LATENT ABSTRACTIONS IN GENERATIVE DIFFUSION MODELS

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ABSTRACT

In this work we study how diffusion-based generative models produce highdimensional data, such as an image, by implicitly relying on a manifestation of a low-dimensional set of latent abstractions, that guide the generative process. We present a novel theoretical framework that extends Nonlinear Filtering (NLF), and that offers a unique perspective on SDE-based generative models. The development of our theory relies on a novel formulation of the joint (state and measurement) dynamics, and an information-theoretic measure of the influence of the system state on the measurement process. According to our theory, diffusion models can be cast as a system of SDE, describing a non-linear filter in which the evolution of unobservable latent abstractions steers the dynamics of an observable measurement process (corresponding to the generative pathways). In addition, we present an empirical study to validate our theory and previous empirical results on the emergence of latent abstractions at different stages of the generative process.

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1 INTRODUCTION

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027 028 029 030 031 032 033 034 035 036 Generative models have become a cornerstone of modern machine learning, offering powerful methods for synthesizing high-quality data across various domains such as image and video synthesis [\(Dhariwal & Nichol, 2021;](#page-10-0) [Ho et al., 2022;](#page-11-0) [He et al., 2022\)](#page-11-1), natural language processing [\(Li et al.,](#page-11-2) [2022b;](#page-11-2) [He et al., 2023;](#page-11-3) [Gulrajani & Hashimoto, 2023;](#page-10-1) [Lou et al., 2024\)](#page-12-0), audio generation [\(Kong](#page-11-4) [et al., 2021;](#page-11-4) [Liu et al., 2022\)](#page-12-1), and molecular structures and general 3D shapes [\(Trippe et al., 2022;](#page-13-0) [Hoogeboom et al., 2022;](#page-11-5) [Luo & Hu, 2021;](#page-12-2) [Zeng et al., 2022\)](#page-13-1), to name a few. These models transform an initial distribution, which is simple to sample from, into one that approximates the data distribution. Among these, diffusion-based models designed through the lenses of Stochastic Differential Equations (SDEs) [\(Song et al., 2021;](#page-13-2) [Ho et al., 2020;](#page-11-6) [Albergo et al., 2023\)](#page-10-2) have gained popularity due to their ability to generate realistic and diverse data samples through a series of stochastic transformations.

037 038 039 040 041 042 043 044 045 In such models, the data generation process, as described by a substantial body of empirical research [\(Chen et al., 2023;](#page-10-3) [Linhardt et al., 2024;](#page-12-3) [Tang et al., 2023\)](#page-13-3), appears to develop according to distinct stages: high-level semantics emerge first, followed by the incorporation of low-level details, culminating in a refinement (denoising) phase. Despite ample evidence, a comprehensive theoretical framework for modeling these dynamics remains underexplored. Indeed, despite recent work on SDE-based generative models [\(Berner et al., 2022;](#page-10-4) [Richter & Berner, 2023;](#page-12-4) [Ye et al., 2022;](#page-13-4) [Raginsky,](#page-12-5) [2024\)](#page-12-5) shed new lights on such models, they fall short of explicitly investigating the emergence of abstract representations in the generative process. We address this gap by establishing a new framework for elucidating how generative models construct and leverage latent abstractions, approached through the paradigm of NLF [\(Bain & Crisan, 2009;](#page-10-5) [Van Handel, 2007;](#page-13-5) [Kutschireiter et al., 2020\)](#page-11-7).

046 047 048 049 050 051 052 053 NLF is used across diverse engineering domains [\(Bain & Crisan, 2009\)](#page-10-5), as it provides robust methodologies for the estimation and prediction of a system's state amidst uncertainty and noise. NLF enables the inference of dynamic latent variables that define the system state based on observed data, offering a Bayesian interpretation of state evolution and the ability to incorporate stochastic system dynamics. The problem we consider is the following: an *unobservable* random variable X is measured through a noisy continuous-time process Y_t , wherein the influence of X on the noisy process is described by an observation function H , with the noise component modeled as a Brownian motion term. The goal is to estimate the a-posteriori measure π_t of the variable X given the entire historical trajectory of the measurement process Y_t .

