# Conditional score-based diffusion models for Bayesian inference in infinite dimensions

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## Abstract

Since their first introduction, score-based diffusion models (SDMs) have been successfully applied to solve a variety of linear inverse problems in finite-dimensional vector spaces due to their ability to efficiently approximate the posterior distribution. However, using SDMs for inverse problems in infinite-dimensional function spaces has only been addressed recently and by learning the unconditional score. While this approach has some advantages, depending on the specific inverse problem at hand, in order to sample from the conditional distribution it needs to incorporate the information from the observed data with a proximal optimization step, solving an optimization problem numerous times. This may not be feasible in inverse problems with computationally costly forward operators. To address these limitations, in this work we propose a method to learn the posterior distribution in infinite-dimensional Bayesian linear inverse problems using amortized conditional SDMs. In particular, we prove that the conditional denoising estimator is a consistent estimator of the conditional score in infinite dimensions. We show that the extension of SDMs to the conditional setting requires some care because the conditional score typically blows up for small times contrarily to the unconditional score. We also discuss the robustness of the learned distribution against perturbations of the observations. We conclude by presenting numerical examples that validate our approach and provide additional insights.

# 1 Introduction

Inverse problems seek to estimate unknown parameters using noisy observations or measurements. One of the main challenges is that they are often ill-posed. A problem is ill-posed if there are no solutions, or there are many (two or more) solutions, or the solution is unstable in relation to small errors in the observations [15]. A common approach to transform the original ill-posed problem into a well-posed one is to formulate it as a least-squares optimization problem that minimizes the difference between observed and predicted data. However, minimization of the data misfit alone negatively impacts the quality of the obtained solution due to the presence of noise in the data and the inherent nullspace of the forward operator [3, 18]. Casting the inverse problem into a Bayesian probabilistic framework allows, instead, for a full characterization of all the possible solutions [27, 41, 43]. The Bayesian approach consists of putting a prior probability distribution describing uncertainty in the parameters of interest, and finding the posterior distribution over these parameters [23]. The prior must be chosen appropriately in order to mitigate the ill-posedness of the

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problem and facilitate computation of the posterior. By adopting the Bayesian formulation, rather than finding one single solution to the inverse problem (e.g., the MAP estimator [6]), a distribution of solutions—the posterior—is finally obtained, whose samples are consistent with the observed data. The posterior distribution can then be sampled to extract statistical information that allows for uncertainty quantification [42].

Over the past few years, deep learning-based methods have been successfully applied to analyze linear inverse problems in a Bayesian fashion. In particular, recently introduced score-based diffusion models (SDMs) [39] have become increasingly popular, due to their ability of producing approximating samples from the posterior distribution [20, 40]. An SDM consists of a diffusion process, which gradually perturbs the data distribution toward a tractable distribution according to a prescribed stochastic differential equation (SDE) by progressively injecting Gaussian noise, and a generative model, which entails a denoising process defined by approximating the time-reversal of the diffusion. Crucially, the denoising stage is also a diffusion process [1] whose drift depends on the logarithmic gradients of the noised data densities, i.e. the scores, which are estimated by [39] using a neural network. Among the advantages SDMs have over other deep generative models is that they produce GANs-level sample quality without suffering from training instabilities [10, 14, 39] and are not affected by mode-collapse as normalizing flows [26]. Additionally, and most importantly to the scope of this work, SDMs have demonstrated superior performance in a variety of inverse problems, such as image inpainting [38, 39], image colorization [39], compressing sensing, and medical imaging [19, 40].

In the aforementioned cases, SDMs have been applied by assuming that the data distribution of interest is supported on a finite-dimensional vector space. However, in inverse problems governed by partial differential equations (PDEs) the unknown parameters to be estimated are functions, e.g., coefficient functions, boundary and initial conditions, or source functions. A straightforward solution may be to discretize the infinite-dimensional input and output function spaces into finite-dimensional vectors, and apply SDMs to learn the posterior. However, theoretical studies of current DMs suggest that performance guarantees do not generalize well on increasing dimensions [7, 9, 33]. This is precisely why Stuart's guiding principle to study a Bayesian inverse problem for functions—"avoid discretization until the last possible moment" [41]—is critical to the use of SDMs.

Motivated by Stuart's principle, in this work we define a conditional score in the infinite-dimensional setting, a critical step for studying Bayesian inverse problems directly in function spaces through SDMs. In particular, we show that using this newly defined score as a reverse drift of the diffusion process yields a generative stage that samples, under specified conditions, from the correct target conditional distribution. We carry out the analysis by focusing on two cases: the case of a Gaussian prior measure and the case of a general class of priors given as a density with respect to a Gaussian measure. Studying the model for a Gaussian prior measure provides illuminating insight, not only because it yields an analytic formula of the score, but also because it gives a full characterization of SDMs in the infinite-dimensional setting, showing under which conditions we are sampling from the correct target conditional distribution and how fast the reverse SDE converges to it. It also serves as a guide for the analysis in the case of a general class of prior measures. Finally, we conclude this work by conducting, in Section 6, an experiment which demonstrates the applicability of our SDM, specifically its ability to approximate non-Gaussian multi-modal distributions, a challenging task that poses difficulties for quite many generative models [2].

#### 1.1 Related works

Our work is primarily motivated by Stuart [41]'s comprehensive mathematical theory for studying PDE-governed inverse problems in a Bayesian fashion [41]. In particular, we are interested in the infinite-dimensional analysis [23, 25], which emphasizes the importance of analyzing PDE-governed inverse problems directly in function space before discretization.

Our paper builds upon a rich and ever expanding body of theoretical and applied works dedicated to SDMs. Song et al. [39] defined SDMs integrating both score-based (Hyvärinen and Dayan [17]; Song and Ermon [38]) and diffusion (Sohl-Dickstein et al. [37]; Ho et al. [16]) models into a single continuous-time framework based on stochastic differential equations. The generative stage in SDMs is based on a result from Anderson [1] proving that the denoising process is also a diffusion process whose drift depends on the scores. This result holds only in vector spaces, which explains the difficulties to extend SDMs to function spaces. Initially, there have been attempts to project the input

functions into a finite-dimensional feature space and then apply SDMs (Dupont et al. [11]; Phillips et al. [32]). However, these approaches are not discretization-independent. It is only very recently that SDMs have been directly studied in function spaces, specifically infinite-dimensional Hilbert spaces. Kerrigan et al. [21] generalized diffusion models to operate directly in function spaces, but they did not consider the time-continuous limit based on SDEs (Song et al. [39]). Lim et al. [29] generalized score matching for trace-class noise corruptions that live in the Hilbert space of the data. However, as Kerrigan et al. [21], they did not investigate the connection to the forward and backward SDEs as Song et al. [39] did in finite dimensions. Two recent works, Pidstrigach et al. [33] and Franzese et al. [13], finally established such connection. In particular, Franzese et al. [13] used results from infinite-dimensional SDEs theory (Föllmer and Wakolbinger [12]; Millet et al. [31]) close to Anderson [1].

Among the mentioned works, Pidstrigach et al. [33] is the closest to ours. We adopt their formalism to establish theoretical guarantees for sampling from the conditional distribution. Another crucial contribution comes from Batzolis et al. [5], as we build upon their proof to show that the score can be estimated by using a conditional denoising score matching objective [44, 38]. A key element in Pidstrigach et al. [33], emphasized also in our analysis, is to obtain an estimate on the expected square norm of the score that needs to be uniform in time. We explicitly compute the expected square norm of the conditional score in the case of a Gaussian prior measure, which shows that a uniform in time estimate is not always true for the conditional score. We provide a set of conditions to be satisfied to ensure a uniform in time estimate for a general class of prior measures. Pidstrigach et al. [33] also proposed a way to perform conditional sampling, building upon the one introduced by Song et al. [40] in a finite-dimensional setting. Their algorithm incorporates the observed data into the unconditional sampling process via a proximal optimization step to generate intermediate samples that are consistent with the measuring acquisition process. In this way, Pidstrigach et al. [33] avoided defining the conditional score. While successful, their method is primarily heuristic. Furthermore, its computational efficiency depends on the specific inverse problem at hand-the algorithm solves an optimization problem at each time step of the diffusion process, for each sampling procedure. In contrast, we can prove, under a set of conditions, that our method samples from the target conditional distribution, and does so by learning an *amortized* version of the conditional score. This addresses a critical gap in the existing literature, as the other approach using infinite-dimensional SDMs focuses on data-specific inference. Amortized methods can be a preferred option in Bayesian inverse problems [4, 22, 24, 34–36], as they reduce inference computational costs by incurring an offline initial training cost for a deep neural network that is capable of approximating the posterior distribution for unseen observed data, provided that we have access to a set of data pairs that adequately represent the underlying joint distribution.

## **1.2 Main contributions**

The main contribution of this work is the analysis of conditional SDMs in infinite-dimensional Hilbert spaces. More specifically,

1) We introduce the conditional score in an infinite-dimensional setting (Section 3).

2) We provide a comprehensive analysis of the forward-reverse conditional SDE framework in the case of a Gaussian prior measure. We explicitly compute the expected square norm of the conditional score, which shows that a uniform in time estimate is not always true for the conditional score. We prove that as long as we start from the invariant distribution of the diffusion process, the reverse SDE converges to the target distribution exponentially fast (Section 4).

3) We provide a set of conditions to be satisfied to ensure a uniform in time estimate for a general class of prior measures. Under these conditions, the conditional score—used as a reverse drift of the diffusion process in SDMs—yields a generative stage that samples from the correct target conditional distribution (Section 5).

4) We prove that the conditional score can be estimated via a conditional denoising score matching objective in infinite dimensions (Section 5).

# 2 Background

Here, we review the definition of unconditional score-based diffusion models (SDMs) in infinitedimensional Hilbert spaces proposed by Pidstrigach et al. [33], as we will adopt the same formalism to define SDMs for conditional settings. We refer to Appendix A for a brief introduction to key tools of probability theory in function spaces.

