad}}^h$ we suppose that the explicit difference scheme (5.22) admits a unique solution $X^h \in \mathcal{X}^h$. Thus, the discrete non-linear solution operator

$$\mathcal{S}^h : \mathcal{U}_{\text{ad}}^h \rightarrow \mathcal{X}^h, \quad X^h = \mathcal{S}^h(U^h) \text{ is the unique solution to (5.22) for } U^h \in \mathcal{U}_{\text{ad}}^h \text{ given the } M \text{ pre-computed Brownian increments}$$

is well defined. Now let us formulate a discrete version of (4.3):

$$\hat{J}^h(U^h) \quad \text{s.t. } U^h \in \mathcal{U}_{\text{ad}}^h, \tag{5.23}$$

where the discrete reduced cost functional \hat{J}^h is given as

$$\hat{J}^h(U^h) = J^h(X^h, U^h) \quad \text{for } U^h \in \mathcal{U}_{\text{ad}}^h \text{ and } X^h = \mathcal{S}^h(U^h)$$

with

$$J^h(X^h, U^h) := \frac{1}{2} \left(\Delta t \sum_{\nu=0}^{N-1} \|c(\mathbb{E}^M[X_\nu^h]) - c_\nu^d\|_{\mathbb{R}^\ell}^2 + \|c(\mathbb{E}^M[X_N^h]) - c_N^d\|_{\mathbb{R}^\ell}^2 + \kappa \|U^h\|_{\mathcal{U}^h}^2 \right)$$

and $X_\nu^h = \{X_\nu^\mu\}_{\mu=1}^M$ for $\nu \in \{0, \dots, N\}$.

6 First-Order Optimality Conditions

In this section, we derive a formula for the gradient of the reduced cost functional $\hat{J} : \mathcal{U}_{\text{ad}} \rightarrow \mathbb{R}$ which allows us to formulate first-order necessary optimality conditions for the continuous problem. Here we focus on the choice $\mathcal{U} = L^2(0, T; \mathbb{R}^r)$. The derivation for the calibration problem is analogously.

First let us introduce the constraint function $e : \mathcal{X} \times \mathcal{U}_{\text{ad}} \rightarrow \mathcal{X}$ by

$$e(X, u) := X(\cdot) - X_\circ - \int_0^{(\cdot)} a(X(s), u(s), s) ds - \int_0^{(\cdot)} b(X(s), u(s), s) dB(s)$$

for $(X, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$. Here, (\cdot) is a placeholder denoting the dependence on t . Using the mapping e , the constraint (3.4) can be expressed as the operator equation

$$e(X, u) = 0 \quad \text{in } \mathcal{X}. \tag{6.1}$$

Due to Definition 3.3, we infer from (6.1) that X is a solution to (3.4) for any given $u \in \mathcal{U}_{\text{ad}}$. Moreover, (4.3) can be expressed equivalently as a non-convex, infinite-dimensional, constrained optimization problem as follows:

$$\min J(X, u) \quad \text{s.t. } (X, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}} \text{ and } e(X, u) = 0 \text{ in } \mathcal{X}. \tag{6.2}$$

It follows from Theorems 3.5 and 4.5 that (6.2) admits a (global) optimal solution $(\bar{X}, \bar{u}) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$ with $\bar{X} = \bar{S}(\bar{u})$ provided that Assumptions 3.2 and 4.1 hold.

6.1 Fréchet Differentiability of the Constraints

To derive the derivative of the constraint function e , we have to ensure Assumption 5.1-2).

Remark 6.1 Let $(x, u) \in \mathbb{R}^d \times \mathcal{U}_{\text{ad}}$. For any $s \in [0, T]$ we have

$$b(x, u(s), s) = [b_1(x, u(s), s) \mid \dots \mid b_m(x, u(s), s)] \in \mathbb{R}^{d \times m}.$$

With Assumption 5.1-2) holding the partial derivative $b_x(x, u(s), s)$ is a linear map from \mathbb{R}^d to $\mathbb{R}^{d \times m}$ for any $s \in [0, T]$. Consequently, $b_x(x, u(s), s)\tilde{x}$ is a $(d \times m)$ matrix for all $\tilde{x} \in \mathbb{R}^d$ and we write

$$\begin{aligned} b_x(x, u(s), s)\tilde{x} &= [b_{1x}(x, u(s), s)\tilde{x} \mid \dots \mid b_{mx}(x, u(s), s)\tilde{x}] \\ &= \sum_{i=1}^d b_{x_i}(x, u(s), s)\tilde{x}_i \in \mathbb{R}^{d \times m} \end{aligned}$$

for any $s \in [0, T]$, where $b_{jx}(x, u(s), s)$ ($1 \leq j \leq m$) denotes the partial derivative of b_j with respect to x . Analogously, we write

$$\begin{aligned} b_u(x, u(s), s)\tilde{u} &= [b_{1u}(x, u(s), s)\tilde{u} \mid \dots \mid b_{mu}(x, u(s), s)\tilde{u}] \\ &= \sum_{i=1}^m b_{u_i}(x, u(s), s)\tilde{u}_i \in \mathbb{R}^{d \times m} \end{aligned}$$

for any $s \in [0, T]$ and $\tilde{u} \in \mathcal{U}$.

Lemma 6.2 Suppose that Assumption 5.1-2) holds. Then the mapping e is continuously Fréchet differentiable on $\mathcal{X} \times \mathcal{U}_{\text{ad}}$. For any $(X, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$ the partial Fréchet derivatives e_X and e_u are given by

$$e_X(X, u)X^\delta = X^\delta(\cdot) - \int_0^{(\cdot)} a_x(X(s), u(s), s)X^\delta(s) ds$$

$$\begin{aligned}
 & - \int_0^{(\cdot)} b_x(\mathbf{X}(s), u(s), s) \mathbf{X}^\delta(s) \, d\mathbf{B}(s) && \text{for } \mathbf{X}^\delta \in \mathcal{X}, \\
 e_u(\mathbf{X}, u) u^\delta &= - \int_0^{(\cdot)} a_u(\mathbf{X}(s), u(s), s) u^\delta(s) \, ds \\
 & - \int_0^{(\cdot)} b_u(\mathbf{X}(s), u(s), s) u^\delta(s) \, d\mathbf{B}(s) && \text{for } u^\delta \in \mathcal{U},
 \end{aligned}$$

respectively, where we have used the notation introduced in Remark 6.1.

Proof The claim follows by similar arguments as the proofs of Lemmas 6.3.3 and 6.3.4 in [25]. In fact, by Assumption 5.1-2) it holds that the coefficients a and b of the SDE are continuously Fréchet differentiable. Now let $\mathbf{X}^\delta \in \mathcal{X}$ and apply Taylor’s formula to a and b with respect to \mathbf{X}

$$a(\mathbf{X}(t) + \mathbf{X}^\delta(t), u(t), t) = a(\mathbf{X}(t), u(t), t) + a_x(\mathbf{X}(t), u(t), t) \mathbf{X}^\delta(t) + \mathcal{O}(\|\mathbf{X}^\delta(t)\|_{\mathbb{R}^d})$$

and

$$b(\mathbf{X}(t) + \mathbf{X}^\delta(t), u(t), t) = b(\mathbf{X}(t), u(t), t) + b_x(\mathbf{X}(t), u(t), t) \mathbf{X}^\delta(t) + \mathcal{O}(\|\mathbf{X}^\delta(t)\|_{\mathbb{R}^d}).$$

Now, we obtain for e_X as defined in the statement of the theorem

$$\begin{aligned}
 & \|e(\mathbf{X} + \mathbf{X}^\delta, u) - e(\mathbf{X}, u) - e_X(\mathbf{X}, u) \mathbf{X}^\delta\|_{\mathcal{X}}^2 \\
 &= \mathbb{E} \left[\int_0^{(\cdot)} \|a(\mathbf{X}(s) + \mathbf{X}^\delta(s), u(s), s) - a(\mathbf{X}(s), u(s), s) - a_x(\mathbf{X}(s), u(s), s) \mathbf{X}^\delta(s)\|_{\mathbb{R}^d}^2 \, ds \right. \\
 &\quad \left. + \int_0^{(\cdot)} \|b(\mathbf{X}(s) + \mathbf{X}^\delta(s), u(s), s) - b(\mathbf{X}(s), u(s), s) - b_x(\mathbf{X}(s), u(s), s) \mathbf{X}^\delta(s)\|_{\mathbb{F}}^2 \, ds \right] \\
 &= \mathbb{E} \left[\int_0^{(\cdot)} \mathcal{O}(\|\mathbf{X}^\delta(s)\|_{\mathbb{R}^d}^2) \, ds \right] = \mathcal{O}(\|\mathbf{X}^\delta\|_{C([0, T]; L^2(\Omega; \mathbb{R}^d))}^2) = \mathcal{O}(\|\mathbf{X}^\delta\|_{\mathcal{X}}^2),
 \end{aligned}$$

where we have used Lemma 2.2. An analogous result holds for the Fréchet differentiability with respect to u . More precisely, for any $u^\delta \in \mathcal{U}$ with $u + u^\delta \in \mathcal{U}_{\text{ad}}$ it holds that

$$\|e(\mathbf{X}, u + u^\delta) - e(\mathbf{X}, u) - e_u(\mathbf{X}, u) u^\delta\|_{\mathcal{X}} = \mathcal{O}(\|u^\delta\|_{\mathcal{U}}).$$

□

In Proposition 6.5 we will prove that the operator $e_X(\mathbf{X}, u) : \mathcal{X} \rightarrow \mathcal{X}$ has a bounded inverse for $(\mathbf{X}, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$. For that purpose we set for all $x = (x_i) \in \mathbb{R}^d$ and f.a.a.