- **054 055 056 057 058 059 060 061** In this work, we establish a connection between SDE-based generative models and NLF by observing that they can be interpreted as *simulations* of NLF dynamics. In our framework, the latent abstraction, which corresponds to certain real-world properties within the scope of classical nonlinear filtering and remains unaffected in a *causal* manner by the posterior process π_t , is implicitly simulated and iteratively refined. We explore the connection between latent abstractions and the a-posteriori process, through the concept of *filtrations* – broadly defined as collections of progressively increasing information sets – and offer a rigorous theory to study the emergence and influence of latent abstractions throughout the data generation process. Our theoretical contributions unfold as follows.
- **062 063 064** In § [2](#page-1-0) we show how to reformulate classical NLF results such that the measurement process is the only available information, and derive the corresponding dynamics of both the latent abstraction and the measurement process. These results are summarized in [Theorem 2](#page-2-0) and [Theorem 3.](#page-3-0)
- **065 066 067 068 069** Given the new dynamics, in [Theorem 4](#page-3-1) we show how to estimate the a-posteriori measure of the NLF model, and present a novel derivation to compute the mutual information between the measurement process and random variables derived from a transformation of the latent abstractions in [Theorem 5.](#page-3-2) Finally, we show in [Theorem 6,](#page-4-0) that the a-posteriori measure is a sufficient statistics for any random variable derived from the latent abstractions, when only having access to the measurement process.
- **070 071 072 073 074 075 076 077 078 079 080 081** Building on these general results, in § [3](#page-4-1) we present a novel perspective on continuous-time scorebased diffusion models, which is summarised in [Equation \(10\).](#page-5-0) We propose to view such generative models as NLF simulators that progress in two stages: first our model updates the a-posteriori measure representing a sufficient statistics of the latent abstractions, second, it uses a projection of the a-posteriori measure to update the measurement process. Such intuitive understanding is the result of several fundamental steps. In [Theorem 7](#page-5-1) and [Theorem 8,](#page-6-0) we show that the common view of score-based diffusion models by which they evolve according to forward (noising) and backward (generative) dynamics is compatible with the NLF formulation, in which there is no need to distinguish between such phases. In other words, the NLF perspective of [Equation \(10\)](#page-5-0) is a valid generative model. In [Appendix H,](#page-19-0) we provide additional results (see [Lemma 1\)](#page-20-0), focusing on the specific case of linear diffusion models, which are the most popular instance of score-based generative models in use today. In $\S 4$, we summarize the main intuitions behind our NLF framework.

082 083 084 085 086 087 088 089 090 091 092 Our results explain, by means of a theoretically sound framework, the emergence of latent abstractions that has been observed by a large body of empirical work [\(Bisk et al., 2020;](#page-10-6) [Bender & Koller, 2020;](#page-10-7) [Li et al., 2022a;](#page-11-8) [Park et al., 2023;](#page-12-6) [Kwon et al., 2023;](#page-11-9) [Chen et al., 2023;](#page-10-3) [Linhardt et al., 2024;](#page-12-3) [Tang](#page-13-3) [et al., 2023;](#page-13-3) [Xiang et al., 2023;](#page-13-6) [Haas et al., 2024\)](#page-10-8). The closest research to our findings is discussed in [\(Sclocchi et al., 2024\)](#page-12-7), albeit from a different mathematical perspective. To root our theoretical results in additional empirical evidence, we conclude our work in § [5](#page-8-0) with a series of experiments on score-based generative models [\(Song et al., 2021\)](#page-13-2), where we 1) validate existing probing techniques to measure the emergence of latent abstractions, 2) compute the mutual information as derived in our framework, and show that it is a suitable approach to measure the relation between the generative process and latent abstractions, 3) introduce a new measurement protocol to further confirm the connections between our theory, and how practical diffusion-based generative models operate.