Let  $\mu_{\text{data}}$  be the target measure, supported on a separable Hilbert space  $(H, \langle \cdot, \cdot \rangle)$ . Consider a forward infinite-dimensional diffusion process  $\{X_t\}_{t=0}^{t=T}$  for continuous time variable  $t \in [0, T]$ , where  $X_0$  is the starting variable and  $X_t$  its perturbation at time t. The diffusion process is defined by the following SDE:

$$dX_t = -\frac{1}{2}X_t dt + \sqrt{C}dW_t,\tag{1}$$

where C is a fixed trace class, positive-definite, symmetric covariance operator from  $C : H \to H$  and  $W_t$  is a Wiener process on H. Here and throughout the paper, the initial conditions and the driving Wiener processes in (1) are assumed independent.

The forward SDE evolves  $X_0 \sim \mu_0$  towards the Gaussian measure  $\mathcal{N}(0, C)$  as  $t \to \infty$ . The goal of score-based diffusion models is to convert the SDE in (1) to a generative model by first sampling  $X_T \sim \mathcal{N}(0, C)$ , and then running the correspondent reverse-time SDE. In the finite-dimensional case, Song et al. [39] show that the reverse-time SDE requires the knowledge of the score function  $\nabla \log p_t(X_t)$ , where  $p_t(X_t)$  is the density of the marginal distributions of  $X_t$  (from now on denoted  $\mathbb{P}_t$ ) with respect to the Lebesgue measure. In infinite-dimensional Hilbert spaces, there is no natural analogue of the Lebesgue measure (for additional details, see [8]) and the density is thus no longer well defined. However, Pidstrigach et al. [33, Lemma 1] notice that, in the finite-dimensional setting where  $H = \mathbb{R}^D$ , the score can be expressed as follows:

$$C\nabla_H \log p_t(x) = -(1 - e^{-t})^{-1} \left( x - e^{-t/2} \mathbb{E}[X_0 | X_t = x] \right),$$
(2)

for t > 0. Since the right-hand side of the expression above is also well-defined in infinite dimensions, Pidstrigach et al. [33] formally define the score as follows:

**Definition 1.** In the infinite-dimensional setting, the score or reverse drift is defined by

$$S(t,x) := -(1-e^{-t})^{-1} \left( x - e^{-t/2} \mathbb{E}[X_0 | X_t = x] \right).$$
(3)

Assuming that the expected square norm of the score is uniformly bounded in time, Pidstrigach et al. [33, Theorem 1] shows that the following SDE

$$dZ_t = \frac{1}{2}Z_t dt + S(T - t, Z_t) dt + \sqrt{C} dW_t, \qquad Z_0 \sim \mathbb{P}_T,$$
(4)

is the time-reversal of (1) and the distribution of  $Z_T$  is thus equal to  $\mu_0$ , proving that the forwardreverse SDE framework of Song et al. [39] generalizes to the infinite-dimensional setting. The reverse SDE requires the knowledge of this newly defined score, and one approach for estimating it is, similarly to [39], by using the denoising score matching loss [44]

$$\mathbb{E}\left[\left\|\widetilde{S}(t,X_t) + (1-e^{-t})^{-1}(X_t - e^{-t/2}X_0)\right\|^2\right],\tag{5}$$

where  $\widetilde{S}(t, X_t)$  is typically approximated by training a neural network.

## **3** The conditional score in infinite dimensions

Analogous to the score function relative to the unconditional SDM in infinite dimensions, we now define the score corresponding to the reverse drift of an SDE when conditioned on observations. We consider a setting where  $X_0$  is an *H*-valued random variable and *H* is an infinite-dimensional Hilbert space. Denote by

$$Y = AX_0 + B \tag{6}$$

a noisy observation given by n linear measurements, where the measurement acquisition process is represented by a linear operator  $A : H \to \mathbb{R}^n$ , and  $B \sim \mathcal{N}(0, C_B)$  represents the noise, with  $C_B$  a  $n \times n$  nonnegative matrix. Within a Bayesian probabilistic framework, solving (6) amounts to putting an appropriately chosen prior probability distribution  $\mu_0$  on  $X_0$ , and sampling from the conditional distribution of  $X_0$  given Y = y.

To the best of our knowledge, the only existing algorithm which performs conditional sampling using infinite-dimensional diffusion models on Hilbert spaces is based on the work of Song et al. [40].

The idea, adapted to infinite dimensions by Pidstrigach et al. [33], is to incorporate the observations into the unconditional sampling process of the SDM via a proximal optimization step to generate intermediate samples that are consistent with the measuring acquisition process.

Our method relies instead on utilizing the score of infinite-dimensional SDMs conditioned on observed *data*, which we introduce in this work. We begin by defining the conditional score, by first noticing that, in finite dimensions, we have the following lemma:

**Lemma 1.** In the finite-dimensional setting where  $H = \mathbb{R}^D$ , we can express the conditional score function as

$$C\nabla_x \log p_t(x|y) = -(1 - e^{-t})^{-1} \left( x - e^{-t/2} \mathbb{E} \left[ X_0 | Y = y, X_t = x \right] \right), \tag{7}$$

for t > 0.

Since the right-hand side of (7) is well-defined in infinite dimensions, by following the same line of thought of Pidstrigach et al. [33] we formally define the score as follows:

**Definition 2.** In the infinite-dimensional setting, the conditional score is defined by

$$S(t, x, y) = -(1 - e^{-t})^{-1} \left( x - e^{-t/2} \mathbb{E} \left[ X_0 | Y = y, X_t = x \right] \right).$$
(8)

**Remark 1.** It is possible to define the conditional score in infinite-dimensional Hilbert spaces by resorting to the results of [12, 31], see Appendix C.1.

For Definition 2 to make sense, we need to show that if we use (8) as the drift of the time-reversal of the SDE in (1) conditioned on y, then it will sample the correct conditional distribution of  $X_0$  given Y = y in infinite dimensions. In the next sections, we will carry out the analysis by focusing on two cases: the case of a Gaussian prior measure  $\mathcal{N}(0, C_{\mu})$ , and the case where the prior of  $X_0$  is given as a density with respect to a Gaussian measure, i.e.,

$$X_0 \sim \mu_0, \qquad \frac{d\mu_0}{d\mu}(x_0) = \frac{e^{-\Phi(x_0)}}{\mathbb{E}_{\mu}[e^{-\Phi(X_0)}]}, \qquad \mu = \mathcal{N}(0, C_{\mu}), \tag{9}$$

where  $C_{\mu}$  is positive and trace class and  $\Phi$  is bounded with  $\mathbb{E}_{\mu}[\|C_{\mu}\nabla_{H}\Phi(X_{0})\|^{2}] < +\infty$ .

# 4 Analysis of the forward-reverse conditional SDE framework for a Gaussian prior measure

We begin our analysis of the forward-reverse conditional SDE framework by examining the case where the prior of  $X_0$  is a Gaussian measure. This case provides illuminating insight, not only because it is possible to get an analytic formula of the score, but also because it offers a full characterization of SDMs in the infinite-dimensional setting, showing under which conditions we are sampling from the correct target conditional distribution and how fast the reverse SDE converges to it. We also show that the conditional score can have a singular behavior at small times when the observations are noiseless, in contrast with the unconditional score under similar hypotheses.

We assume that  $\Phi = 0$  in (9). All distributions in play are Gaussian:

$$X_0 \sim \mathcal{N}(0, C_\mu),\tag{10}$$

$$X_t | X_0 \sim \mathcal{N}(e^{-t/2} X_0, (1 - e^{-t})C), \tag{11}$$

$$X_t | X_0 \sim \mathcal{N}(e^{-t/2} X_0, (1 - e^{-t})C),$$
(11)  
$$X_0 | Y \sim \mathcal{N}(M_o Y, C_o),$$
(12)

$$X_t | Y \sim \mathcal{N} \left( e^{-t/2} M_o Y, e^{-t} C_o + (1 - e^{-t}) C \right), \tag{13}$$

where

$$M_o = C_{\mu}A^*(AC_{\mu}A^* + C_B)^{-1}, \qquad C_o = C_{\mu} - C_{\mu}A^*(AC_{\mu}A^* + C_B)^{-1}AC_{\mu}.$$
 (14)

By Mercer theorem [30], there exist  $(\mu_j)$  and an orthonormal basis  $(v_j)$  in H such that  $\mu_j \ge 0$  and  $C_{\mu}v_j = \mu_j v_j \ \forall j$ . As we have assumed that  $C_{\mu}$  is trace class, we have  $\sum_j \mu_j < +\infty$ . We assume that the functions  $v_i$  are eigenfunctions of C and we denote by  $\lambda_i$  the corresponding eigenvalues.

We assume an observational model corresponding to observing a finite-dimensional subspace of H spanned by  $v_{\eta(1)}, \dots, v_{\eta(n)}$  corresponding to  $g_k = v_{\eta(k)}, \ k = 1, \dots, n$ , where  $g_j \in H$  is such that  $(Af)_j = \langle g_j, f \rangle$ . We denote  $\mathcal{I}^{(n)} = \{\eta(1), \dots, \eta(n)\}$ . We assume moreover  $C_B = \sigma_B^2 I_n$ .

Let  $Z_t$  be the solution of reverse-time SDE:

$$dZ_t = \frac{1}{2}Z_t dt + S(T - t, Z_t, y)dt + \sqrt{C}dW_t, \quad Z_0 \sim X_T | Y = y.$$
(15)

We want to show that the reverse SDE we have just formulated in (15) indeed constitutes a reversal of the stochastic dynamics from the forward SDE in (1) conditioned on y.