$t \in [0, T]$

$$\begin{aligned} \mathbf{a}(x, t) &= a_x(\mathbf{X}(\cdot, t), u(t), t)x = \sum_{i=1}^d a_{x_i}(\mathbf{X}(\cdot, t), u(t), t)x_i \in \mathbb{R}^d \quad \text{in } \Omega \text{ a.s.,} \\ \mathbf{b}(x, t) &= b_x(\mathbf{X}(\cdot, t), u(t), t)x = \sum_{i=1}^d b_{x_i}(\mathbf{X}(\cdot, t), u(t), t)x_i \in \mathbb{R}^{d \times m} \quad \text{in } \Omega \text{ a.s.,} \end{aligned} \tag{6.3}$$

where we have used the notation introduced in Remark 6.1 and ‘a.s.’ stands for ‘almost surely’. Note that both $\mathbf{a}(\cdot, t)$ and $\mathbf{b}(\cdot, t)$ are linear mappings on \mathbb{R}^d f.a.a. $t \in [0, T]$ and in Ω a.s. However, due to the dependence on \mathbf{X} the functions \mathbf{a} and \mathbf{b} contain random-valued coefficients. Therefore, we can not utilize Assumption 4.3 together with [57, Theorem 6.14] in the proof of Proposition 6.5 below; cf. Remark 4.4. For that reason we introduce the following hypothesis.

Assumption 6.3 Let $(\mathbf{X}, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$ hold and the mappings \mathbf{a}, \mathbf{b} be given as in (6.3). Suppose that there exists a constant $L_{\mathbf{a}\mathbf{b}} \geq 0$ satisfying

$$\|a_x(\mathbf{X}(t), u(t), t)\|_F \leq L_{\mathbf{a}\mathbf{b}} \quad \text{f.a.a. } t \in [0, T] \text{ and in } \Omega \text{ a.s.,} \tag{6.4a}$$

$$\left(\sum_{i=1}^d \|b_{x_i}(\mathbf{X}(t), u(t), t)\|_F^2 \right)^{1/2} \leq L_{\mathbf{a}\mathbf{b}} \quad \text{f.a.a. } t \in [0, T] \text{ and in } \Omega \text{ a.s.} \tag{6.4b}$$

Further, we suppose that

$$\mathbb{E} \left[\int_0^T \|\mathbf{a}(0, t)\|_{\mathbb{R}^d}^2 + \|\mathbf{b}(0, t)\|_F^2 dt \right] \leq L_{\mathbf{a}\mathbf{b}}^2, \tag{6.5}$$

i.e., $\mathbf{a}(0, \cdot) \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$ and $\mathbf{b}(0, \cdot) \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m})$ hold.

In the next lemma, we prove that Assumption 6.3 implies condition (RC) from [57, p. 49] which is given by (6.5) and (6.6) below. Notice that condition (RC) ensures the existence of a unique solution to linear SDEs with random coefficient functions. This fact will be used in Proposition 6.5 below in an essential manner.

Lemma 6.4 Let $(\mathbf{X}, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$ hold and the mappings \mathbf{a}, \mathbf{b} be given as in (6.3). Suppose that Assumption 6.3 holds true. Then we have

$$\|\mathbf{a}(\varphi(t), t) - \mathbf{a}(\phi(t), t)\|_{\mathbb{R}^d} \leq L_{\mathbf{a}\mathbf{b}} \|\varphi - \phi\|_{C([0, T]; \mathbb{R}^d)} \quad \text{f.a.a. } t \in [0, T] \text{ and in } \Omega \text{ a.s.,} \tag{6.6a}$$

$$\|\mathbf{b}(\varphi(t), t) - \mathbf{b}(\phi(t), t)\|_F \leq L_{\mathbf{a}\mathbf{b}} \|\varphi - \phi\|_{C([0, T]; \mathbb{R}^d)} \quad \text{f.a.a. } t \in [0, T] \text{ and in } \Omega \text{ a.s.,} \tag{6.6b}$$

where φ, ϕ are chosen arbitrarily in $C([0, T]; \mathbb{R}^d)$.

Proof For arbitrarily $\varphi, \phi \in C([0, T]; \mathbb{R}^d)$ and $u \in \mathcal{U}_{\text{ad}}$ we get f.a.a. $t \in [0, T]$ and in Ω a.s.

$$\begin{aligned} \|\alpha(\varphi(t), t) - \alpha(\phi(t), t)\|_{\mathbb{R}^d} &= \|a_x(\mathbf{X}(t), u(t), t)(\varphi(t) - \phi(t))\|_{\mathbb{R}^d} \\ &\leq \|a_x(\mathbf{X}(t), u(t), t)\|_{\mathbb{F}} \|\varphi(t) - \phi(t)\|_{\mathbb{R}^d} \leq \|a_x(\mathbf{X}(t), u(t), t)\|_{\mathbb{F}} \|\varphi - \phi\|_{C([0, T]; \mathbb{R}^d)}, \end{aligned}$$

where \mathbf{X} is any element in \mathcal{X} . Utilizing (6.4a) we infer that (6.6a) is valid. Analogously, we derive f.a.a. $t \in [0, T]$ and in Ω a.s.

$$\begin{aligned} \|\mathbf{b}(\varphi(t), t) - \mathbf{b}(\phi(t), t)\|_{\mathbb{F}} &= \left\| \sum_{i=1}^d b_{x_i}(\mathbf{X}(t), u(t), t)(\varphi_i(t) - \phi_i(t)) \right\|_{\mathbb{F}} \\ &\leq \sum_{i=1}^d \|b_{x_i}(\mathbf{X}(t), u(t), t)\|_{\mathbb{F}} |\varphi_i(t) - \phi_i(t)| \\ &\leq \left(\sum_{i=1}^d \|b_{x_i}(\mathbf{X}(t), u(t), t)\|_{\mathbb{F}}^2 \right)^{1/2} \|\varphi(t) - \phi(t)\|_{\mathbb{R}^d} \\ &\leq \left(\sum_{i=1}^d \|b_{x_i}(\mathbf{X}(t), u(t), t)\|_{\mathbb{F}}^2 \right)^{1/2} \|\varphi - \phi\|_{C([0, T]; \mathbb{R}^d)}, \end{aligned}$$

where again \mathbf{X} is any element in \mathcal{X} . Hence, (6.4b) implies (6.6b). □

Proposition 6.5 *Suppose that Assumptions 5.1 and 6.3 hold, and let $(\mathbf{X}, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$. Then the linear operator $e_{\mathbf{X}}(\mathbf{X}, u) : \mathcal{X} \rightarrow \mathcal{X}$ is bijective and its inverse $e_{\mathbf{X}}(\mathbf{X}, u)^{-1}$ is a bounded operator.*

Proof Suppose that $(\mathbf{X}, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$ and $\mathbf{Y} \in \mathcal{X}$ are given arbitrarily. Then there exist a measurable initial condition \mathbf{Y}_\circ and measurable coefficients $\tilde{\mathbf{a}} \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)$, $\tilde{\mathbf{b}} = [\tilde{\mathbf{b}}_1 | \dots | \tilde{\mathbf{b}}_m] \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m})$ with

$$\mathbf{Y}(t) = \mathbf{Y}_\circ + \int_0^t \tilde{\mathbf{a}}(s) \, ds + \int_0^t \tilde{\mathbf{b}}(s) \, d\mathbf{B}(s) \quad \text{for } t \in [0, T]. \tag{6.7}$$

We have to show that there exists a unique $\mathbf{X}^\delta \in \mathcal{X}$ satisfying

$$e_{\mathbf{X}}(\mathbf{X}, u)\mathbf{X}^\delta = \mathbf{Y} \quad \text{in } \mathcal{X}. \tag{6.8}$$

By Lemma 6.2 and (6.7), equation (6.8) is equivalent to

$$\begin{aligned} \mathbf{X}^\delta(\cdot) - \int_0^{(\cdot)} \underbrace{a_x(\mathbf{X}(s), u(s), s)\mathbf{X}^\delta(s)}_{=: \mathbf{a}(\mathbf{X}^\delta(s), s) \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d)} \, ds - \int_0^{(\cdot)} \underbrace{b_x(\mathbf{X}(s), u(s), s)\mathbf{X}^\delta(s)}_{=: \mathbf{b}(\mathbf{X}^\delta(s), s) \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m})} \, d\mathbf{B}(s) \\ = \mathbf{Y}_\circ + \int_0^t \tilde{\mathbf{a}}(s) \, ds + \int_0^t \tilde{\mathbf{b}}(s) \, d\mathbf{B}(s) \quad \text{for } t \in [0, T]. \end{aligned}$$

We set

$$\begin{aligned} \hat{\mathbf{a}}(\mathbf{X}^\delta(\cdot), \cdot) &= \mathbf{a}(\mathbf{X}^\delta(\cdot), \cdot) + \tilde{\mathbf{a}} \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d), \\ \hat{\mathbf{b}}(\mathbf{X}^\delta(\cdot), \cdot) &= \mathbf{b}(\mathbf{X}^\delta(\cdot), \cdot) + \tilde{\mathbf{b}} \in \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^{d \times m}). \end{aligned} \tag{6.9}$$

Then $\mathbf{X}^\delta \in \mathcal{X}$ is the solution to the linear SDE with random coefficients

$$\begin{cases} d\mathbf{X}^\delta(t) = \hat{\mathbf{a}}(\mathbf{X}^\delta(t), t) dt + \hat{\mathbf{b}}(\mathbf{X}^\delta(t), t) d\mathbf{B}(t) & \text{for } t \in (0, T], \\ \mathbf{X}^\delta(0) = \mathbf{Y}_\circ. \end{cases}$$

Utilizing Assumption 6.3 and Lemma 6.4 it follows from [57, Theorem 6.16] that there exists a unique $\mathbf{X}^\delta \in \mathcal{X}$ satisfying $\mathbf{X}^\delta = e_{\mathcal{X}}(\mathbf{X}, u)^{-1} \mathbf{Y} \in \mathcal{X}$. Thus, $e_{\mathcal{X}}(\mathbf{X}, u)^{-1}$ is bijective. Moreover, we infer from [57, Theorem 6.16] that there is a constant $C > 0$ such that

$$\sup_{t \in [0, T]} \mathbb{E}[\|\mathbf{X}^\delta(t)\|_{\mathbb{R}^d}^2] \leq C(1 + \mathbb{E}[\|\mathbf{Y}_\circ\|_{\mathbb{R}^d}^2]) \tag{6.10}$$

for all $\mathbf{Y} \in \mathcal{X}$. Applying (6.9) and Lemma 6.4 we estimate

$$\begin{aligned} \int_0^T \|\hat{\mathbf{a}}(\mathbf{X}^\delta(t), t)\|_{\mathbb{R}^d}^2 dt &\leq 2 \int_0^T \|\tilde{\mathbf{a}}(t)\|_{\mathbb{R}^d}^2 + \|\mathbf{a}(\mathbf{X}^\delta(t), t)\|_{\mathbb{R}^d}^2 dt \\ &\leq 2 \int_0^T \|\tilde{\mathbf{a}}(t)\|_{\mathbb{R}^d}^2 + 2 \|\mathbf{a}(\mathbf{X}^\delta(t), t) - \mathbf{a}(0, t)\|_{\mathbb{R}^d}^2 + 2 \|\mathbf{a}(0, t)\|_{\mathbb{R}^d}^2 dt \\ &\leq 2 \int_0^T \|\tilde{\mathbf{a}}(t)\|_{\mathbb{R}^d}^2 dt + 4 \int_0^T L_{\mathbf{a}\mathbf{b}}^2 \|\mathbf{X}^\delta(t)\|_{\mathbb{R}^d}^2 + \|\mathbf{a}(0, t)\|_{\mathbb{R}^d}^2 dt \quad \text{in } \Omega \text{ a.s.} \end{aligned}$$