- 2 NONLINEAR FILTERING
- **096 097 098 099 100 101 102 103 104 105** Consider two random variables Y_t and X, corresponding to a stochastic **measurement** process (Y_t) of some underlying **latent abstraction** (X) . We construct our universe sample space Ω as the combination of the space of continuous functions in the interval [0, T] ($T \in \mathbb{R}^+$) and of a complete separable metric space S, i.e., $\Omega = \mathcal{C}([0,T], \mathbb{R}^N) \times S$. On this space, we consider the joint *canonical* process $Z_t(\omega) = [Y_t, X] = [\omega_t^y, \omega^x]$ for all $\omega \in \Omega$, with $\omega = [\omega^y, \omega^x]$. In this work we indicate with $\sigma(\cdot)$ sigma-algebras. Consider the growing filtration naturally induced by the canonical process $\mathcal{F}^{Y,X}_t = \sigma(Y_{0 \le s \le t}, X)$ (a short-hand for $\sigma(\sigma(Y_{0 \le s \le t}) \cup \sigma(X))$), and define $\mathcal{F} = \mathcal{F}^{Y,X}_T$. We build the probability triplet (Ω, \mathcal{F}, P) , where the probability measure P is selected such that the process $\{Z_{0\leq t\leq T}, \mathcal{F}_{0\leq t\leq T}^{Y,X}\}$ has the following SDE representation
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$$
Y_t = Y_0 + \int_0^t H(Y_s, X, s) \mathrm{d} s + W_t,\tag{1}
$$

108 109 110 where $\{W_{0\leq t\leq T},\mathcal{F}_{0\leq t\leq T}^{Y,X}\}$ is a Brownian motion with initial value 0 and $H:\Omega\times[0,T]\to\mathbb{R}^N$ is an *observation* process. All standard technical assumptions are available in [Appendix A.](#page-14-0)

111 112 113 114 115 Next, we provide the necessary background on NLF, to pave the way for understanding its connection with the generative models of interest. The most important building block of the NLF literature is represented by the **conditional probability measure** $P[X \in A | \mathcal{F}_t^{\bar{Y}}]$ (notice the reduced filtration $\mathcal{F}_t^Y \subset \mathcal{F}_t^{Y,X}$), which summarizes, a-posteriori, the distribution of X given observations of the measurement process until time t, that is, $Y_{0 \le s \le t}$.

116 117 118 119 Theorem 1. *[Thm 2.1 [\(Bain & Crisan, 2009\)](#page-10-5)] Consider the probability triplet* (Ω, \mathcal{F}, P) *, the metric space* S *and its Borel sigma-algebra* B(S)*. There exists a (probability measure valued* P(S)*) process* $\{\pi_{0\leq t\leq T},\mathcal{F}^Y_{0\leq t\leq T}\}$, with a progressively measurable modification, such that for all $A\in\mathcal{B}(\mathcal{S})$, the *conditional probability measure* $P[X \in A \, | \, \mathcal{F}_t^Y]$ *is well defined and is equal to* $\pi_t(A)$ *.*

120 121 122 The conditional probability measure is extremely important, as the fundamental goal of nonlinear filtering is the solution of the following problem. Here, we introduce the quantity ϕ , which is a random variable derived from the latent abstractions X.