To this aim, we will need the following lemma:

**Lemma 2.** We define  $Z^{(j)} = \langle v_j, Z \rangle$ ,  $p^{(j)} = \lambda_j / \mu_j$  for all j. We also define  $y^{(j)} = y_{\eta(j)}$  for  $j \in \mathcal{I}^{(n)}$  and  $y^{(j)} = 0$  otherwise, and  $q^{(j)} = \mu_j / \sigma_B^2$  for  $j \in \mathcal{I}^{(n)}$  and  $q^{(j)} = 0$  otherwise. Then we can write for all j

$$dZ_t^{(j)} = \mu^{(x,j)} (T-t) Z_t^{(j)} dt + \mu^{(y,j)} (T-t) y^{(j)} dt + \sqrt{\lambda_j} dW^{(j)},$$
(16)

with  $W^{(j)}$  independent and identically distributed standard Brownian motions,

$$\mu^{(x,j)}(t) = \frac{1}{2} - \frac{e^t p^{(j)}(1+q^{(j)})}{1+(e^t-1)p^{(j)}(1+q^{(j)})}, \qquad \mu^{(y,j)}(t) = \frac{e^{t/2} p^{(j)} q^{(j)}}{1+(e^t-1)p^{(j)}(1+q^{(j)})}.$$
 (17)

*Proof.* The proof is a Gaussian calculation. It relies on computing  $\langle S, v_j \rangle$ , which yields an analytic formula. See Appendix B.

Lemma 2 enables us to discuss when we are sampling from the correct target conditional distribution  $X_0|Y \sim \mathcal{N}(M_o Y, C_o)$ . We can make a few remarks:

1) In the limit  $T \to \infty$ , we get  $\mu^{(x,j)}(T-t) \to -1/2$  and  $\mu^{(y,j)}(T-t) \to 0$ .

2) If  $j \notin \mathcal{I}^{(n)}$  then we have the same mode dynamics as in the unconditional case. Thus we sample from the correct target distribution if T is large or if we start from  $Z_0^{(j)} \sim \mathcal{N}(0, \Sigma_0^{(j)})$  for  $\Sigma_0^{(j)} = \mu_j e^{-T} + \lambda_j (1 - e^{-T})$ , which is the distribution of  $X_T^{(j)} = \langle X_T, v_j \rangle$  given Y = y. 3) If  $j \in \mathcal{I}^{(n)}$  and we start from  $Z_0^{(j)} \sim \mathcal{N}(\bar{z}_0^{(j)}, \Sigma_0^{(j)})$ , then we find  $Z_T^{(j)} \sim \mathcal{N}(\bar{z}_T^{(j)}, \Sigma_T^{(j)})$  with

$$\Sigma_T^{(j)} = \Sigma_0^{(j)} \left( \frac{e^T}{(1 + (e^T - 1)p^{(j)}(1 + q^{(j)}))^2} \right) + \frac{\mu_j}{1 + q^{(j)}} \left( 1 - \frac{1}{(1 + (e^T - 1)p^{(j)}(1 + q^{j)}))} \right),$$
(18)

$$\bar{z}_T^{(j)} = \frac{\bar{z}_0^{(j)} e^{T/2}}{1 + (e^T - 1)p^{(j)}(1 + q^{(j)})} + \frac{y^{(j)}q^{(j)}}{1 + q^{(j)}} \left(1 - \frac{1}{1 + (e^T - 1)p^{(j)}(1 + q^{(j)})}\right).$$
(19)

The distribution of  $X_0^{(j)} = \langle X_0, v_j \rangle$  given Y = y is  $\mathcal{N}(y^{(j)}q^{(j)}/(1+q^{(j)}), \mu_j/(1+q^{(j)})$ . As  $\bar{z}_T^{(j)} \to y^{(j)}q^{(j)}/(1+q^{(j)})$  and  $\Sigma_T^{(j)} \to \mu_j/(1+q^{(j)})$  as  $T \to +\infty$ , this shows that we sample from the exact target distribution (the one of  $X_0$  given Y = y) for T large. 4) If we start the reverse-time SDE from the correct model

$$\bar{z}_{0}^{(j)} = \frac{e^{-T/2}y^{(j)}q^{(j)}}{1+q^{(j)}}, \qquad \Sigma_{0}^{(j)} = \frac{\mu_{j}e^{-T}}{1+q^{(j)}} + \lambda_{j}(1-e^{-T}),$$
(20)

then indeed  $Z_T^{(j)} \sim \mathcal{N}(y^{(j)}q^{(j)}/(1+q^{(j)}), \mu_j/(1+q^{(j)}))$ . This shows that, for any  $T, Z_T$  has the same distribution as  $X_0$  given Y = y, which is the exact target distribution. We can show similarly that  $Z_{T-t}$  has the same distribution as  $X_t$  given Y = y for any  $t \in [0, T]$ .

5) In the case that  $\sigma_B = 0$  so that we observe the mode values perfectly for  $j \in \mathcal{I}^{(n)}$ , then

$$\mu^{(x,j)}(t) = \frac{1}{2} - \frac{e^t}{e^t - 1}, \qquad \mu^{(y,j)}(t) = \frac{e^{t/2}}{e^t - 1}, \tag{21}$$

and indeed  $\lim_{t\uparrow T} Z_t^{(j)} = y^{(j)}$  a.s. Indeed the  $t^{-1}$  singularity at the origin drives the process to the origin like in the Brownian bridge.

Our analysis shows that, as long as we start from the invariant distribution of the diffusion process, we are able to sample from the correct target conditional distribution and that happens exponentially fast. This proves that the score of Definition (2) is the reverse drift of the SDE in (15). Additionally, the analysis shows that the score is uniformly bounded, except when there is no noise in the observations, blowing up near t = 0.

**Remark 2.** Note that, for  $q^{(j)} = 0$ , we obtain the unconditional model:

$$dZ_t^{(j)} = \mu^{(j)}(T-t)Z_t^{(j)}dt + \sqrt{\lambda_j}dW^{(j)}, \text{ with } \mu^{(j)}(t) = \frac{1}{2} - \frac{e^t p^{(j)}}{1 + (e^t - 1)p^{(j)}}.$$
 (22)

If  $C = C_{\mu}$ , the square expectation of the norm and the Lipschitz constant of the score are uniformly bounded in time:  $\sup_{j,t \in [0,T]} |\mu^{(j)}(t)| = 1/2$ .

**Proposition 1.** The score is  $S(t, x, y) = \sum_{j} S_{G}^{(j)}(t, \langle x, v_{j} \rangle, y^{(j)})v_{j}, \ S_{G}^{(j)}(t, x^{(j)}, y^{(j)}) = (\mu^{(x,j)}(T-t) - 1/2) x^{(j)} + \mu^{(y,j)}(T-t)y^{(j)}$  and it satisfies

$$\mathbb{E}[\|S(t, X_t, y)\|_H^2 | Y = y] = \sum_j \frac{e^t (1 + q^{(j)})}{1 + (e^t - 1)p^{(j)}(1 + q^{(j)})} \frac{\lambda_j^2}{\mu_j}.$$
(23)

Proof. The proof is a Gaussian calculation given in Appendix B.

In the unconditional setting, we have  $\mathbb{E}[\|S(t, X_t)\|_H^2] = \sum_j \frac{e^t}{1 + (e^t - 1)p^{(j)}} \frac{\lambda_j^2}{\mu_j}$  which is equal to  $\sum_j \lambda_j$  when  $C = C_{\mu}$ . It is indeed uniformly bounded in time. In the conditional and noiseless setting ( $\sigma_B = 0$ ), we have  $\mathbb{E}[\|S(t, X_t, y)\|_H^2|Y = y] =$ 

 $\sum_{j \notin \mathcal{I}^{(n)}} \frac{e^t}{1 + (e^t - 1)p^{(j)}} \frac{\lambda_j^2}{\mu_j} + \sum_{j \in \mathcal{I}^{(n)}} \frac{\lambda_j}{1 - e^{-t}}$ , which blows up as 1/t as  $t \to 0$ . This result shows that the extension of the score-based diffusion models to the conditional setting is not trivial.

# 5 Well-posedness for the reverse SDE for a general class of prior measures

We are now ready to consider the case of a general class of prior measures given as a density with respect to a Gaussian measure. The analysis of this case resembles the one of Pidstrigach et al. [33] for the unconditional setting. The main challenge is the singularity of the score for small times, an event that in the Gaussian case was observed in the noiseless setting. We will provide a set of conditions to be satisfied by  $\Phi$  in (9), so that the conditional score is bounded uniformly in time. The existence of this bound is needed to make sense of the forward-reverse conditional SDE, and to prove the accuracy and stability of the conditional sampling.

We start the analysis by recalling that, in the infinite-dimensional case, the conditional score is (8). It is easy to get a first estimate:

$$\mathbb{E}[\|S(t, X_t, y)\|_H^2 | Y = y] \le (1 - e^{-t})^{-1} \mathrm{Tr}(C).$$
(24)

The proof follows from Jensen inequality and the law of total expectation, see Appendix C. Note that (24) is indeed an upper bound of (23) since  $\text{Tr}(C) = \sum_{j} \lambda_{j}$ .

Note that the bound (24) is also valid for the unconditional score  $S(t, x) = -(1 - e^{-t})^{-1}(x - e^{-t/2}\mathbb{E}[X_0|X_t = x])$ . We can observe that the upper bound (24) blows up in the limit of small times. We can make a few comments:

1) The bound (24) is convenient for positive times, but the use of Jensen's inequality results in a very crude bound for small times. As shown in the previous section, we know that there exists a bound (22) for the unconditional score in the Gaussian case that is uniform in time.

2) The singular behavior as 1/t at small time t is, however, not artificial. Such a behavior is needed in order to drive the state to the deterministic initial condition when there are exact observations. This behavior has been exhibited by (21) and (23) in the Gaussian case when  $\sigma_B = 0$ . This indicates that the following assumption (25) is not trivial in the conditional setting.

For Definition 2 to make sense in the more general case where the prior of  $X_0$  is given as a density with respect to a Gaussian measure, we will need to make the following assumption.