Analogously, we find that

$$\begin{aligned} \int_0^T \|\hat{\mathbf{b}}(\mathbf{X}^\delta(t), t, \cdot)\|_{\mathbb{F}}^2 dt &\leq 2 \int_0^T \|\tilde{\mathbf{b}}(t)\|_{\mathbb{F}}^2 dt \\ &\quad + 4 \int_0^T L_{\mathbf{a}\mathbf{b}}^2 \|\mathbf{X}^\delta(t)\|_{\mathbb{R}^d}^2 + \|\mathbf{b}(0, t)\|_{\mathbb{F}}^2 dt \quad \text{in } \Omega \text{ a.s.} \end{aligned}$$

Let $\mathbf{Y} \in \mathcal{X}$ with $\|\mathbf{Y}\|_{\mathcal{X}} \leq 1$ be chosen arbitrarily. Then, \mathbf{Y} has a representation as in (6.7) so that we have

$$\|\mathbf{Y}\|_{\mathcal{X}}^2 = \mathbb{E}[\|\mathbf{Y}_\circ\|_{\mathbb{R}^d}^2] + \mathbb{E}\left[\int_0^T \|\tilde{\mathbf{a}}(t)\|_{\mathbb{R}^d}^2 + \|\tilde{\mathbf{b}}(t)\|_{\mathbb{F}}^2 dt\right] \leq 1. \tag{6.11}$$

Utilizing Assumption 6.3 as well as equations (6.11) and (6.10) it follows that

$$\|e_{\mathcal{X}}(\mathbf{X}, u)^{-1} \mathbf{Y}\|_{\mathcal{X}}^2 = \|\mathbf{X}^\delta\|_{\mathcal{X}}^2$$

$$\begin{aligned}
 &= \mathbb{E}[\|Y_\circ\|_{\mathbb{R}^d}^2] + \mathbb{E}\left[\int_0^T \|\hat{a}(X^\delta(t), t)\|_{\mathbb{R}^d}^2 + \|\hat{b}(X^\delta(t), t)\|_F^2 dt\right] \\
 &\leq 2\left(\mathbb{E}[\|Y_\circ\|_{\mathbb{R}^d}^2] + \mathbb{E}\left[\int_0^T \|\tilde{a}(t)\|_{\mathbb{R}^d}^2 + \|\tilde{b}(t)\|_F^2 dt\right]\right) + 8L_{ab}^2 \int_0^T \mathbb{E}[\|X^\delta(t)\|_{\mathbb{R}^d}^2] dt \\
 &\quad + 4\mathbb{E}\left[\int_0^T \|a(0, t)\|_{\mathbb{R}^d}^2 + \|b(0, t)\|_F^2 dt\right] \\
 &\leq 2 + 8L_{ab}^2 T \sup_{t \in [0, T]} \mathbb{E}[\|X^\delta(t)\|_{\mathbb{R}^d}] + 4L_{ab}^2 \leq c_1 + c_2 \left(1 + \mathbb{E}[\|Y_\circ\|_{\mathbb{R}^d}^2]\right) \leq c_1 + 2c_2
 \end{aligned}$$

for constants $c_1 := 2 + 4L_{ab}^2$ and $c_2 := 8L_{ab}^2 TC$ which do not depend on Y . Consequently,

$$\|e_X(X, u)^{-1}\|_{L(\mathcal{X})} = \sup_{\|Y\|_{\mathcal{X}} \leq 1} \|e_X(X, u)^{-1}Y\|_{\mathcal{X}} \leq c_1 + 2c_2,$$

where $L(\mathcal{X})$ denotes the Banach space of all linear and bounded mappings from \mathcal{X} to \mathcal{X} supplied by the usual operator norm. This implies that the bijective mapping $e_X(X, u)^{-1}$ is also bounded. □

Remark 6.6 It follows from Proposition 6.5 that the Fréchet derivative

$$e'(X, u) = (e_X(X, u) | e_u(X, u)) : \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X}$$

is surjective. This implies a constraint qualification which allows us to formulate first-order necessary optimality conditions for (4.3); cf., e.g., [38, p. 243].

6.2 Fréchet Differentiability of the Objective

Next, we turn to the cost functional defined in (4.2); c.f. [25, Lemma 6.3.5].

Lemma 6.7 *Let Assumption 5.1-1) be satisfied. Then the cost functional J is continuously Fréchet differentiable at every $(X, u) \in \mathcal{X} \times \mathcal{U}_{ad}$. Introducing*

$$\begin{aligned}
 g_1(t) &= C'(\mathbb{E}[X(t)])^\top (C(\mathbb{E}[X(t)]) - c^d(t)) \in \mathbb{R}^d \text{ for } t \in [0, T], \\
 g_2 &= C'(\mathbb{E}[X(T)])^\top (C(\mathbb{E}[X(T)]) - c_T^d) \in \mathbb{R}^d
 \end{aligned} \tag{6.12}$$

we have

$$\langle J_X(X, u), X^\delta \rangle_{\mathcal{X}, \mathcal{X}} = \mathbb{E}\left[\int_0^T g_1(t)^\top X^\delta(t) dt\right] + \mathbb{E}[g_2^\top X^\delta(T)] \text{ for all } X^\delta \in \mathcal{X}, \tag{6.13a}$$

$$\langle J_u(X, u), u^\delta \rangle_{\mathcal{U}, \mathcal{U}} = \kappa \int_0^T u(t)^\top u^\delta(t) dt \text{ for all } u^\delta \in \mathcal{U}. \tag{6.13b}$$

Proof Notice that the Jacobian $C'(x)$ belongs to $\mathbb{R}^{\ell \times d}$ for every $x \in \mathbb{R}^d$. Let $(X, u) \in \mathcal{X} \times \mathcal{U}_{\text{ad}}$ be chosen arbitrarily. Then, it follows that

$$\begin{aligned} \langle J_X(X, u), X^\delta \rangle_{\mathcal{X}', \mathcal{X}} &= \int_0^T (C(\mathbb{E}[X(t)]) - c^d(t))^\top C'(\mathbb{E}[X(t)]) \mathbb{E}[X^\delta(t)] dt \\ &\quad + (C(\mathbb{E}[X(T)]) - c_T^d)^\top C'(\mathbb{E}[X(T)]) \mathbb{E}[X^\delta(T)] \\ &= \int_0^T g_1(t)^\top \mathbb{E}[X^\delta(t)] dt + g_2^\top \mathbb{E}[X^\delta(T)] \\ &= \mathbb{E} \left[\int_0^T g_1(t)^\top X^\delta(t) dt \right] + \mathbb{E}[g_2^\top X^\delta(T)] \quad \text{for all } X^\delta \in \mathcal{X}, \end{aligned}$$

which immediately gives (6.13a). The proof of (6.13b) is straightforward. □

6.3 Derivation of the Gradient for the Reduced Cost

In the sequel we follow [27, Section 1.6.2] and [25, Section 6.3]. We suppose that Assumptions 5.1 and 6.3 hold. Let $u \in \mathcal{U}_{\text{ad}}$ be given and $X_u = \mathcal{S}(u) \in \mathcal{X}$. Then, $e(\mathcal{S}(u), u) = 0$ is valid in \mathcal{X} . Due to Lemma 6.2, the mapping e is Fréchet differentiable. Thus, we have

$$0 = \frac{d}{du} [e(\mathcal{S}(u), u)] u^\delta = e_X(\mathcal{S}(u), u) \mathcal{S}'(u) u^\delta + e_u(\mathcal{S}(u), u) u^\delta \quad \text{in } \mathcal{X} \tag{6.14}$$

for all $u^\delta \in \mathcal{U}$. From Proposition 6.5 and (6.14), we derive the formula

$$\mathcal{S}'(u) = -e_X(\mathcal{S}(u), u)^{-1} e_u(\mathcal{S}(u), u) \quad \text{in } L(\mathcal{U}, \mathcal{X}'), \tag{6.15}$$

where $L(\mathcal{U}, \mathcal{X}')$ stands for the Banach space of all linear and bounded operators from \mathcal{U} to \mathcal{X} . Furthermore, it follows that

$$\begin{aligned} \langle \hat{J}'(u), u^\delta \rangle_{\mathcal{U}', \mathcal{U}} &= \frac{d}{dt} [J(\mathcal{S}(u), u)] u^\delta = \langle J_X(\mathcal{S}(u), u), \mathcal{S}'(u) u^\delta \rangle_{\mathcal{X}', \mathcal{X}} + \langle J_u(\mathcal{S}(u), u), u^\delta \rangle_{\mathcal{U}', \mathcal{U}} \\ &= \langle \mathcal{S}'(u)^* J_X(\mathcal{S}(u), u) + J_u(\mathcal{S}(u), u), u^\delta \rangle_{\mathcal{U}', \mathcal{U}} \end{aligned}$$

for all $u^\delta \in \mathcal{U}$, which yields directly

$$\hat{J}'(u) = \mathcal{S}'(u)^* J_X(\mathcal{S}(u), u) + J_u(\mathcal{S}(u), u) \quad \text{in } \mathcal{U}'. \tag{6.16}$$