123 124 125 Problem 1. *For any fixed* ϕ : $S \to \mathbb{R}$ *bounded and measurable, given knowledge of the measurement process* $Y_{0 \leq s \leq t}$, compute $\mathbb{E}_{P}[\phi(X) | \mathcal{F}_{t}^{Y}]$. This amounts to computing

$$
\langle \pi_t, \phi \rangle = \int_{\mathcal{S}} \phi(x) \mathrm{d}\pi_t(x). \tag{2}
$$

128 129 130 131 132 133 In simple terms, [Problem 1](#page-2-1) involves studying the existence of the a-posteriori measure and the implementation of efficient algorithms for its update, using the flowing stream of incoming information Y_t . We first focus our attention on the existence of an analytic expression for the value of the a-posteriori expected measure π_t . Then, we quantify the interaction dynamics between observable measurements and ϕ , through the lenses of mutual information $\mathcal{I}(Y_{0\leq s\leq t};\phi)$, which is an extension of the problems considered in [\(Newton, 2008;](#page-12-8) [Duncan, 1970;](#page-10-9) [1971;](#page-10-10) [Mitter & Newton, 2003\)](#page-12-9).

134 135 2.1 TECHNICAL PRELIMINARIES

136 137 138 139 140 We set the stage of our work by revisiting the measurement process Y_t , and express it in a way that does not require access to unobservable information. Indeed, while Y_t is naturally adapted w.r.t. its own filtration \mathcal{F}_t^Y , and consequently to any other growing filtration \mathcal{R}_t such $\mathcal{F}_t^{Y,X} \supseteq \mathcal{R}_t \supseteq \mathcal{F}_t^Y$, the representation in [Equation \(1\)](#page-1-1) is in general not adapted, letting aside degenerate cases.

141 142 143 144 145 146 147 Let's consider the family of growing filtrations $\mathcal{R}_t = \sigma(\mathcal{R}_0 \cup \sigma(Y_{0 \leq s \leq t} - Y_0))$, where $\sigma(Y_0) \subseteq$ $\mathcal{R}_0 \subseteq \sigma(X, Y_0)$. Intuitively \mathcal{R}_0 allows to modulate between the two extreme cases of knowing only the initial conditions of the SDE, that is Y_0 , to the case of complete knowledge of the whole latent abstraction X, and anything in between. As shown hereafter, the original process Y_t associated to the space (Ω, \mathcal{F}, P) which solves [Equation \(1\),](#page-1-1) also solves [Equation \(4\),](#page-3-3) that is adapted on the reduced filtration \mathcal{R}_t . This allows us to reason about the partial observation of the latent abstraction (\mathcal{R}_0) vs $\sigma(X, Y_0)$), without incurring in the problem of the measurement process Y_t being statistically dependent of the whole latent abstraction X.

148 149 150 151 152 153 154 Armed with such representation, we study under which change of measure the process $Y_t - Y_0$ behaves as a Brownian motion [\(Theorem 3\)](#page-3-0). This serves the purpose of simplifying the calculation of the expected value of ϕ given Y_t, as described in [Problem 1.](#page-2-1) Indeed, if Y_t − Y₀ is a Brownian motion independent of ϕ , its knowledge does not influence our best guess for ϕ , i.e. the conditional expected value. Moreover, our alternative representation is instrumental for the efficient and simple computation of the mutual information $\mathcal{I}(Y_{0 \leq s \leq t}; \phi)$, where the different measures involved in the Radon-Nikodym derivatives will be compared against the same reference Brownian measures.

155 156 The first step to define our representation is provided by the following

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157 158 159 Theorem 2. *[\[Proof\].](#page-14-1) Consider the the probability triplet* (Ω, \mathcal{F}, P) *, the process in [Equation](#page-1-1)* (1) *defined on it, and the growing filtration* $\mathcal{R}_t = \sigma(\mathcal{R}_0 \cup \sigma(Y_{0 \le s \le t} - Y_0))$ *. Define a new stochastic process*

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$$
V_t^{\mathcal{R}} \stackrel{\text{def}}{=} Y_t - Y_0 - \int_0^t \mathbb{E}_{\mathcal{P}}(H(Y_s, X, s) | \mathcal{R}_s) \mathrm{d}s. \tag{3}
$$

Then, $\{W_{0\leq t\leq T}^{\mathcal{R}}, \mathcal{R}_{0\leq t\leq T}\}$ is a Brownian motion. Notice that if $\mathcal{R}_t=\mathcal{F}_t^{Y,X}$, then $W_t^{\mathcal{R}}=W_t$.