**Assumption 1.** For any  $y \in \mathbb{R}^n$ , we have

$$\sup_{t \in [0,T]} \mathbb{E} \left[ \| S(t, X_t, y) \|_H^2 | Y = y \right] < \infty.$$
(25)

We are now ready to state the analogous result to Pidstrigach et al. [33, Theorem 1]. **Proposition 2.** *Under Assumption 1, the solution of the reverse-time SDE* 

$$dZ_t = \frac{1}{2} Z_t dt + S(T - t, Z_t, y) dt + \sqrt{C} dW_t, \qquad Z_0 \sim X_T | Y = y,$$
(26)

satisfies  $Z_T \sim X_0 | Y = y$ .

*Proof.* Given Assumption 1, the proof follows the same steps as the one given in [33] for the unconditional score. See Appendix C for the full proof.  $\Box$ 

Assumption 1 is satisfied under some appropriate conditions. We give in the following proposition one such set of conditions. It shows that it is possible to get an upper bound in (24) that is uniform in time provided some additional conditions are fulfilled.

**Proposition 3.** We assume that the conditional version of  $C_{\mu}$  in (9) and C in (1) have the same basis of eigenfunctions  $(v_j)$  and we define  $X_t^{(j)} = \langle X_t, v_j \rangle$  and  $S^{(j)}(t, x, y) = \langle S(t, x, y), v_j \rangle$  so that in (1)  $S(t, x, y) = \sum_j S^{(j)}(t, x, y)v_j$ . We assume an observational model as described in Section 4 and that the  $p^{(j)}(1+q^{(j)})$  are uniformly bounded with respect to j and that C is of trace class. We make a modified version of assumption in (9) as follows. We assume that 1) the conditional distribution of  $X_0$  given Y = y is absolutely continuous with respect to the Gaussian measure  $\mu$  with a Radon-Nikodym derivative proportional to  $\exp(-\Phi(x_0, y))$ ; 2) we have  $\Phi(x_0, y) = \sum_j \Phi^{(j)}(x_0^{(j)}, y)$ ,  $x_0^{(j)} = \langle x_0, v_j \rangle$ ; 3) for  $\psi^{(j)}(x^{(j)}, y) = \exp(-\Phi^{(j)}(x^{(j)}, y))$  we have

$$\frac{1}{K} \le |\psi^{(j)}(x^{(j)}, y)| \le K, \qquad |\psi^{(j)}(x^{(j)}, y) - \psi^{(j)}(x^{(j)'}, y)| \le L|x^{(j)'} - x^{(j)}|, \qquad (27)$$

where K and L do not depend on j. Then Assumption 1 holds true.

Proof. The proof is given in Appendix C.

To use the new score function of Definition 2 for sampling from the posterior, we need to define a way to estimate it. In other words, we need to define a loss function over which the difference between the true score and a neural network  $s_{\theta}(t, x_t, y)$  is minimized in  $\theta$ . A natural choice for the loss function is

$$\mathbb{E}_{t \sim U(0,T), x_t, y \sim \mathcal{L}(X_t, Y)} \left[ \|S(t, x_t, y) - s_{\theta}(t, x_t, y)\|_H^2 \right],$$
(28)

however it cannot be minimized directly since we do not have access to the ground truth conditional score  $S(t, x_t, y)$ . Therefore, in practice, a different objective has to be used. Batzolis et al. [5] proved that, in finite dimensions, a denoising score matching loss can be used:

$$\mathbb{E}_{t \sim U(0,T), x_0, y \sim \mathcal{L}(X_0,Y), x_t \sim \mathcal{L}(X_t | X_0 = x_0)} \left[ \| C \nabla_{x_t} \ln p(x_t | x_0) - s_{\theta}(t, x_t, y) \|^2 \right].$$
(29)

This expression involves only  $\nabla_{x_t} \log p(x_t|x_0)$  which can be computed analytically from the transition kernel of the forward diffusion process, also in infinite dimensions. In the following proposition, we build on the arguments of Batzolis et al. [5] and provide a proof that the conditional denoising estimator is a consistent estimator of the conditional score in infinite dimensions.

**Proposition 4.** Under Assumption 1, the minimizer in  $\theta$  of

$$\mathbb{E}_{x_0,y\sim\mathcal{L}(X_0,Y),x_t\sim\mathcal{L}(X_t|X_0=x_0)} \left[ \| -(1-e^{-t})^{-1}(x_t-e^{-t/2}x_0) - s_{\theta}(t,x_t,y) \|_H^2 \right]$$
(30)

is the same as the minimizer of

$$\mathbb{E}_{x_t, y \sim \mathcal{L}(X_t, Y)} \left[ \|S(t, x_t, y) - s_\theta(t, x_t, y)\|_H^2 \right].$$
(31)

The same result holds if we add  $t \sim \mathcal{U}(0,T)$  in the expectations.

*Proof.* The proof combines some of the arguments of Batzolis et al. [5] and steps of the proof of Lemma 2 in [33], see Appendix C.  $\Box$ 

**Remark 3.** A statement of robustness can be written as in [33, Theorem 2].

## 6 Numerical experiment

We have presented theoretical results on the amortized learning of infinite-dimensional conditional distributions using SDMs. To put this theory into practice, we propose a stylized example where we learn to sample from a non-Gaussian, multi-modal conditional distribution. Our goal is to showcase the ability of the presented learning framework to capture nontrivial conditional distributions.

To enable learning in function spaces, we parameterize the conditional score  $s_{\theta}(t, x_t, y)$  using discretization-invariant Fourier neural operators [FNOs; 28]. This parameterization enables mapping input triplets  $(t, x_t, y)$  to the score conditioned on y at time t. Once trained—by minimizing the objective function in equation (29) with respect to  $\theta$ —we use the FNO as an approximation to the conditional score to sample new realizations of the conditional distribution by simulating the reverse-time SDE in equation (15). Our implementation is based on Li et al. [28] and includes a fully-connected lifting layer, five Fourier neural layers, and a final layer that maps the lifted domain back to the desired shape of the conditional score. We refer to Appendix D for more information about the architecture.

Inspired by Phillips et al. [32], we use the relation  $y = ax_0^2 + \varepsilon$  with  $\varepsilon \sim \Gamma(1, 2)$  and  $a \sim \mathcal{U}\{-1, 1\}$  evaluated on a uniformly sampled grid of 25 evaluation points in [-3, 3] to create joint training pairs  $x_0, y \sim \mathcal{L}(X_0, Y)$ . We draw  $10^5$  training pairs and train the FNO over 200 epochs with a batchsize of 512 using an initial learning rate of  $10^{-3}$ , decaying to  $5 \times 10^{-4}$  over the epochs with a power-law rate of -1/3. The results are summarized in Figure 1. By juxtaposing the true and predicted conditional samples in the top row we can confirm that we are able to learn this bi-modal, non-Gaussian conditional distribution. We further investigate the accuracy of the learned conditional distribution by comparing two one dimensional problem, we argue our choice of architecture and training framework (cf. equation 29) have the potential to be applied to larger-scale problems.



Figure 1: Conditional sampling verification. Top row illustrates the true function samples from the conditional distribution (left) and samples via the score-based model (right). Bottom row indicates pointwise marginals for two different points.

## 7 Conclusions

This is a foundational paper. Our analysis shows that conditional SDMs can be applied to define a discretization-invariant method that *is able to perform conditional sampling directly on infinite-dimensional Hilbert spaces*. Note that the method we propose in this work is data-driven, with the exception of the data pairs used to learn the score, that are informed by the measurement acquisition process, and uses Fourier neural operators [FNOs; 28] for obtaining (amortized) approximations of the score.

## A Probability measures on infinite-dimensional Hilbert spaces

In this section, we briefly present some fundamental notions related to probability measures on infinite-dimensional spaces, specifically separable Hilbert spaces  $(H, \langle \cdot, \cdot \rangle)$ . There is abundant literature on the subject. For more details we refer to Da Prato [8], Kerrigan et al. [21], Pidstrigach et al. [33], Stuart [41] and references therein.

## A.1 Gaussian measures on Hilbert spaces

**Definition 3.** Let  $(\Omega, \mathcal{F}, \mathbb{P})$  be a probability space. A measurable function  $X : \Omega \to H$  is called a Gaussian random element (GRE) if for any  $h \in H$ , the random variable  $\langle h, X \rangle$  has a scalar Gaussian distribution.

Every GRE X has a mean element  $m \in H$  defined by

$$m = \int_{\Omega} X(\omega) d\mathbb{P}(\omega),$$

and a linear covariance operator  $C: H \to H$  defined by

$$Ch = \int_{\Omega} \langle h, X(\omega) \rangle X(\omega) d\mathbb{P}(\omega) - \langle m, h \rangle m, \quad \forall h \in H.$$

We denote  $X \sim \mathcal{N}(m, C)$  for a GRE in H with mean element m and covariance operator C. It can be shown that the covariance operator of a GRE is trace class, positive-definite and symmetric. Conversely, for any trace class, positive-definite and symmetric linear operator  $C : H \to H$  and every  $m \in H$ , there exists a GRE with  $X \sim \mathcal{N}(m, C)$ . This leads us to the following definition:

**Definition 4.** If X is a GRE, the pushforward of  $\mathbb{P}$  through X, denoted by  $\mathbb{P}_X$ , is called a Gaussian probability measure on H. We will write  $\mathbb{P}_X = \mathcal{N}(m, C)$ .

Let  $X \sim \mathcal{N}(m, C)$ . We can make a few remarks:

1) For any  $h \in H$ , we have  $\langle h, X \rangle \sim \mathcal{N}(\langle h, m \rangle, \langle Ch, h \rangle)$ .

2) *C* is compact. By Mercer theorem [30] there exists  $(\lambda_j)$  and an orthonormal basis of eigenfunctions  $(v_j)$  such that  $\lambda_j \ge 0$  and  $Cv_j = \lambda_j v_j \forall j$ . We consider the infinite-dimensional case in which  $\lambda_j > 0 \forall j$ .