Next, we introduce the Lagrange multiplier $\mathcal{G} \in \mathcal{X}'$ by

$$e_X(\mathcal{S}(u), u)^* \mathcal{G} = -J_X(\mathcal{S}(u), u) \quad \text{in } \mathcal{X}', \tag{6.17}$$

where $e_X(\mathcal{S}(u), u)^* : \mathcal{X}' \rightarrow \mathcal{X}'$ stands for the dual of $e_X(\mathcal{S}(u), u) : \mathcal{X} \rightarrow \mathcal{X}$ satisfying

$$\langle e_X(\mathcal{S}(u), u)^* \mathcal{F}, X^\delta \rangle_{\mathcal{X}', \mathcal{X}} = \langle \mathcal{F}, e_X(\mathcal{S}(u), u) X^\delta \rangle_{\mathcal{X}', \mathcal{X}} \quad \text{for all } (\mathcal{F}, X^\delta) \in \mathcal{X}' \times \mathcal{X}.$$

It follows from (6.17) that

$$\mathcal{G} = -e_X(\mathcal{S}(u), u)^{-*} J_X(\mathcal{S}(u), u) \quad \text{in } \mathcal{X}'. \quad (6.18)$$

In (6.18), we denote by $e_X(\mathcal{S}(u), u)^{-*} : \mathcal{X}' \rightarrow \mathcal{X}'$ the inverse of $e_X(\mathcal{S}(u), u)^*$. Moreover, (6.18) is equivalent to

$$\langle \mathcal{G}, \mathbf{X}^\delta \rangle_{\mathcal{X}', \mathcal{X}} = -\langle e_X(\mathcal{S}(u), u)^{-*} J_X(\mathcal{S}(u), u), \mathbf{X}^\delta \rangle_{\mathcal{X}', \mathcal{X}} \quad \text{for all } \mathbf{X}^\delta \in \mathcal{X}. \quad (6.19)$$

Using (6.15) and (6.18) we find that

$$\begin{aligned} \mathcal{S}'(u)^* J_X(\mathcal{S}(u), u) &= \left[-e_X(\mathcal{S}(u), u)^{-1} e_u(\mathcal{S}(u), u) \right]^* J_X(\mathcal{S}(u), u) \\ &= e_u(\mathcal{S}(u), u)^* \left[-e_X(\mathcal{S}(u), u)^{-*} J_X(\mathcal{S}(u), u) \right] \\ &= e_u(\mathcal{S}(u), u)^* \mathcal{G} \quad \text{in } \mathcal{U}', \end{aligned} \quad (6.20)$$

where the operator $e_u(\mathcal{S}(u), u)^*$ maps from \mathcal{X}' to \mathcal{U}' . Inserting the last expression in (6.16) we derive

$$\hat{J}'(u) = \mathcal{S}'(u)^* J_X(\mathcal{S}(u), u) + J_u(\mathcal{S}(u), u) = e_u(\mathcal{S}(u), u)^* \mathcal{G} + J_u(\mathcal{S}(u), u) \quad \text{in } \mathcal{U}'.$$

For arbitrary $\mathbf{X}^\delta \in \mathcal{X}$ let $\mathbf{Y}^\delta = \mathbf{Y}^\delta(\mathbf{X}^\delta) \in \mathcal{X}$ be the unique solution to

$$e_X(\mathcal{S}(u), u) \mathbf{Y}^\delta = \mathbf{X}^\delta \quad \text{in } \mathcal{X}. \quad (6.21)$$

In particular, we have

$$\mathbf{Y}^\delta(t) - \int_0^t a_x(\mathbf{X}(s), u(s), s) \mathbf{Y}^\delta(s) \, ds - \int_0^t b_x(\mathbf{X}(s), u(s), s) \mathbf{Y}^\delta(s) \, d\mathbf{B}(s) = \mathbf{X}^\delta(t) \quad (6.22)$$

for all $t \in [0, T]$, where we have applied the notation introduced in Remark 6.1. Then, we infer from (6.19) that

$$\begin{aligned} \langle \mathcal{G}, \mathbf{X}^\delta \rangle_{\mathcal{X}', \mathcal{X}} &= -\langle e_X(\mathcal{S}(u), u)^{-*} J_X(\mathcal{S}(u), u), e_X(\mathcal{S}(u), u) \mathbf{Y}^\delta \rangle_{\mathcal{X}', \mathcal{X}} \\ &= -\langle J_X(\mathcal{S}(u), u), \mathbf{Y}^\delta \rangle_{\mathcal{X}', \mathcal{X}} \quad \text{for all } \mathbf{X}^\delta \in \mathcal{X} \end{aligned} \quad (6.23)$$

and for the associated $\mathbf{Y}^\delta \in \mathcal{X}$ solving (6.21). Now we study the specific problem introduced in Example 4.2. Using (6.13a) we have

$$\langle \mathcal{G}, \mathbf{X}^\delta \rangle_{\mathcal{X}', \mathcal{X}} = \mathbb{E} \left[\int_0^T \mathbf{g}_1(t)^\top \mathbf{Y}^\delta(t) \, dt \right] + \mathbb{E}[\mathbf{g}_2^\top \mathbf{Y}^\delta(T)] \quad (6.24)$$

with \mathbf{g}_1 and \mathbf{g}_2 from (6.12).

In the following, we want to represent the functional $\mathcal{G} \in \mathcal{X}'$ in the form $\mathcal{G} = \ell_{\Lambda}$ (see Lemma 2.2) with a suitably chosen $\Lambda \in \mathcal{X}$. Slightly changing the notation, we write $\Lambda = \Phi(\Lambda_o, -A, Z)$ with $(\Lambda_o, -A, Z) \in \mathbb{X}$ (see (2.5)), and get

$$\ell_{\Lambda}(X^{\delta}) = \mathbb{E} \left[X^{\delta}(T)^{\top} \Lambda(T) + \int_0^T X^{\delta}(t)^{\top} A(t) dt \right] = \langle (X_o, a, b), (\Lambda_o, \Lambda, Z) \rangle_{\mathbb{X}} \tag{6.25}$$

for $X^{\delta} = \Phi(X_o, a, b)$, where the second equality follows from Lemma 2.2. Note that this can be seen as a Riesz representation in the space \mathbb{X} . Let $Y^{\delta} = \Phi(Y_o, \tilde{a}, \tilde{b})$. From (6.22), we know that we have

$$X^{\delta} = Y^{\delta} - \Phi(0, a_x Y^{\delta}, b_x Y^{\delta}), \tag{6.26}$$

where we abbreviated $a_x = a_x(X(\cdot), u(\cdot), \cdot)$ and $b_x = b_x(X(\cdot), u(\cdot), \cdot)$. Recall that $b(X, u, \cdot) = (b_1(X, u, \cdot) | \dots | b_m(X, u, \cdot))$ and $Z = (Z_1 | \dots | Z_m)$. Therefore, the Frobenius inner product, defined in (2.3), of $b_x Y^{\delta}$ and Z is given by

$$\langle b_x Y^{\delta}, Z \rangle_F = \sum_{j=1}^m (b_{jx} Y^{\delta})^{\top} Z_j = (Y^{\delta})^{\top} \left(\sum_{j=1}^m b_{jx}^{\top} Z_j \right). \tag{6.27}$$

With (6.25)–(6.27), we obtain

$$\begin{aligned} \ell_{\Lambda}(X^{\delta}) &= \ell_{\Lambda}(Y^{\delta}) - \langle (0, a_x Y^{\delta}, b_x Y^{\delta}), (\Lambda_o, \Lambda, Z) \rangle_{\mathbb{X}} \\ &= \mathbb{E} \left[\int_0^T Y^{\delta}(t)^{\top} (A(t) - a_x(X(t), u(t), t)^{\top} \Lambda(t) - \sum_{j=1}^m b_{jx}(X(t), u(t), t)^{\top} Z_j(t)) dt \right] \\ &\quad + \mathbb{E}[Y^{\delta}(T)^{\top} \Lambda(T)]. \end{aligned}$$

Comparing this with (6.24), we see that the representation $\langle \mathcal{G}, X^{\delta} \rangle_{\mathcal{X}', \mathcal{X}} = \ell_{\Lambda}(X^{\delta})$ holds for all $X^{\delta} \in \mathcal{X}$ if

$$\begin{aligned} \mathbb{E} \left[\int_0^T Y^{\delta}(t)^{\top} (A(t) - a_x(X(t), u(t), t)^{\top} \Lambda(t) - \sum_{j=1}^m b_{jx}(X(t), u(t), t)^{\top} Z_j(t) - g_1(t)) dt \right] \\ + \mathbb{E}[Y^{\delta}(T)^{\top} (\Lambda(T) - g_2)] = 0 \end{aligned}$$

which yields

$$A(\cdot) = a_x(X(\cdot), u(\cdot), \cdot)^{\top} \Lambda(\cdot) + \sum_{j=1}^m b_{jx}(X(\cdot), u(\cdot), \cdot)^{\top} Z_j(\cdot) + g_1(\cdot) \quad \text{in } \mathbb{L}_{\mathcal{F}}^2(\mathbb{R}^d),$$

$$\Lambda(T) = g_2.$$

As $\Lambda = \Phi(\Lambda_\circ, -A, Z)$, we see that Λ satisfies the following (linear) BSDE (cf., e.g., [39]):

$$\begin{cases} d\Lambda(t) = -\left(\mathbf{g}_1(t) + a_x(\mathbf{X}(t), u(t), t)^\top \Lambda(t) + \sum_{j=1}^m b_{jx}(\mathbf{X}(t), u(t), t)^\top \mathbf{Z}_j(t)\right) dt \\ \quad + \mathbf{Z}(t) d\mathbf{B}(t) \quad \text{for all } t \in [0, T), \\ \Lambda(T) = \mathbf{g}_2. \end{cases} \tag{6.28a}$$

Moreover, if the solution pair (Λ, Z) to (6.28a) is computed, then

$$\Lambda_\circ = \Lambda(0) \tag{6.28b}$$

holds. Now we turn to the representation of the gradient $\nabla \hat{J}(u) \in \mathcal{U}$ of the reduced cost functional \hat{J} at a given admissible control $u \in \mathcal{U}_{\text{ad}}$. Recall that

$$\langle \nabla \hat{J}(u), u^\delta \rangle_{\mathcal{U}} = \langle \hat{J}'(u), u^\delta \rangle_{\mathcal{U}', \mathcal{U}} \quad \text{for all } u^\delta \in \mathcal{U}$$

holds, i.e., the gradient $\nabla \hat{J}(u) \in \mathcal{U}$ is the Riesz representant of $\hat{J}'(u) \in \mathcal{U}'$. Utilizing (6.20) and $\mathcal{G} = \ell_\Lambda$, we find

$$\begin{aligned} \langle \mathcal{S}'(u)^* J_X(\mathcal{S}(u), u), u^\delta \rangle_{\mathcal{U}', \mathcal{U}} &= \langle e_u(\mathcal{S}(u), u)^* \mathcal{G}, u^\delta \rangle_{\mathcal{U}', \mathcal{U}} = \langle \mathcal{G}, e_u(\mathcal{S}(u), u) u^\delta \rangle_{\mathcal{X}', \mathcal{X}} \\ &= \ell_\Lambda(e_u(\mathcal{S}(u), u) u^\delta). \end{aligned}$$