162 163 Following [Theorem 2,](#page-2-0) the process ${Y_{0 \leq t \leq T}, \mathcal{R}_{0 \leq t \leq T}}$ has SDE representation

$$
Y_t = Y_0 + \int_0^t \mathbb{E}_{\mathcal{P}}(H(Y_s, X, s) | \mathcal{R}_s) ds + W_t^{\mathcal{R}}.
$$
 (4)

Next, we derive the change of measure necessary for the process $\tilde{W}_t \stackrel{\text{def}}{=} Y_t - Y_0$ to be a Brownian motion w.r.t to the filtration \mathcal{R}_t . To do this, we apply the Girsanov theorem [\(Øksendal, 2003\)](#page-12-10) to \tilde{W}_t which, in general, admits a \mathcal{R} – adapted representation $\int_0^t \mathbb{E}_{P}(H(Y_s, X, s) | \mathcal{R}_s) ds + W_t^{\mathcal{R}}$.

Theorem 3. *[\[Proof\].](#page-15-0)* Define the new probability space $(\Omega, \mathcal{R}_T, Q^{\mathcal{R}})$ via the measure $Q^{\mathcal{R}}(A)$ = $\mathbb{E}_{\mathrm{P}}\left[\mathbf{1}(A)(\psi_T^{\mathcal{R}})^{-1}\right]$, for $A\in\mathcal{R}_T$, where

$$
\psi_t^{\mathcal{R}} \stackrel{\text{def}}{=} \exp\biggl(\int_0^t \mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) \,|\, \mathcal{R}_s] \mathrm{d}Y_s - \frac{1}{2} \int_0^t \|\mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) \,|\, \mathcal{R}_s]\|^2 \mathrm{d}s\biggr),\tag{5}
$$

and

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$$
Q^{\mathcal{R}}|_{\mathcal{R}_t} = \mathbb{E}_{P}\left[\mathbf{1}(A)\mathbb{E}_{P}[(\psi_T^{\mathcal{R}})^{-1} | \mathcal{R}_t]\right] = \mathbb{E}_{P}\left[\mathbf{1}(A)(\psi_t^{\mathcal{R}})^{-1}\right].
$$

Then, the stochastic process $\{\tilde{W}_{0\leq t\leq T}, \mathcal{R}_{0\leq t\leq T}\}$ *is a Brownian motion on the space* $(\Omega, \mathcal{R}_T, Q^\mathcal{R})$ *.*

A direct consequence of [Theorem 3](#page-3-0) is that the process \tilde{W}_t is independent of any \mathcal{R}_0 measurable random variable under the measure Q^R . Moreover, it holds that for all $\mathcal{R}'_t \subseteq \mathcal{R}_t$, $Q^R |_{\mathcal{R}'_t} = Q^{\mathcal{R}'} |_{\mathcal{R}'_t}$.

2.2 A-POSTERIORI MEASURE AND MUTUAL INFORMATION

184 185 186 187 188 As we did in § [2](#page-1-0) for the process π_t , here we introduce a new process π_t^R which represents the conditional law of X given the filtration $\mathcal{R}_t = \sigma(\mathcal{R}_0 \cup \sigma(Y_{0 \le s \le t} - Y_0))$. More precisely, for all $A \in \mathcal{B}(\mathcal{S})$, the conditional probability measure $P[X \in A \mid \mathcal{R}_t]$ is well defined and is equal to $\pi_t^{\mathcal{R}}(A)$. Moreover, for any $\phi : \mathcal{S} \to \mathbb{R}$ bounded and measurable, $\mathbb{E}_{\mathcal{P}}[\phi(X) | \mathcal{R}_t] = \langle \pi_t^{\mathcal{R}}, \phi \rangle$. Notice that if $\mathcal{R} = \mathcal{F}^Y$ then $\pi^{\mathcal{R}}$ reduces to π .