3) Suppose m = 0 (we call the Gaussian measure of X centered). The expected square norm of X is given by

$$\mathbb{E}[\|X\|_{H}^{2}] = \mathbb{E}\left[\sum_{j=1}^{\infty} \langle v_{j}, X \rangle^{2}\right] = \sum_{j=1}^{\infty} \langle Cv_{j}, v_{j} \rangle = \sum_{j=1}^{\infty} \lambda_{j} = \sum_{j=1}^{\infty} \operatorname{Tr}(C),$$

which is finite since C is trace class.

#### A.2 Absolutely continuous measures and the Feldman-Hajek theorem

Here we introduce the notion of absolute continuity for measures.

**Definition 5.** Let  $\mu$  and  $\nu$  be two probability measures on H equipped with its Borel  $\sigma$ -algebra  $\mathcal{B}(H)$ . Measure  $\mu$  is absolutely continuous with respect to  $\nu$  (we write  $\mu \ll \nu$ ) if  $\mu(\Sigma) = 0$  for all  $\Sigma \in \mathcal{B}(H)$  such that  $\nu(\Sigma) = 0$ .

**Definition 6.** If  $\mu \ll \nu$  and  $\nu \ll \mu$  then  $\mu$  and  $\nu$  are said to be equivalent and we write  $\mu \sim \nu$ . If  $\mu$  and  $\nu$  are concentrated on disjoint sets then they are called singular; in this case we write  $\mu \perp \nu$ .

Another notion that will be used throughout the paper is the Radon-Nikodym derivative.

**Theorem 1.** Let  $\mu$  and  $\nu$  be two measures on  $(H, \mathcal{B}(H))$  and  $\nu$  be  $\sigma$ -finite. If  $\mu \ll \nu$ , then there exists a  $\nu$ -measurable function f on H such that

$$\mu(A') = \int_{A'} f d\nu, \quad \forall A' \in \mathcal{B}(H).$$

Furthermore, f is unique  $\nu$ -a.e. and is called the Radon-Nikodym derivative of  $\mu$  with respect to  $\nu$ . It is denoted by  $d\mu/d\nu$ .

#### **Remark 4.** In the paper, we will sometimes refer to f as the density of $\mu$ with respect to $\nu$ .

We are finally able to state the Feldman-Hajek theorem in its general form. **Theorem 2.** *The following statements hold.* 

- 1. Gaussian measures  $\mu = \mathcal{N}(m_1, C_1)$ ,  $\nu = \mathcal{N}(m_2, C_2)$  are either singular or equivalent.
- 2. They are equivalent if and only if the following conditions hold:
  - (i)  $\nu$  and  $\mu$  have the same Cameron-Martin space  $H_0 = C_1^{1/2}(H) = C_2^{1/2}(H)$ .
  - (*ii*)  $m_1 m_2 \in H_0$ .
  - (iii) The operator  $(C_1^{-1/2}C_2^{1/2})(C_1^{-1/2}C_2^{1/2})^* I$  is a Hilbert-Schmidt operator on the closure  $\overline{H_0}$ .
- 3. If  $\mu$  and  $\nu$  are equivalent and  $C_1 = C_2 = C$ , then  $\nu$ -a.s. the Radon-Nikodym derivative  $d\mu/d\nu$  is given by

$$\frac{a\mu}{d\nu}(h) = e^{\Psi(h)},$$
  
where  $\Psi(h) = \langle C^{-1/2}(m_1 - m_2), C^{-1/2}(h - m_2) \rangle - \frac{1}{2} \|C^{-1/2}(m_1 - m_2)\|_H^2 \forall h \in H.$ 

#### A.3 Bayes' theorem for inverse problems

Let H and K be separable Hilbert spaces, equipped with the Borel  $\sigma$ -algebra, and  $A : H \to K$  a measurable mapping. We want to solve the inverse problem of finding X from Y, where

$$Y = A(X) + B$$

and  $B \in K$  denotes the noise. We adopt a Bayesian approach to this problem. We let  $(X, Y) \in H \times K$  be a random variable and compute X|Y. We first specify (X, Y) as follows: 1) Prior:  $X \sim \mu_0$  measure on H.

2) Noise:  $B \sim \eta_0$  measure on K, with B independent from X.

The random variable Y|X is then distributed according to the measure  $\eta_x$ , the translate of  $\eta_0$  by A(X). We assume that  $\eta_x \ll \eta_0$ . Thus for some potential  $\Psi : H \times K \to \mathbb{R}$ ,

$$\frac{d\eta_x}{d\eta_0}(y) = e^{-\Psi(x,y)}$$

The potential  $\Psi(\cdot, y)$  satisfying the above formula is often termed the negative log likelihood of the problem. Now define  $\nu_0$  to be the product measure  $\nu_0 = \mu_0 \times \eta_0$ . We can finally state the following infinite-dimensional analogue of the Bayes' theorem.

**Theorem 3.** Assume that  $\Psi : H \times K \to \mathbb{R}$  is  $\nu_0$ -measurable and define

$$Z(y) = \int e^{-\Psi(x,y)} d\mu_0.$$

Then

$$\frac{d\mu_0(\cdot|Y=y)}{d\mu_0}(x) = \frac{1}{Z(y)}e^{-\Psi(x,y)},$$

where  $\mu_0(\cdot|Y=y)$  is the conditional distribution of X given Y=y.

## **B** Proofs of Section 4

#### **B.1** Proofs of Lemma 2 and Proposition 1

We assume that  $C_{\mu}$  in (9) and C in (1) have the same basis of eigenfunctions  $(v_j)$  and that  $C_{\mu}v_j = \mu_j v_j$ ,  $Cv_j = \lambda_j v_j \forall j$ . We define  $X_t^{(j)} = \langle X_t, v_j \rangle$ ,  $y^{(j)} = \langle y, v_j \rangle$  and  $S^{(j)}(t, x, y) = \langle S(t, x, y), v_j \rangle$  so that in (1)  $S(t, x, y) = \sum_j S^{(j)}(t, x, y)v_j$ . We assume  $j \in \mathcal{I}^{(n)}$  so that we consider a mode corresponding to an observation. We then have

$$dX_t^{(j)} = -\frac{1}{2}X_t^{(j)}dt + \sqrt{\lambda^{(j)}}dW_t^{(j)},$$

with  $W^{(j)}$  standard Brownian motions which are independent for the different modes j. Note also that with  $C_{\mu}$  and C having the same basis of eigenfunctions the system of modes is diagonalized so that the  $X_{i}^{(j)}$  processes are independent with respect to mode j, both for the observed and un-observed modes. Thus we have

$$X_0^{(j)} = \sqrt{\mu_j} \eta_0^{(j)}, \quad Y^{(j)} = X_0^{(j)} + \sigma_B \eta_1^{(j)}, \quad X_t^{(j)} = X_0^{(j)} e^{-t/2} + \sqrt{\lambda_j (1 - e^{-t})} \eta_2^{(j)},$$

for  $\eta_i^{(j)}$  independent standard Gaussian random variables. We then seek

$$x_0^{(j,y)} = \mathbb{E}[X_0^{(j)} \mid X_t = x, Y = y] = \mathbb{E}[X_0^{(j)} \mid X_t^{(j)} = x^{(j)}, Y^{(j)} = y^{(j)}],$$

which in this Gaussian setting is the  $L^2$  projection of  $X_0^{(j)}$  onto  $X_t^{(j)}$  and  $Y^{(j)}$ . Thus we can write  $x_0^{(j,y)} = ax^{(j)} + by^{(j)}$  with (a, b) solving

$$\mathbb{E}[(aX_t^{(j)} + bY^{(j)} - X_0^{(j)})Y^{(j)}] = 0, \quad \mathbb{E}[(aX_t^{(j)} + bY^{(j)} - X_0^{(j)})X_t^{(j)}] = 0,$$

which gives

$$a = \frac{e^{t/2}}{1 + (e^t - 1)p^{(j)}(1 + q^{(j)})}, \qquad b = \frac{p^{(j)}q^{(j)}(e^t - 1)}{1 + (e^t - 1)p^{(j)}(1 + q^{(j)})},$$

for  $p^{(j)} = \lambda_j / \mu_j, q^{(j)} = \mu^{(j)} / \sigma^2$ .

We then get in view of (8)

$$S^{(j)}(t,x,y) = -\left(\frac{e^t p^{(j)}(1+q^{(j)})}{1+(e^t-1)p^{(j)}(1+q^{(j)})}\right)x^{(j)} + \left(\frac{e^{t/2}p^{(j)}q^{(j)}}{1+(e^t-1)p^{(j)}(1+q^{(j)})}\right)y^{(j)}.$$
 (32)

Note that with some abuse of notation we then have

$$S^{(j)}(t, x, y) = S^{(j)}(t, x^{(j)}, y^{(j)}),$$

which is important since then also the time reversed system diagonalizes. We remark that for an unobserved mode we get by a similar, but easier, calculation

$$S^{(j)}(t,x,y) = -\left(\frac{e^t p^{(j)}}{1 + (e^t - 1)p^{(j)}}\right) x^{(j)},$$

which simply corresponds to setting  $\sigma_B = \infty$  in (32).

Consider next  $\mathbb{E}[S^{(j)}(t, x, y)^2]$ . Note first that

$$\begin{split} \mathbb{E}[X_t^{(j)} \mid Y = y] &= \left(\frac{q^{(j)}e^{-t/2}}{1+q^{(j)}}\right)y^{(j)},\\ \operatorname{Var}[X_t^{(j)} \mid Y = y] &= e^{-t}\operatorname{Var}[X_t^{(j)} \mid Y = y] + \lambda_j(1-e^{-t})\\ &= \left(1 + (e^t - 1)p^{(j)}(1+q^{(j)})\right)\left(\frac{\mu_j e^{-t}}{1+q^{(j)}}\right). \end{split}$$

We can then easily check that the score is conditionally centered  $\mathbb{E}[S^{(j)}(t, X_t, Y) | Y = y] = 0$  and we then get

$$\begin{split} \mathbb{E}[(S^{(j)}(t,X_t,Y))^2 \mid Y = y] &= \left(\frac{e^t p^{(j)}(1+q^{(j)})}{1+(e^t-1)p^{(j)}(1+q^{(j)})}\right)^2 \operatorname{Var}[X_t^{(j)} \mid Y = y] \\ &= \frac{e^t \mu_j(p^{(j)})^2(1+q^{(j)})}{1+(e^t-1)p^{(j)}(1+q^{(j)})}, \end{split}$$

which gives Proposition 1 upon summing over the mode index j, where we define  $q^{(j)} = 0$  for the unobserved modes.