By Lemma 6.2, we know that $e_u(\mathcal{S}(u), u) u^\delta = \Phi(0, \tilde{\alpha}, \tilde{\mathbf{b}}) \in \mathcal{X}$ with

$$\tilde{\alpha}(t) := -a_u(\mathbf{X}(t), u(t), t) u^\delta(t), \quad \tilde{\mathbf{b}}(t) := -b_u(\mathbf{X}(t), u(t), t) u^\delta(t), \quad t \in (0, T).$$

From this and Lemma 2.2-2), we obtain

$$\begin{aligned} \langle \mathcal{S}'(u)^* J_X(\mathcal{S}(u), u), u^\delta \rangle_{\mathcal{U}', \mathcal{U}} &= \ell_\Lambda(\Phi(0, \tilde{\alpha}, \tilde{\mathbf{b}})) = \langle (0, \tilde{\alpha}, \tilde{\mathbf{b}}), (\Lambda_\circ, \Lambda, \mathbf{Z}) \rangle_{\mathbb{X}} \\ &= \langle \tilde{\alpha}, \Lambda \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)} + \langle \tilde{\mathbf{b}}, \mathbf{Z} \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^{d \times m})}. \end{aligned} \tag{6.29}$$

Noting that the control u is deterministic, we rewrite the first term on the right-hand side as

$$\begin{aligned} \langle \tilde{\alpha}, \Lambda \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)} &= \langle -a_u(\mathbf{X}(\cdot), u(\cdot), \cdot) u^\delta, \Lambda \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^d)} = \langle u^\delta, -a_u(\mathbf{X}(\cdot), u(\cdot), \cdot)^\top \Lambda \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^r)} \\ &= \mathbb{E} \left[\int_0^T u^\delta(t)^\top (-a_u(\mathbf{X}(t), u(t), t))^\top \Lambda(t) dt \right] \\ &= \int_0^T u^\delta(t)^\top \mathbb{E} \left[(-a_u(\mathbf{X}(t), u(t), t))^\top \Lambda(t) \right] dt \\ &= \left\langle \mathbb{E} \left[-a_u(\mathbf{X}(\cdot), u(\cdot), \cdot)^\top \Lambda \right], u^\delta \right\rangle_{\mathcal{U}}. \end{aligned}$$

In the same way, we obtain for the second term on the right-hand side of (6.29)

$$\begin{aligned} \langle \tilde{\mathbf{b}}, \mathbf{Z} \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^{d \times m})} &= \langle -b_u(\mathbf{X}(\cdot), u(\cdot), \cdot)u^\delta, \mathbf{Z} \rangle_{\mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^{d \times m})} \\ &= \left\langle \mathbb{E} \left[- \sum_{j=1}^m b_{ju}(\mathbf{X}(\cdot), u(\cdot), \cdot)^\top \mathbf{Z}_j \right], u^\delta \right\rangle_{\mathcal{U}}; \end{aligned}$$

cf. (6.27) for the description of the Frobenius inner product. Inserting this into (6.29) and using (6.16) and (6.13b), we see that

$$\begin{aligned} \langle \hat{J}'(u), u^\delta \rangle_{\mathcal{U}, \mathcal{U}} &= \langle \mathcal{S}'(u)^* J_{\mathbf{X}}(\mathcal{S}(u), u) + J_u(\mathcal{S}(u), u), u^\delta \rangle_{\mathcal{U}, \mathcal{U}} \\ &= \left\langle \mathbb{E} \left[- a_u(\mathbf{X}, u, \cdot)^\top \mathbf{\Lambda} - \sum_{j=1}^m b_{ju}(\mathbf{X}, u, \cdot)^\top \mathbf{Z}_j \right] + \kappa u, u^\delta \right\rangle_{\mathcal{U}}. \end{aligned} \tag{6.30}$$

Summarizing, we have proved the following theorem.

Theorem 6.8 *Suppose that Assumptions 5.1 and 6.3 hold. Moreover, the cost functional is given by (4.2) and (6.28) is uniquely solvable. Then, for any $u \in \mathcal{U}_{\text{ad}}$ the gradient of \hat{J} is given as*

$$\nabla \hat{J}(u) = \kappa u - \mathbb{E} \left[a_u(\mathbf{X}(\cdot), u(\cdot), \cdot)^\top \mathbf{\Lambda} + \sum_{j=1}^m b_{ju}(\mathbf{X}(\cdot), u(\cdot), \cdot)^\top \mathbf{Z}_j \right] \in \mathcal{U}, \tag{6.31}$$

where the pair $(\mathbf{\Lambda}, \mathbf{Z}) \in \mathcal{X} \times \mathbb{L}^2_{\mathcal{F}}(\mathbb{R}^{d \times m})$ solves (6.28).

Remark 6.9 Let us compare $\nabla \hat{J}$ for the case $\mathcal{U} = \mathcal{U}^c$ with the gradient $\nabla \hat{J}^h$ (given in (5.20) for the discretized problem. For this case we can write (6.31) as

$$\nabla \hat{J}(u) = \kappa u - \mathbb{E} \left[\int_0^T a_u(\mathbf{X}(t), u, t)^\top \mathbf{\Lambda} + \sum_{j=1}^m b_{ju}(\mathbf{X}(t), u, t)^\top \mathbf{Z}_j dt \right]. \tag{6.32}$$

Recall that the discrete gradient (5.20) is

$$\begin{aligned} \nabla \hat{J}^h(u) &= \kappa u - \mathbb{E}^M \left[\sum_{v=1}^{N-1} a_u(\mathbf{X}_v^\mu, u, t_v)^\top \mathbf{\Lambda}_{v+1}^\mu \Delta t \right] \\ &\quad + \mathbb{E}^M \left[\sum_{v=1}^{N-1} \sum_{j=1}^m b_{ju}(\mathbf{X}_v^\mu, u, t_v)^\top \left(\Delta B_{v,j}^\mu \mathbf{\Lambda}_{v+1}^\mu \right) \right]. \end{aligned}$$

The first difference between (5.20) and (6.32) is that the integral over time in the continuous gradient turns to a sum over the time intervals discrete gradient. This is not surprising. However, we point out that in the discrete case, the coefficient function

a_u and the adjoint variable Λ are not evaluated at the same timestep, but at t_v and t_{v+1} , respectively. The crucial difference is in the last part. In the continuous case, the stochastic variable Z appears that is absent in the discrete gradient. Instead, in the latter case, the (pre-computed) Brownian increments ΔB multiplied with Λ appear. This is consistent with the numerical scheme to solve backward SDEs presented in [23, Section 3.3]. Furthermore, recall that the time increment is incorporated in the Brownian increment. Hence, the discretization factor Δt only appears in the deterministic part.

Our discussion raises the question whether optimization and discretization commute in the sense that the optimize-before-discretize and discretize-before-optimize approaches lead to similar results for sufficiently fine mesh sizes. We are currently investigating this question.

The following result follows directly from Theorem 6.8 and [27, Theorem 1.46].

Corollary 6.10 *Suppose that all assumptions of Theorem 6.8 hold. We assume that $\bar{u} \in \mathcal{U}_{\text{ad}}$ is a local solution to (4.5). Then, first-order necessary optimality conditions are given by the variational inequality*

$$\left\langle \kappa \bar{u} + \mathbb{E} \left[-a_u(\bar{X}, \bar{u}, \cdot)^\top \bar{\Lambda} - \sum_{j=1}^m b_{ju}(\bar{X}, \bar{u}, \cdot)^\top \bar{Z}_j \right], u - \bar{u} \right\rangle_{\mathcal{U}} \geq 0 \text{ for all } u \in \mathcal{U}_{\text{ad}},$$

where $\bar{X} = \mathcal{S}(\bar{u})$ holds and (Λ, Z) solves (6.28) for $(X, u) = (\bar{X}, \bar{u})$.

7 Numerical Experiments

In this section, we explain our optimization strategy. Afterwards, we perform numerical experiments. In the first one, we find an optimal control such that the mean and variance of the governing process follow precisely the prescribed data. The governing process in this case is the well-known mean-reverting Ornstein–Uhlenbeck process. In the second one, we calibrate a model consisting of systems of SDEs by finding optimal parameters. The specific model is the so-called Stochastic Prandtl–Tomlinson (SPT) model that is used to study microrheological processes of viscous fluids.

Let us mention that in both examples our cost functionals are not of the specific form introduced in Example 4.2.

Exploiting the discrete optimality system and using the Euler–Maruyama (EM) scheme [26, 41], we construct a stochastic gradient method that is summarized in Algorithm 1. During the process of solving the model and adjoint SDE, we utilize the parallelization technique of multi-threading in order to speed up the calculations. This is possible since each realization is independent of the other ones. While updating the control, we apply a projection onto \mathcal{U}_{ad} or $\mathcal{U}_{\text{ad}}^c$ utilizing the standard projection operator $\mathcal{P}_{\mathcal{U}_{\text{ad}}}$ that is based on a componentwise projection.

Hence, we apply a stochastic gradient method using fixed batch sizes M^ℓ . Convergence properties can be found in [8]. In our examples, we use with some initial $s_0 > 0$

the stepsize rule

$$s_\ell = s_0/\ell \quad \text{with } \ell \in \mathbb{N} \tag{7.1}$$

for the stochastic gradient method.

Algorithm 1 Stochastic Gradient Method for Stochastic Optimal Control

Require: Initial discrete control guess $u^0 = (u_1^0, \dots, u_r^0)^\top$ in case of $\mathcal{U} = [u_a, u_b]$ (calibration problem) or $U^{h,0} = [u_0^0 | \dots | u_{N-1}^0]$ in case of $\mathcal{U} = L^2(0, T; \mathbb{R}^r)$ (time-dependent controls), tolerance $tol > 0$, maximum iteration depth $\ell_{\max} \in \mathbb{N}$;

- 1: Set $\ell = 0$, initialize $E \gg tol$;
 - 2: **while** $E > tol$ **and** $\ell < \ell_{\max}$ **do**
 - 3: Generate $M^\ell \in \mathbb{N}$ random numbers (call the set of the random numbers $\mathcal{M}^\ell \in \mathbb{N}^{M^\ell}$);
 - 4: Solve the discretized state model using the EM scheme;
 - 5: Solve the associated adjoint model using the EM scheme;
 - 6: Assemble the gradient $\nabla \hat{J}^h(u^\ell)$ and $\nabla \hat{J}^h(U^{h,\ell})$, respectively, of the reduced cost and compute $E = \|\nabla \hat{J}^h(u^\ell)\|_{\mathcal{U}^c}$ and $E = \|\nabla \hat{J}^h(U^{h,\ell})\|_{\mathcal{U}^h}$, respectively;
 - 7: Calculate stepsize s_ℓ using (7.1);
 - 8: Determine a new control $u^{\ell+1}$ and $U^{h,\ell+1}$, respectively, by applying a projected stochastic gradient step;
 - 9: Set $\ell = \ell + 1$;
 - 10: **end while**
 - 11: **return** u^ℓ and $U^{h,\ell}$, respectively.
-

Remark 7.1 The random numbers \mathcal{M}^ℓ in Algorithm 1 change in every optimization iteration, but stay the same within an iteration.

7.1 Time-Dependent Ornstein–Uhlenbeck Process

In the context of (3.4) we have $d = 1, m = 1, r = 2$ and therefore $\mathcal{U} := L^2(0, T; \mathbb{R}^2)$. For a fixed parameter $\theta > 0$, the stochastic process $X(t) \in L^2(\Omega; \mathbb{R})$ solves the linear SDE

$$dX(t) = \theta(u_1(t) - X(t)) dt + u_2(t) dB(t) \text{ for } t \in (0, T], \quad X(0) = X_\circ \tag{7.2}$$

with an initial condition $X_\circ \in L^2(\Omega)$ and the time-dependent coefficients $u = (u_1, u_2) \in \mathcal{U}$. We set

$$a(x, u, t) = \theta(u_1 - x), \quad b(x, u, t) = u_2$$

for $(x, u, t) \in \mathbb{R} \times \mathbb{R}^r \times [0, T]$ and $u = (u_1, u_2)$.

Then, (7.2) can be expressed in the form (3.4). Recall that for $X \in L^2(\Omega)$ the variance is defined as

$$\mathbb{V}[X] := \mathbb{E}[X - \mathbb{E}[X]]^2 = \int_{\Omega} (X - \mathbb{E}[X])^2 d\mathbb{P} = \int_{\Omega} (X(\omega) - \mathbb{E}[X])^2 d\mathbb{P}(\omega).$$

Now we introduce the cost functional as

$$J(X, u) := \frac{1}{2} \|\mathbb{E}[X(\cdot)] - \eta^d(\cdot)\|_{L^2(0,T)}^2 + \frac{1}{2} \|\mathbb{V}[X(\cdot)] - \sigma^d(\cdot)\|_{L^2(0,T)}^2 + \frac{1}{2} |\mathbb{E}[X(T)] - \eta_T^d|^2 + \frac{1}{2} |\mathbb{V}[X(T)] - \sigma_T^d|^2 + \frac{\kappa}{2} \|u\|_{\mathcal{U}}^2 \quad (7.3)$$

with

$$\eta^d(t) = \sin\left(\frac{2\pi t}{T}\right) - 1, \quad \sigma^d(t) = 0.2\left(\cos\left(\frac{2\pi t}{T}\right) + 2\right), \quad \eta_T^d = \eta^d(T), \\ \sigma_T^d = \sigma^d(T)$$

for $t \in [0, T]$. Setting for $t \in [0, T]$ and $X \in \mathcal{X}$

$$j(X) = \frac{1}{2} \|\mathbb{E}[X(\cdot)] - \eta^d\|_{L^2(0,T)}^2 + \frac{1}{2} \|\mathbb{V}[X(\cdot)] - \sigma^d\|_{L^2(0,T)}^2, \\ j_T(X) = \frac{1}{2} \|\mathbb{E}[X(T)] - \eta_T^d\|_{L^2(0,T)}^2 + \frac{1}{2} \|\mathbb{V}[X(T)] - \sigma_T^d\|_{L^2(0,T)}^2$$

the cost (7.3) and our optimization problem can be expressed as (4.1) and (4.3), respectively.

Remark 7.2 (1) Note that the coefficient functions a and b are independent of t and affine linear in x and u . In particular, both coefficients are Lipschitz continuous in x and u . Moreover, a and b are time-independent. Furthermore, (3.3) holds for $u \in \mathcal{U}$. Hence, Assumptions 3.2 and 4.3 are fulfilled.

- (2) For the cost functional it holds that it is continuous as a composition of continuous functions and moreover bounded from below by zero. Furthermore, the parts of the functional only containing the expected value are convex as a composition of non-decreasing functions and a convex function. However, since the variance is not a convex function, the parts with the variance are not convex. Consequently, Assumption 4.1 is only partially satisfied.
- (3) Note that a and b are continuously differentiable and hence Assumption 5.1-2) is fulfilled. Furthermore, $a_x(x, u(t), t) = -\theta$ and $b_x(x, u(t), t) = 0$ hold for $(x, u) \in \mathbb{R} \times \mathcal{U}$ and $t \in [0, T]$. Thus, (6.6) is clearly valid by choosing $L_{ab} = \theta$ and $L_{ab} = 0$, respectively. Thus, Assumption 6.3 is fulfilled.

Utilizing the notation introduced in Sect. 5.3, it turns out that for $\mu = 1, \dots, M$ and $\nu = 0, \dots, N - 1$, the first-order necessary optimality system of the discrete optimization problem is given with $\mu = 1, \dots, M$ by

$$\begin{cases} X_{\nu+1}^\mu = X_\nu^\mu + (\theta(U_{1\nu}^h - X_\nu^\mu)) \Delta t + U_{2\nu}^h \Delta B_\nu^\mu, & \nu = 0, \dots, N - 1 \\ X_0^\mu = X_\circ^\mu, \end{cases} \quad (7.4a)$$

$$\begin{cases} \Lambda_v^\mu = \Lambda_{v+1}^\mu - \theta \Lambda_{v+1}^\mu \Delta t + \Delta t \left(\mathbb{E}^M[X_v^M] - \eta_v^d \right) \\ \quad + 2\Delta t \left(\mathbb{V}^M[X_v^M] - \sigma_v^d \right) \left(X_v^\mu - \mathbb{E}^M[X_v^M] \right), & v = N - 1, \dots, 0, \\ \Lambda_N^\mu = \left(\mathbb{E}^M[X_N^h] - \eta_T^d \right) + 2 \left(\mathbb{V}^M[X_N^h] - \sigma_T^d \right) \left(X_N^\mu - \mathbb{E}^M[X_N^h] \right), \end{cases} \tag{7.4b}$$

$$\nabla \hat{J}_v^h(u) := \kappa u_v - \frac{1}{M} \sum_{\mu=1}^M \left(\begin{pmatrix} \theta \\ 0 \end{pmatrix} \Delta t + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Delta B_v^\mu \right) \Lambda_{v+1}^\mu \quad \text{for } v = 0, \dots, N - 1 \tag{7.4c}$$

with

$$\begin{aligned} X^h &= \{ X_v^\mu \in \mathbb{R} \mid \mu = 1, \dots, M, v = 0, \dots, N \}, \\ U^h &= [u_0 | \dots | u_{N-1}] \in \mathbb{R}^{2 \times N}, \quad u_v = (U_{1v}^h, U_{2v}^h)^\top \in \mathbb{R}^2 \quad (v = 0, \dots, N - 1), \\ \Lambda^h &= \{ \Lambda_v^\mu \in \mathbb{R} \mid \mu = 1, \dots, M, v = 0, \dots, N \}. \end{aligned}$$

In the sequel, we set the regularization parameter to zero, i.e. $\kappa = 0$. Notice that (7.4c) can in this case be written as

$$\nabla \hat{J}_v^h(u) = \mathbb{E}^M \left[\begin{pmatrix} \theta \Delta t \Lambda_{v+1}^M \\ \Delta B_v \Lambda_{v+1}^M \end{pmatrix} \right] = \begin{pmatrix} \theta \Delta t \mathbb{E}^M[\Lambda_{v+1}^M] \\ \mathbb{E}^M[\Delta B_v \Lambda_{v+1}^M] \end{pmatrix}. \tag{7.5}$$

Recall that $\mathbb{E}[\Delta B_{v+1}] = 0$. However, since we used the ΔB_v^μ to derive X_{v+1} and with this Λ_{v+1} , it holds that Λ_{v+1} is not independent of ΔB_v . Therefore, the second component of the gradient in (7.5) is non-zero.

In the next figures, we present the results of our optimization strategy for the Ornstein–Uhlenbeck process (7.2). For this example, we choose the initial condition X_\circ to obey the normal distribution with mean $\eta^d(0)$ and standard deviation $\sigma^d(0)$.