# C Proofs of Section 5

#### C.1 Discussion about an alternative approach

The following lemma is a complementary result related to Remark 1. It shows that we can actually derive the expression of the score from the results contained in Millet et al. [31]. The result is powerful, but requires the verification of technical conditions.

Lemma 3. Under the conditions stated in Proposition 3 the score is defined by

$$S(x, y, t) = -(1 - e^{-t})^{-1} \left( x - e^{-t/2} \mathbb{E} \left[ X_0 | X_t = x, Y = y \right] \right)$$
(33)

and the time reversed diffusion takes the form in (15).

Proof. Define

$$X^{(j)} = \langle v_i, X \rangle$$
 for  $Cv_i = \lambda_i v_i$ .

Then

$$dX^{(j)} = -\frac{1}{2}X^{(j)}dt + \sqrt{\lambda_j}dW^{(j)} \text{ for } W^{(j)} = \langle v_j, W \rangle,$$
(34)

and where we assume that C is of trace class. This is then an infinite dimensional system of the type considered in Millet et al. [31]. We proceed to verify some conditions stated in Millet et al. [31]: (i) the coefficients of the system (34) satisfy standard growth and Lipschitz continuity conditions (assumption (H1, H4) satisfied); (ii) the coefficients depend on finitely many coordinates (assumption (H2) satisfied); the system is time independent and diagonal (assumption (H5) satisfied). Moreover define  $\check{x}^{(j)} = (x_1, \cdots, x_{j-1}, x_{j+1}, \cdots)$ , then the law of  $X_t^{(j)}$  given  $\check{X}_t^{(j)}$  has for t > 0 density  $p_t(x^{(j)}|\check{X}_t^{(j)} = \check{x}^{(j)}, Y = y)$  with respect to Lebesgue measure and so that for  $t_0 > 0$  and each j:  $\int_{t_0}^T \mathbb{E}[|\partial_{x^{(j)}} \log(p_t(x^{(j)})|Y = y)dt < \infty$ . Then it follows from Theorems 3.1 and 4.3 in Millet et al. [31] that the time reversed problem is associated with the well-posed martingale problem defined by the coefficients in (15) for the score being:

$$\langle v_j, S(x,y,t) \rangle = \frac{\lambda_j \frac{\partial}{\partial x^j} \left( p_t(x^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, Y = y) \right)}{p_t(x^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, Y = y)},$$

with the convention that the right hand side is null on the set  $\{p_t(x^{(j)}|\check{X}_t^{(j)}=\check{x}^{(j)},Y=y)=0\}$ . It then follows for t>0

$$\begin{split} \langle v_j, S(x, y, t) \rangle \\ &= \int_{\mathbb{R}} d\mu_0(x_0^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, Y = y) \frac{\lambda_j \frac{\partial}{\partial x^j} \left( p_t(x^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, X_0^{(j)} = x_0^{(j)}, Y = y) \right)}{p_t(x^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, Y = y)}. \end{split}$$

We then get

$$\begin{split} \langle v_j, S(x, y, t) \rangle &= -\int_{\mathbb{R}} d\mu_0(x_0^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, Y = y) \\ & \times \left( \frac{x^j - e^{-t/2} x_0^{(j)}}{1 - e^{-t}} \right) \frac{\left( p_t(x^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, X_0^{(j)} = x_0^{(j)}, Y = y) \right)}{p_t(x^{(j)} | \check{X}_t^{(j)} = \check{x}^{(j)}, Y = y)} \\ &= -\int_{\mathbb{R}} d\mu_0(x_0^{(j)} | X_t = x, Y = y) \left( \frac{x^j - e^{-t/2} x_0^{(j)}}{1 - e^{-t}} \right). \end{split}$$

## C.2 A preliminary lemma

The following lemma is the equivalent of [33, Lemma 3]. It is used in the forthcoming proof of Proposition 2.

**Lemma 4.** In the finite-dimensional setting  $x \in \mathbb{R}^D$ , we have for any  $0 \le s \le t \le T$ :

$$\nabla \log p_{t,y}(x_t) = e^{(t-s)/2} \mathbb{E}_y \big[ \nabla \log p_{s,y}(X_s) | X_t = x_t \big],$$

where  $\mathbb{E}_y$  is the expectation with respect to the distribution of  $X_0$  and W given Y = y and  $p_{t,y}$  is the pdf of  $X_t$  under this distribution.

Proof. We can write

$$p_{t,y}(x_t) = \int_{\mathbb{R}^D} p_{s,y}(x_s) p_{t|s,y}(x_t|x_s) dx_s$$

where  $p_{t|s,y}(\cdot|x_s)$  is the pdf of  $X_t$  given Y = y and  $X_s = x_s$ . It is, in fact, equal to the pdf of  $X_t$  given  $X_s = x_s$ , which is the pdf of the multivariate Gaussian distribution with mean  $\exp(-(t-s)/2)x_s$  and covariance  $(1 - \exp(-(t-s)))C$ . Therefore

$$p_{t,y}(x_t) = \int_{\mathbb{R}^D} p_{s,y}(x_s) p_{t|s}(x_t|x_s) dx_s$$

We can then deduce that

$$\begin{split} \nabla p_{t,y}(x_t) &= \frac{1}{(2\pi)^{D/2}(1-e^{-(t-s)})^{1/2}\det(C)^{1/2}} \int_{\mathbb{R}^D} dx_s p_{s,y}(x_s) \\ &\times \nabla_{x_t} \exp\left(-\frac{1}{2(1-e^{-(t-s)})}(x_t - \exp(-(t-s)/2)x_s)^T C^{-1}(x_t - \exp(-(t-s)/2)x_s)\right) \\ &= -\frac{e^{(t-s)/2}}{(2\pi)^{D/2}(1-e^{-(t-s)})^{1/2}\det(C)^{1/2}} \int_{\mathbb{R}^D} dx_s p_{s,y}(x_s) \\ &\times \nabla_{x_s} \exp\left(-\frac{1}{2(1-e^{-(t-s)})}(x_t - \exp(-(t-s)/2)x_s)^T C^{-1}(x_t - \exp(-(t-s)/2)x_s)\right) \\ &= \frac{e^{(t-s)/2}}{(2\pi)^{D/2}(1-e^{-(t-s)})^{1/2}\det(C)^{1/2}} \int_{\mathbb{R}^D} dx_s \nabla_{x_s}(p_{s,y}(x_s)) \\ &\times \exp\left(-\frac{1}{2(1-e^{-(t-s)})}(x_t - \exp(-(t-s)/2)x_s)^T C^{-1}(x_t - \exp(-(t-s)/2)x_s)\right) \\ &= e^{(t-s)/2} \int_{\mathbb{R}^D} dx_s \nabla_{x_s}(p_{s,y}(x_s)) p_{t|s}(x_t|x_s), \end{split}$$

which gives

$$\nabla p_{t,y}(x_t) = e^{(t-s)/2} \int_{\mathbb{R}^D} p_{t|s}(x_t|x_s) p_{s,y}(x_s) \nabla \log p_{s,y}(x_s) dx_s.$$

Using again that  $p_{t|s,y}(\cdot|x_s) = p_{t|s}(\cdot|x_s)$  and  $p_{t|s,y}(x_t|x_s) = \frac{p_{(s,t),y}(x_s,x_t)}{p_{s,y}(x_s)}$ , we get

$$\nabla p_{t,y}(x_t) = e^{(t-s)/2} \int_{\mathbb{R}^D} p_{t|s,y}(x_t|x_s) p_{s,y}(x_s) \nabla \log p_{s,y}(x_s) dx_s$$
$$= e^{(t-s)/2} \int_{\mathbb{R}^D} p_{(s,t),y}(x_s, x_t) \nabla \log p_{s,y}(x_s) dx_s.$$

Since  $\nabla \log p_{t,y}(x_t) = \frac{\nabla p_{t,y}(x_t)}{p_{t,y}(x_t)}$  and  $p_{s|t,y}(x_s|x_t) = \frac{p_{(s,t),y}(x_s,x_t)}{p_{t,y}(x_t)}$  we get that  $\nabla \log p_{t,y}(x_t) = e^{(t-s)/2} \int_{\mathbb{R}^D} p_{s|t,y}(x_s|x_t) \nabla \log p_{s,y}(x_s) dx_s$  $= e^{(t-s)/2} \mathbb{E}_y [\nabla \log p_{s,y}(X_s) | X_t = x_t].$ 

### C.3 Proof of Proposition 2

The proof adapts the one of [33] to the conditional setting. The only difference is that the expectation is  $\mathbb{E}_y$ , which affects the distribution of  $X_0$  but not the one of W. Moreover, Lemma 4 shows that the key to the proof (the reverse-time martingale property of the finite-dimensional score) is still valid. Here  $\mathbb{E}_y$  is the expectation with respect to the distribution of  $X_0$  and W given Y = y.