Since (7.2) is a linear SDE, the trajectory of mean and variance can be calculated as (see, e.g., [40, Chapter 3, Theorem 3.2 and Example 5.2])

$$\begin{aligned} \mathbb{E}[X(t)] &= e^{-\theta t} \mathbb{E}[X_\circ] + e^{-\theta t} \theta \int_0^t u_1(s) e^{\theta s} ds, \\ \mathbb{V}[X(t)] &= e^{-2\theta t} \mathbb{V}[X_\circ] + e^{-2\theta t} \int_0^t u_2^2(s) e^{2\theta s} ds. \end{aligned} \tag{7.6}$$

Hence, we can derive the best controls u in the sense that they will lead to a perfect tracking of the desired trajectories of mean and variance:

$$u_1^*(t) = (\eta^d)'(t) \frac{1}{\theta} + \eta^d(t) \quad \text{and} \quad (u_2^*)^2(t) = 2\theta(\sigma^d)(t) + \sqrt{\sigma^d(t)}(\sqrt{\sigma^d})'(t). \tag{7.7}$$

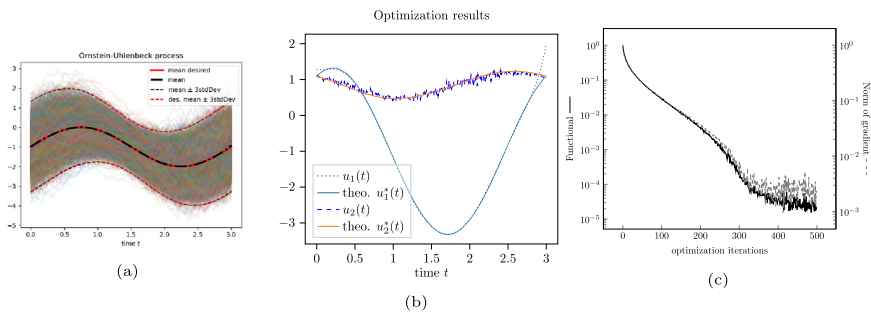


Fig. 1 Results for the example of Sect. 7.1. **a** Trajectories of all trials (grayed out), desired moments (red) calculated moments (black) while applying the control calculated by Algorithm 1; **b** Calculated controls u and u together with controls u_1^* and u_2^* defined in (7.7) for a perfect tracking; **c** Convergence history of relative functional (solid) and Euclidean norm of the relative gradient (dashed) over the optimization iterations (cf. (7.8))

The success of the method given in Algorithm 1 is evident in Fig. 1. The method manages to find controls u_1 and u_2 such that the trajectory of the mean value and the variance of the solution of the model equation follows the desired one. In Fig. 1(a), the trajectories of all M trials are plotted together with the calculated and desired moments. In Fig. 1(b), the control that is calculated with our optimization method is plotted together with the theoretical control ($u_1^*(t), u_2^*(t)$) that leads to a perfect tracking. One obtains a very good agreement for $u_1(t)$. For $u_2(t)$ there is higher noise. However, for more iterations of the stochastic gradient method, the noise gets smaller. Finally, in Fig. 1(c), we plot the convergence history of the (relative) functional and the relative norm of the gradient over the optimization iterations ℓ . and the analogous holds for the relative gradient.

More specifically, the relative functional is given by

$$\hat{J}^h(\mathbf{U}^{h,\ell})/|\hat{J}^h(\mathbf{U}^{h,0})|, \tag{7.8}$$

7.2 Stochastic Prandtl–Tomlinson (SPT) Model

The SPT model is a non-equilibrium bath model in which a tracer particle, also called colloidal, is assumed to be immersed in a suspension of micelles; see, e.g., [29, 30, 43] and the references therein and see [47, 48] for the origins of this models in the deterministic case. In this setting, the internal forces between the particles lead to non-Markovian behavior of the movement of the colloidal due to the memory of the system. The goal is to study the properties of the suspension by tracing the colloidal.

To model the complex fluid, the colloidal particle is investigated with a coupling to one or more bath particles that describe the background. The system of differential equations describing the position of the tracer and K bath particles is given by

$$dX_1(t) = \frac{1}{\gamma_1} \left(-\partial_x V_{\text{ext}}(X_1(t), t) - \sum_{k=2}^{K+1} V'_{\text{int},k}(X_1(t) - X_k(t)) \right) dt + \frac{1}{\gamma_1} dB_1(t),$$

$$dX_k(t) = \frac{1}{\gamma_k} V'_{\text{int},k}(X_1(t) - X_k(t)) + \frac{1}{\gamma_k} dB_k(t) \quad \text{for } k = 2, \dots, K + 1, \tag{7.9}$$

for $t \in (0, T]$, where for $(x, t) \in \mathbb{R} \times [0, T]$

$$V_{\text{ext}}(x, t) = \frac{\kappa_{\text{ext}}}{2} (x - v_0 t)^2 \quad \text{and} \quad V_{\text{int},k}(x) = V_{0,k} \cos\left(\frac{2\pi x}{d_k}\right) \quad \text{for } k = 2, \dots, K + 1.$$

The system (7.9) is completed with the initial condition $X_i(0) = X_{i,o}^{eq}, i = 1, \dots, K + 1$, where $X_{i,o}^{eq} \in L^2(\Omega; \mathbb{R})$ is the equilibrium distribution of the corresponding particle given the external potential $V_{\text{ext}}(X, 0)$. In system (7.9), the variable X_1 denotes the position of the tracer particle and the X_k 's the position of the bath particle $p_k, k = 2, \dots, K + 1$. The $\gamma_i > 0, i = 1, \dots, K + 1$, are the friction coefficients of the corresponding particle and are assumed to be known. The external potential V_{ext} may be applied using optical traps (laser beams) of strength $\kappa_{\text{ext}} > 0$ to realize harmonic potentials. This potential has a trapping effect, which means that the particle cannot leave the potential easily. This trap is then pulled with a constant velocity v_0 through the surrounding medium. The internal forces between the tracer and the bath particles are denoted by $V_{\text{int},k}$ for $k = 2, \dots, K + 1$. The force

$$“\xi_k(t) = \dot{B}_k(t)” \quad \text{for } t \in [0, T] \text{ and } k = 1, \dots, K + 1$$

resembles a random force for which the following mean value relation and fluctuation-dissipation theorem must hold

$$\mathbb{E}[\xi_i(t)] = 0, \quad \mathbb{E}[\xi_i(t)\xi_j(t')] = 2k_B T \gamma_i \delta_{ij} \delta(t - t') \quad \text{for } i, j = 1, \dots, K + 1, \tag{7.10}$$

where $k_B > 0$ is Boltzmann's constant and $T > 0$ the temperature of the bath. The requirements (7.10) are fulfilled by Brownian motion, hence we can apply our setting above.

Remark 7.3 Notice that in [29, 30], the authors did not specify any initial condition within the SPT model (7.9). The reason for this is that the system needs to be in equilibrium. To realize this numerically, we need to integrate over the transient phase in order to generate sensible data that will be used to calculate the simulation data. To generate X_o^{eq} , any initial condition can be used and the model needs to evolve for a certain equilibration time $t_{eq} > 0$. Then, we use the state of the system after t_{eq} as X_o^{eq} . In order to account for a possible high equilibration time, one needs to resort to parallelization techniques such as multi-threading that we use in our simulations.

The goal is to identify the pairs $\{(V_{0,k}, d_k)\}_{k=2}^{K+1} \subset \mathbb{R}^2$ for each bath particle $p_k, k = 2, \dots, K + 1$, within (7.9), such that experimental data is matched as good as possible. For $r = 2K$ we define the parameter vector $u = [u_1, \dots, u_{2K}]^\top \in \mathcal{U}^c := \mathbb{R}^r$ with

$$u_{2k-3} = V_{0,k} \quad \text{and} \quad u_{2k-2} = \frac{1}{d_k} \quad \text{for } k = 2, \dots, K + 1.$$

It follows that

$$\begin{aligned} V_{\text{int},k}(x) &= u_{2k-3} \cos(2\pi u_{2k-2}x) && \text{for } k = 2, \dots, K+1, \\ V'_{\text{int},k}(x) &= -2\pi u_{2k-3} u_{2k-2} \sin(2\pi u_{2k-2}x) && \text{for } k = 2, \dots, K+1. \end{aligned}$$

We suppose that $u_a \in \mathcal{U}^c$ satisfies $u_a > 0$ component-wise in \mathbb{R}^{2K} . Further, the state variable consists of the tracer particle X_1 and the bath particles X_2, \dots, X_{K+1} . Hence, for $d = K + 1$ and $t \in [0, T]$ we define the following state vector

$$X(t) := (X_1(t), \dots, X_d(t))^T \in \mathbb{R}^d.$$

The SDE for X is given by (3.4), where the coefficient functions a and b are given for every $(x, u, t) \in \mathbb{R}^d \times \mathbb{R}^r \times [0, T]$ as

$$\begin{aligned} a_1(x, u, t) &= \frac{1}{\gamma_1} \left(-\partial_x V_{\text{ext}}(x_1, t) - \sum_{k=2}^d V'_{\text{int},k}(x_1 - x_k) \right) \\ &= \frac{1}{\gamma_1} \left(-\kappa_{\text{ext}}(x_1 - v_0 t) + 2\pi \sum_{k=2}^d u_{2k-2} u_{2k-3} \sin(2\pi u_{2k-2}(x_1 - x_k)) \right) \\ a_i(x, u, t) &= \frac{1}{\gamma_i} V'_{\text{int},i}(x_1 - x_i) = -\frac{2\pi}{\gamma_i} u_{2i-2} u_{2i-3} \sin(2\pi u_{2i-2}(x_1 - x_i)) \end{aligned} \quad (7.11a)$$

for $i = 2, \dots, d$ and

$$b_i(x, u, t) = 1/\gamma_i, \quad i = 1, \dots, d. \quad (7.11b)$$

Notice that the b_i 's are constant and therefore independent of (x, u, t) . Moreover, we have that

$$a_x(x, u, t) = ((\partial_{x_j} a_i(x, u, t))) \in \mathbb{R}^{d \times d} \quad (7.12)$$

with

$$\begin{aligned} \partial_{x_1} a_1(x, u, t) &= -\frac{\kappa_{\text{ext}}}{\gamma_1} + \frac{4\pi^2}{\gamma_1} \sum_{k=2}^{K+1} u_{2k-2}^2 u_{2k-3} \cos(2\pi u_{2k-2}(x_1 - x_k)), \\ \partial_{x_j} a_1(x, u, t) &= -\frac{4\pi^2}{\gamma_1} u_{2k-2}^2 u_{2k-3} \cos(2\pi u_{2k-2}(x_1 - x_j)), \quad j = 2, \dots, K+1, \\ \partial_{x_1} a_i(x, u, t) &= -\frac{4\pi^2}{\gamma_i} u_{2i-2}^2 u_{2i-3} \cos(2\pi u_{2i-2}(x_1 - x_i)), \quad i = 2, \dots, K+1, \\ \partial_{x_i} a_i(x, u, t) &= \frac{4\pi^2}{\gamma_i} u_{2i-2}^2 u_{2i-3} \cos(2\pi u_{2i-2}(x_1 - x_i)), \quad i = 2, \dots, K+1. \end{aligned}$$