To prove Proposition 2, we are left to show that the solution of the reverse-time SDE

$$dZ_t = \frac{1}{2}Z_t dt + S(T - t, Z_t, y)dt + \sqrt{C}W_t, \quad Z_0 \sim X_T | Y = y$$
(35)

satisfies  $Z_T \sim X_0 | Y = y$ . We recall that  $X_t$  is the solution to the SDE

$$dX_t = -\frac{1}{2}X_t dt + \sqrt{C}dW_t, \quad X_0 \sim \mu_0$$

We first notice that  $X_t$  is given by the following stochastic convolution:

$$X_t = e^{-t/2} X_0 + \int_0^t e^{-(t-s)/2} \sqrt{C} dW_s.$$

For  $P^D$  the orthogonal projection on the subspace of H spanned by  $v_1, \ldots, v_D$  (the eigenfunctions of C),  $X_t^D = P^D(X_t)$  are solutions to

$$dX_t^D = -\frac{1}{2}X_t^D dt + \sqrt{(C^D)}dW_t^D,$$

where

$$C^D = P^D C P^D, \quad W^D_t = P^D W_t.$$

We define  $X_t^{D:M} = X_t^M - X_t^D$ . Then

6

$$X_t^{D:M} = e^{-t/2} X_0^{D:M} + \int_0^t e^{-(t-s)/2} \sqrt{(C^{D:M})} dW_s^{D:M}$$

where the superscript D: M indicates the projection onto span $\{v_{D+1}, \ldots, v_M\}$ . It holds that

$$\mathbb{E}_{y} \Big[ \sup_{t \leq T} \|X_{t}^{D:M}\|_{H}^{2} \Big] \leq 2e^{-t} \mathbb{E}_{y} [\|X_{0}^{D:\infty}\|_{H}^{2}] + 2(1 - e^{-t}) \sum_{i=D+1}^{\infty} \lambda_{i} \to 0$$

as  $D \to \infty$ , where we used Doob's  $L^2$  inequality to bound the stochastic integral. Therefore  $(X_t^N)$  is a Cauchy sequence and converges to  $X_t$  in  $L^2(\mathbb{P}_y)$ . Consequently, the distribution of  $X_t^N$  given Y = y converges to the distribution of  $X_t$  given Y = y as  $N \to +\infty$ .

Recall that

$$S(t, X_t, y) = -(1 - e^{-t})^{-1} \mathbb{E}_y [X_t - e^{-t/2} X_0 \mid X_t],$$

and recall that

$$C^{D}\nabla \log p_{t,y}^{D}(X_{t}^{1:D}) = -(1-e^{-t})^{-1}P^{D}\mathbb{E}_{y}[X_{t}-e^{-t/2}X_{0} \mid X_{t}^{1:D}].$$

In particular, due to the tower property of the conditional expectations,

$$C^{D} \nabla \log p_{t,y}^{D}(X_{t}^{1:D}) = \mathbb{E}_{y}[S(t, X_{t}, y) \mid X_{t}^{1:D}].$$

Since, by Assumption 1,

$$\mathbb{E}_{y}[\|S(t, X_t, y)\|_{H}^2] < \infty,$$

the quantities  $\mathbb{E}_y[X_t - e^{-t/2}X_0 \mid X_t^{1:D}]$  are bounded in  $L^2(\mathbb{P}_y)$  and will converge to the limit,  $\mathbb{E}_y[S(t, X_t, y) \mid X_t] = S(t, X_t, y)$ , by the Martingale convergence theorem. We get rid of the projection  $P^D$  by

$$(1 - e^{-t})\mathbb{E}_{y}[\|C^{D}\nabla\log p_{t,y}^{D}(X_{t}^{1:D}) - S(t, X_{t}, y)\|_{H}^{2}]$$

$$= \mathbb{E}_{y}[\|P^{D}\mathbb{E}_{y}[X_{t} - e^{-t/2}X_{0} \mid X_{t}^{1:D}] - \mathbb{E}_{y}[X_{t} - e^{-t/2}X_{0} \mid X_{t}]\|_{H}^{2}]$$

$$\leq \mathbb{E}_{y}[\|\mathbb{E}_{y}[X_{t} - e^{-t/2}X_{0} \mid X_{t}^{1:D}] - \mathbb{E}_{y}[X_{t} - e^{-t/2}X_{0} \mid X_{t}]\|_{H}^{2}]$$

$$+ \mathbb{E}_{y}[\|(I - P^{D})\mathbb{E}_{y}[X_{t} - e^{-t/2}X_{0} \mid X_{t}^{1:D}]\|_{H}^{2}]$$

$$\leq \mathbb{E}_{y}[\|\mathbb{E}[X_{t} - e^{-t/2}X_{0} \mid X_{t}^{1:D}] - \mathbb{E}_{y}[X_{t} - e^{-t/2}X_{0} \mid X_{t}]\|_{H}^{2}]$$

$$+ \mathbb{E}_{y}[\|(I - P^{D})(X_{t} - e^{-t/2}X_{0})\|_{H}^{2}].$$

The first term vanishes due to our previous discussion. The second term vanishes since

$$\mathbb{E}_{y}[\|(I - P^{D})(X_{t} - e^{-t/2}X_{0})\|_{H}^{2}] = \mathbb{E}_{y}[\|(I - P^{D})\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_{s}\|_{H}^{2}]$$
$$= \mathbb{E}[\|(I - P^{D})\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_{s}\|_{H}^{2}]$$
$$= (1 - e^{-t})\sum_{i=D+1}^{\infty}\lambda_{j} \to 0$$

as  $D \to \infty$ .

We now make use of the fact that  $\nabla \log p_{t,y}^D$  is a square-integrable Martingale in the reverse-time direction by Lemma 4. We therefore get a sequence of continuous  $L^2$ -bounded Martingales converging to a stochastic process. Since the space of continuous  $L^2$ -bounded martingale is closed and pointwise convergence translates to uniform convergence, we get that S is a  $L^2$ -bounded martingale, with the convergence of of  $C^D \nabla \log p_{t,y}^D$  to S being uniform in time.

We have that

$$Z_t^D - Z_0^D - \frac{1}{2} \int_0^t Z_s ds - \int_0^t C^D \nabla \log p_{s,y}^D(Z_s) = \sqrt{C} W_t^D.$$

Since all the terms on the left-hand side converge in  $L^2$ , uniformly in t, so does the right-hand side. Using again the closedness of the spaces of Martingales and Levy's characterization of Wiener process, we find that  $\sqrt{C}W_t^D$  converges to  $\sqrt{C}W_t$ . Therefore

$$Z_t = Z_0 + \frac{1}{2}Z_s ds + \int_0^t S(t, Z_t, y) + \sqrt{C}W_t^D.$$

Therefore,  $Z_t$  is indeed a solution to (35) and  $Z_T \sim X_0 | Y = y$ . Using uniqueness of the solution we then conclude that this holds for any solution  $Z_t$ .

## C.4 Proof of (24)

$$\begin{split} \mathbb{E}[\|S(t, X_t, y)\|_{H}^{2}|Y = y] &= (1 - e^{-t})^{-2} \mathbb{E}[\|\mathbb{E}[X_t - e^{-t/2}X_0|Y = y, X_t]\|_{H}^{2}|Y = y] \\ &= (1 - e^{-t})^{-2} \mathbb{E}[\|\mathbb{E}[\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_s|Y = y, X_t]\|_{H}^{2}|Y = y] \\ &\leq (1 - e^{-t})^{-2} \mathbb{E}[\mathbb{E}[\|\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_s\|_{H}^{2}|Y = y, X_t]|Y = y] \\ &= (1 - e^{-t})^{-2} \mathbb{E}[\|\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_s\|_{H}^{2}|Y = y] \\ &= (1 - e^{-t})^{-2} \mathbb{E}[\|\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_s\|_{H}^{2}] \\ &= (1 - e^{-t})^{-1} \mathbb{E}[\|\int_{0}^{t} e^{-(t-s)/2}\sqrt{C}dW_s\|_{H}^{2}] \\ &= (1 - e^{-t})^{-1} \mathrm{Tr}(C). \end{split}$$

## C.5 Proof of Proposition 3

Note that with the assumptions in Proposition 3 with  $C_{\mu}$  and C having the same basis of eigenfunctions and the separability assumption on the Radon-Nikodym derivative for the modes, the system for the modes again diagonalizes. However, in this case the (conditional) distribution for  $X_0^{(j)}$  is non-Gaussian in general and the change of measure with repect to the Gaussian measure characterized

by  $\psi^{(j)}(x^{(j)}, y)$ . We let the superscript g denote the Gaussian case with  $\psi \equiv 1$ , then we have:  $S^{(j)}(t, x, y)$ 

$$\begin{aligned} &= -(1 - e^{-t})^{-1} \left( x^{(j)} - e^{-t/2} \mathbb{E}[X_0^{(j)} | X_t = x, Y = y] \right) \\ &= -(1 - e^{-t})^{-1} \left( x^{(j)} - e^{-t/2} \int_{\mathbb{R}} x_0 \left( \frac{\mu_{x_0, x_t^{(j)} | y}^{(j, g)}(x_0, x^{(j)}) \psi^{(j)}(x_0, y)}{\mu_{x_t^{(j)} | y}^{(j)}(x^{(j)})} \right) dx_0 \right) \\ &= (1 - e^{-t})^{-1} \left( e^{-t/2} \int_{\mathbb{R}} x_0 \left( \frac{\mu_{x_0, x_t^{(j)} | y}^{(j, g)}(x_0 + x^{(j)} e^{t/2}, x^{(j)}) \psi^{(j)}(x_0 + x^{(j)} e^{t/2}, y)}{\mu_{x_t^{(j)} | y}^{(j)}(x^{(j)})} \right) dx_0 \right) \\ &= S_G^{(j)}(t, x, y) T^{(j)}(t, x^{(j)}, y) + \tilde{R}^{(j)}(t, x^{(j)}, y), \end{aligned}$$

for  $S_G^{(j)}$  the mode score in the Gaussian case given in (32) and with

$$\begin{split} T^{(j)}(t,x^{(j)},y) &= \left(\frac{\mu_{x_t^{(j)}|y}^{(j,g)}(x^{(j)})\psi^{(j)}(x^{(j)}e^{t/2},y)}{\mu_{x_t^{(j)}|y}^{(j)}(x^{(j)})}\right),\\ \tilde{R}^{(j)}(t,x^{(j)},y) &= (1-e^{-t})^{-1}e^{-t/2}\\ &\times \int_{\mathbb{R}} x_0 \left(\frac{\mu_{x_0,x_t^{(j)}|y}^{(j,g)}(x_0+x^{(j)}e^{t/2},x^{(j)})\left(\psi^{(j)}(x_0+x^{(j)}e^{t/2},y)-\psi^{(j)}(x^{(j)}e^{t/2},y)\right)}{\mu_{x_t^{(j)}|y}(x^{(j)})}\right) dx_0. \end{split}$$

We have for  $\phi_{\lambda}$  the centered Gaussian density at second moment  $\lambda$ 

$$T^{(j)}(t,x^{(j)},y) = \frac{\int_{\mathbb{R}} \phi_{\lambda_t^{(j)}}(x^{(j)} - ve^{-t/2}) \phi_{\mu_y^{(j)}}(v - x_y^{(j)}) dv}{\int_{\mathbb{R}} \phi_{\lambda_t^{(j)}}(x^{(j)} - ve^{-t/2}) \phi_{\mu_y^{(j)}}(v - x_y^{(j)}) \psi^{(j)}(v,y) / \psi^{(j)}(x^{(j)}e^{t/2},y) dv},$$

for  $\lambda_t^{(j)} = \lambda_j(1 - e^{-t}), \mu_y^{(j)} = \mu_j/(1 + q^{(j)})$  and  $x_y^{(j)} = y^{(j)}q^{(j)}/(1 + q^{(j)})$  for  $y^{(j)} = \langle y, v_j \rangle$ . Here  $x_y^{(j)}, \mu_y^{(j)}$  are repectively the mean and variance of  $X_0^{(j)}$  given y and where we used the parameterization set forth in Section B.1. We then have

$$|T^{(j)}(t, x^{(j)}, y)| \le K^2, \quad \lim_{t \downarrow 0} T^{(j)}(t, x^{(j)}y) = 1.$$

We moreover have

$$\begin{split} |\tilde{R}^{(j)}(t,x^{(j)},y)| &\leq e^{-t/2}(1-e^{-t})^{-1}L\left(\frac{\int_{\mathbb{R}} x_0^2 \phi_{\lambda_t^{(j)}}(x^{(j)}-x_0e^{-t/2})\phi_{\mu_y^{(j)}}(x_0-x_y^{(j)})dx_0}{\int_{\mathbb{R}} \phi_{\lambda_t^{(j)}}(x^{(j)}-ve^{-t/2})\phi_{\mu_y^{(j)}}(v-x_y^{(j)})\psi^{(j)}(v,y)dv}\right) \\ &\leq e^{-t/2}(1-e^{-t})^{-1}LK\left(\frac{\int_{\mathbb{R}} x_0^2 \phi_{\lambda_t^{(j)}}(x^{(j)}-x_0e^{-t/2})\phi_{\mu_y^{(j)}}(x_0-x_y^{(j)})dx_0}{\int_{\mathbb{R}} \phi_{\lambda_t^{(j)}}(x^{(j)}-ve^{-t/2})\phi_{\mu_y^{(j)}}(v-x_y^{(j)})dv}\right). \end{split}$$

We then find

$$\limsup_{t \downarrow 0} |\tilde{R}^{(j)}(t, x^{(j)}, y)| \le \lambda^{(j)} L K,$$

and, moreover

$$\begin{split} |\tilde{R}^{(j)}(t,x^{(j)},y)| &\leq \\ \lambda_j L K e^{t/2} \left( \frac{1}{1 + (e^t - 1)p^{(j)}(1 + q^{(j)})} + \lambda_j \frac{(x_y^{(j)} - x^{(j)}e^{t/2})^2}{(\mu_y^{(j)})^2} \frac{(e^t - 1)}{(1 + (e^t - 1)p^{(j)}(1 + q^{(j)}))^2} \right) \end{split}$$

Consider in the Gaussian case in (23) a mode so that  $p^{(j)}(1+q^{(j)}) \uparrow \infty$  and  $\lambda_j$  fixed, then the contribution of this mode to the score norm blows up in the small time limit. The situation with

 $p^{(j)}(1+q^{(j)})\uparrow\infty$  would happen for instance in a limit of perfect mode observation so that  $\sigma_B\downarrow 0$ and thus  $q^{(j)}\uparrow\infty$ . Indeed in the limit of small (conditional) target mode variability relative to the diffusion noise parameter the score drift becomes large for small time to drive the mode to the conditional target distribution. We here thus assume  $p^{(j)}(1+q^{(j)})$  is uniformly bounded with respect to mode (j index), moreover, that C is of trace class. We then find that Assumption 1 is satisfied with the following bound

$$\sup_{t \in [0,T]} \mathbb{E} \left[ \|S(t, X_t, y)\|_H^2 | Y = y \right]$$
  
$$\leq 2 \left( \sum_j \lambda_j e^T \left( K^4 p^{(j)} (1 + q^{(j)}) + 2\lambda_j e^T (LK)^2 \left( 1 + 3 \left( p^{(j)} (1 + q^{(j)}) (e^T - 1) \right)^4 \right) \right) \right).$$

We remark that in the case that we do not have a uniform bound on the  $p^{(j)}(1+q^{(j)})$ 's it follows from (24) that the rate of divergence of the square score norm is at most  $t^{-1}$  as  $t \downarrow 0$  with C of trace class.

#### C.6 Proof of Proposition 4

We start from (31):

$$\mathbb{E}_{x_t,y\sim\mathcal{L}(X_t,Y)}\left[\|S(t,x_t,y) - s_{\theta}(t,x_t,y)\|_{H}^{2}\right] = \mathbb{E}_{x_t,y\sim\mathcal{L}(X_t,Y)}\left[\|S(t,x_t,y)\|_{H}^{2}\right] \\ + \mathbb{E}_{x_t,y\sim\mathcal{L}(X_t,Y)}\left[\|s_{\theta}(t,x_t,y)\|_{H}^{2}\right] - 2\mathbb{E}_{x_t,y\sim\mathcal{L}(X_t,Y)}\left[\left\langle S(t,x_t,y), s_{\theta}(t,x_t,y)\right\rangle\right].$$

From Definition 1 we have

$$\begin{split} & \mathbb{E}_{x_{t},y\sim\mathcal{L}(X_{t},Y)}\left[\left\langle S(t,x_{t},y),s_{\theta}(t,x_{t},y)\right\rangle\right] \\ &= -(1-e^{-t})^{-1}\mathbb{E}_{x_{t},y\sim\mathcal{L}(X_{t},Y)}\left[\left\langle x_{t}-e^{-t/2}\mathbb{E}_{x_{0}\sim\mathcal{L}(X_{0}|X_{t}=x_{t},Y=y)}[x_{0}],s_{\theta}(t,x_{t},y)\right\rangle\right] \\ &= -(1-e^{-t})^{-1}\mathbb{E}_{x_{t},y\sim\mathcal{L}(X_{t},Y)}\left[\mathbb{E}_{x_{0}\sim\mathcal{L}(X_{0}|X_{t}=x_{t},Y=y)}\left[\left\langle x_{t}-e^{-t/2}x_{0},s_{\theta}(t,x_{t},y)\right\rangle\right]\right] \\ &= -(1-e^{-t})^{-1}\mathbb{E}_{(x_{0},x_{t},y)\sim\mathcal{L}(X_{0},X_{t},Y)}\left[\left\langle x_{t}-e^{-t/2}x_{0},s_{\theta}(t,x_{t},y)\right\rangle\right]. \end{split}$$

We obtain that

$$\begin{aligned} & \mathbb{E}_{x_t, y \sim \mathcal{L}(X_t, Y)} \left[ \| S(t, x_t, y) - s_{\theta}(t, x_t, y) \|_{H}^{2} \right] \\ &= B + \mathbb{E}_{(x_0, x_t, y) \sim \mathcal{L}(X_0, X_t, Y)} \left[ \| - (1 - e^{-t})^{-1} (x_t - e^{-t/2} x_0) - s_{\theta}(t, x_t, y) \|_{H}^{2} \right], \end{aligned}$$

with

$$B = \mathbb{E}_{x_t, y \sim \mathcal{L}(X_t, Y)} \left[ \|S(t, x_t, y)\|_H^2 \right] - \mathbb{E}_{(x_0, x_t) \sim \mathcal{L}(X_0, X_t)} \left[ \|(1 - e^{-t})^{-1} (x_t - e^{-t/2} x_0)\|_H^2 \right]$$
  
that does not depend on  $\theta$ . Since  $\mathcal{L}(X_t | X_0 = x_0, Y = y) = \mathcal{L}(X_t | X_0 = x_0)$  we finally get that

$$\mathbb{E}_{x_t, y \sim \mathcal{L}(X_t, Y)} \Big[ \|S(t, x_t, y) - s_{\theta}(t, x_t, y)\|_H^2 \Big] \\= B + \mathbb{E}_{x_0, y \sim \mathcal{L}(X_0, Y), x_t \sim \mathcal{L}(X_t | X_0 = x_0)} \Big[ \| - (1 - e^{-t})^{-1} (x_t - e^{-t/2} x_0) - s_{\theta}(t, x_t, y)\|_H^2 \Big].$$

# **D** Numerical experiment details

In this section, we provide additional details regarding our numerical experiment. As mentioned in the main text, we synthesized a conditional distribution using the relation  $y = ax_0^2 + \varepsilon$ , where  $\varepsilon \sim \Gamma(1, 2)$  and  $a \sim \mathcal{U}\{-1, 1\}$ . Here,  $\Gamma$  refers to the Gamma distribution, and  $\mathcal{U}\{-1, 1\}$  denotes the uniform distribution over the set  $\{-1, 1\}$ . Subsequently, we used our approach to approximate the conditional distribution of y given x. The hyperparameters described in the main text were selected by comparing the validation loss over 1024 samples. The training process takes approximately 15 minutes on a GeForce RTX 2080 Ti GPU device. Regarding the diffusion process, we followed the approach outlined in Ho et al. [16] and employed standard Gaussian noise with linearly increasing variance for the forward process, which was discretized into 500 timesteps. The initial Gaussian noise variance was set to  $10^{-4}$  and linearly increased over the timesteps until it reached  $2 \times 10^{-2}$ .

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