We also find for

$$a_u(x, u, t) = ((\partial_{u_j} a_i(x, u, t))) \in \mathbb{R}^{d \times r},$$

with the following components. For the right-hand side a_1 corresponding to the tracer particle, we calculate

$$\begin{aligned} \partial_{u_{2k-3}} a_1(x, u, t) &= \frac{2\pi}{\gamma_1} u_{2k-2} \sin(2\pi u_{2k-2}(x_1 - x_k)), \\ \partial_{u_{2k-2}} a_1(x, u, t) &= \frac{2\pi}{\gamma_1} \left(u_{2k-3} \sin(2\pi u_{2k-2}(x_1 - x_k)) \right. \\ &\quad \left. + 2\pi u_{2k-3} u_{2k-2}(x_1 - x_k) \cos(2\pi u_{2k-2}(x_1 - x_k)) \right). \end{aligned} \tag{7.13}$$

For the other right-hand sides $a_i, i = 2, \dots, d$, we calculate

$$\begin{aligned} \partial_{u_{2i-3}} a_i &= -\frac{2\pi}{\gamma_i} u_{2i-2} \sin(2\pi u_{2i-2}(x_1 - x_i)), \\ \partial_{u_{2i-2}} a_i &= -\frac{2\pi}{\gamma_i} \left(u_{2i-3} \sin(2\pi u_{2i-2}(x_1 - x_i)) \right. \\ &\quad \left. + 2\pi u_{2i-2} u_{2i-3}(x_1 - x_i) \sin(2\pi u_{2i-2}(x_1 - x_i)) \right). \end{aligned} \tag{7.14}$$

All other components vanish, i.e. $\partial_{u_j} a_i = 0$ if $i \neq j$ for $j = 1, \dots, d, i = 2, \dots, d$ since the position of each particle depends not on parameters of the other particles. Hence, $\partial_u a(x, u, t)$ has the structure

$$\begin{pmatrix} \partial_{u_1} a_0 & \partial_{u_2} a_0 & \dots & \dots & \dots & \dots & \partial_{u_{2K}} a_0 \\ \partial_{u_1} a_1 & 0 & 0 & \partial_{u_K} a_1 & 0 & \dots & 0 \\ 0 & \ddots & 0 & 0 & \ddots & 0 & \vdots \\ \vdots & 0 & \ddots & 0 & 0 & \ddots & 0 \\ 0 & \dots & 0 & \partial_{u_K} a_K & 0 & 0 & \partial_{u_{2K}} a_{N_p} \end{pmatrix}.$$

Notice that $\partial_u b = 0$ and $\partial_x b = 0$. We define the following continuous problem

$$\min J(\mathbf{X}, u) = \frac{1}{2} \left\| [\mathcal{C}(\mathbf{X})](\cdot) - c^d(\cdot) \right\|_{L^2(0, T)}^2 + \frac{1}{2} \left\| [\mathcal{C}(\mathbf{X})](T) - c^d(T) \right\|_2^2, \tag{7.15a}$$

$$\text{s.t. } (\mathbf{X}, u) \in \mathcal{X} \times \mathbb{R}^{2N_p} \text{ solves (7.9),} \tag{7.15b}$$

where we have set

$$[\mathcal{C}(\mathbf{X})](t) := \frac{\mathbb{E}[Y_1(t)Y_1(0)]}{\mathbb{E}[Y_1^2(t)]} \text{ and } Y_1(t) = X_1(t) - \mathbb{E}[X_1(t)], \tag{7.16}$$

The term $[C(X)](t)$ stands for the (normalized) correlation function and is connected to the *mean conditional displacement* that is used in [30]. Notice that it holds for all t that

$$[C(X)](t) = \frac{\text{Cov}(Y_1(t), Y_1(0))}{\mathbb{V}[Y_1(t)]},$$

since $\mathbb{E}[Y_1(t)] = 0$ by the definition of Y_1 .

Remark 7.4 (1) The coefficients functions a and b are given by (7.11). Hence, they consist of functions that are either affine linear in x and u or smooth and bounded and therefore fulfill the Lipschitz property. Moreover, by linearity and boundedness, they also fulfill (3.3). Consequently, Assumption 3.2 holds also for the SPT model.

(2) Also the coefficients functions a and b are continuously differentiable functions as a composition of smooth functions. Their first partial derivatives are given by (7.13), (7.14), (7.2). Furthermore, the derivatives are bounded in X due to the boundedness of the sin function and bounded in u due to our assumptions on \mathcal{U}_{ad} . Thus, Assumption 5.1-2) and Assumption 6.3 are fulfilled.

(3) We do not have the convexity of \mathcal{C} since it contains the variance. But assuming that the variance of X_u is not vanishing, we have continuous differentiability of the functional as a composition of continuous differentiable functions and hence that Assumption 5.1-1) is fulfilled. Furthermore, the functional is also bounded from below by zero, since it consists of norms. Consequently, Assumption 4.1 is only partially satisfied.

Now, we formulate the discretized model and the discretized adjoint model to the problem (7.15). For this, we define the discrete version of \mathcal{C} as follows:

$$c_v^M(X^h) := \frac{\mathbb{E}^M[Y_{1,v}^h Y_{1,0}^h]}{\mathbb{E}^M[(Y_{1,v}^h)^2]} \quad \text{for } v = 1, \dots, N \text{ and } Y_{1,v}^h = X_{1,v}^h - \mathbb{E}^M[X_{1,v}^h].$$

Recall the definition of \mathbb{E}^M in (5.11). Notice that the derivative of the functional with respect to $X_{1,v}^\mu, v \in \{1, \dots, N\}, \mu \in \{1, \dots, M\}$ is given by

$$\begin{aligned} & (c_v^M(X^h) - c_v^d) \left(\frac{1}{M^2} \sum_{\mu'=1}^M (Y_{1,v}^{\mu'})^2 Y_{1,0}^\mu - \frac{1}{M^2} \sum_{\mu'=1}^M (Y_{1,v}^{\mu'} Y_{1,0}^{\mu'}) 2Y_{1,v}^\mu \right) \left(\frac{1}{M} \sum_{\mu'=1}^M (Y_{1,v}^{\mu'})^2 \right)^{-2} \\ &= \frac{1}{M} (c_v^M(X^h) - c_v^d) \mathbb{E}^M[(Y_{1,v}^h)^2] (Y_{1,0}^\mu - 2c_v^M(X^h) Y_{1,v}^\mu) (\mathbb{E}^M[(Y_{1,v}^h)^2])^{-2} \\ &= \frac{1}{M} (c_v^M(X^h) - c_v^d) \frac{Y_{1,0}^\mu - 2c_v^M(X^h) Y_{1,v}^\mu}{\mathbb{E}^M[(Y_{1,v}^h)^2]} \end{aligned}$$

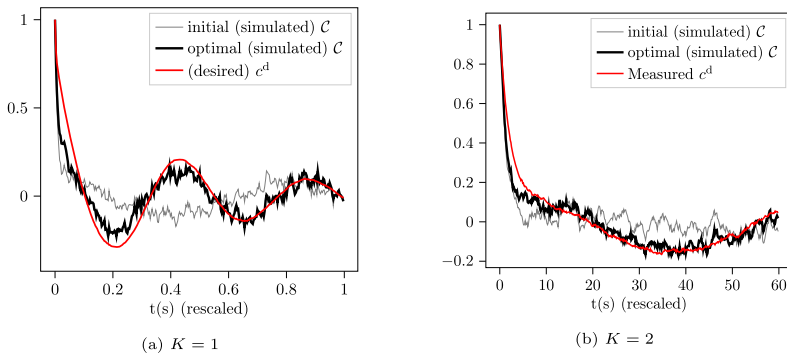


Fig. 2 Results of numerical experiments for (7.15). Simulation of X_u defined in (7.16) using the initial (grey) and optimal (black) guess of parameters for \mathbf{a} $K = 1$ and \mathbf{b} $K = 2$, each time compared with the desired c^d (red)

Thus, we can write the derivative of the functional with respect to the state variable $\mathbf{X}^h = (X_i^h)_{i=1,\dots,d}$ as

$$J_{\mathbf{X}^h}^h(\mathbf{X}_v^\mu) = \begin{cases} \frac{1}{M} (C_v^M(\mathbf{X}^h) - c^d) \frac{Y_{1,0}^\mu - 2C_v^M(\mathbf{X}^h)Y_{1,v}^\mu}{\mathbb{E}^M[(Y_{1,v}^h)^2]} & \text{if } i = 1, \\ 0 & \text{otherwise.} \end{cases} \tag{7.17}$$

We introduce the adjoint variable $\Lambda^h = \{\Lambda_v^\mu\} \in \mathcal{X}^h$. Using (5.19a) and (7.12), we can formulate the discrete adjoint equation that evolves backwards in time for $v = N - 1, \dots, 0$

$$\Lambda_v^\mu = (I + \Delta t a_x^v(\mathbf{X}_v^\mu, u))^\top \Lambda_{v+1}^\mu + \Delta t J_{\mathbf{X}^h}^h(\mathbf{X}_v^\mu) \quad \text{for } \mu = 1, \dots, m \tag{7.18a}$$

with the terminal condition

$$\Lambda_N^\mu = J_{\mathbf{X}^h}^h(\mathbf{X}_N^\mu) \quad \text{for } \mu = 1, \dots, m. \tag{7.18b}$$

Furthermore, the discrete gradient is given by

$$\nabla \hat{J}^h(\mathbf{u}) = \frac{1}{M} \frac{1}{N-1} \sum_{\mu=1}^M \sum_{v=0}^{N-1} (a_u^v(\mathbf{X}_v^\mu, u))^\top \Lambda_{v+1}^\mu. \tag{7.19}$$

For the first numerical experiment using the SPT model, we consider a single bath particle, i.e. we set $K = 1$. In Fig. 2, we present the results. The plot in Fig. 2(a) shows the simulation of (7.9) using the initial guess of the parameters and the simulation using the parameters obtained by Algorithm 1.

For a second test, we consider (7.15) with two bath-particles, i.e. $K = 2$. In this case, we observed that a longer calibration time is needed, also because the equilibration time t_{eq} is longer (cf. Remark 7.3). We plot the results in Fig. 2(b).

It is evident, that our method manages to find optimal parameters in order to match the desired behavior of the model.

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Declarations

Conflict of interest The authors have no relevant financial or non-financial interests to disclose.

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