189 190 191 Armed with [Theorem 3,](#page-3-0) we are ready to derive the expression for the a-posteriori measure $\pi_t^{\mathcal{R}}$ and the mutual information between observable measurements and the unavailable information about the latent abstractions, that materialize in the random variable ϕ .

192 193 194 Theorem 4. [\[Proof\].](#page-15-1) The measure-valued process $\pi^{\mathcal{R}}_t$ solves in weak sense (see [Appendix D](#page-15-1) for a *precise definition), the following* SDE

$$
\pi_t^{\mathcal{R}} = \pi_0^{\mathcal{R}} + \int_0^t \pi_s^{\mathcal{R}} \left(H(Y_s, \cdot, s) - \langle \pi_s^{\mathcal{R}}, H(Y_s, \cdot, s) \rangle \right) \left(\mathrm{d}Y_s - \langle \pi_s^{\mathcal{R}}, H(Y_s, \cdot, s) \rangle \mathrm{d}s \right), \tag{6}
$$

197 *where the initial condition* π_0 *satisfies* $\pi_0^{\mathcal{R}}(A) = \text{P}[X \in A | \mathcal{R}_0]$ *for all* $A \in \mathcal{B}(\mathcal{S})$ *.*

198 199 200 201 202 203 204 When $\mathcal{R} = \mathcal{F}^Y$, [Equation \(6\)](#page-3-4) is the well-know Kushner-Stratonovitch (or Fujisaki-Kallianpur-Kunita) equation (see e.g. Bain $& Crisan (2009)$ $& Crisan (2009)$). A proof for uniqueness of the solution of [Equation \(6\)](#page-3-4) can be approached by considering the strategies in [\(Fotsa-Mbogne & Pardoux, 2017\)](#page-10-11), but is outside the scope of this work. The (recursive) expression in [Equation \(6\)](#page-3-4) is particularly useful for engineering purposes since, in general, it is usually not known in which variables $\phi(X)$, representing latent abstractions, we could be interested in. Keeping track of the *whole distribution* $\pi_t^{\mathcal{R}}$ at time t is the most cost-effective solution, as we will show later.

205 206 207 Our next goal is to quantify the interaction dynamics between observable measurements and latent abstractions that materialize through the variable $\phi(X)$ (from now on we write only ϕ for the sake of brevity): in [Theorem 5](#page-3-2) we derive the mutual information $\mathcal{I}(Y_{0 \leq s \leq t}; \phi)$.

208 209 Theorem 5. *[\[Proof\]](#page-16-0)* The mutual information between observable measurements $Y_{0\leq s\leq t}$ and ϕ is *defined as:*

$$
\mathcal{I}(Y_{0\leq s\leq t};\phi) \stackrel{\text{def}}{=} \int \log \frac{\mathrm{d}P_{\#Y_{0\leq s\leq t},\phi}}{\mathrm{d}P_{\#Y_{0\leq s\leq t}} \mathrm{d}P_{\# \phi}} \mathrm{d}P_{\#Y_{0\leq s\leq t},\phi}.
$$
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213 214 *It holds that such quantity is equal to* $\mathbb{E}_{\mathrm{P}}\left[\log\frac{d\mathrm{P} \mid \pi_t}{d\mathrm{P} \mid \pi_t^{\chi} d\mathrm{P} \mid \sigma(\phi)}\right]$ *, which can be simplified as follows:*

$$
\mathcal{I}(Y_0;\phi) + \frac{1}{2} \mathbb{E}_{\mathcal{P}} \left[\int_0^t \left\| \mathbb{E}_{\mathcal{P}} [H(X,Y_s,s) \,|\, \mathcal{F}_s^Y] - \mathbb{E}_{\mathcal{P}} [H(X,Y_s,s) \,|\, \mathcal{R}_s] \right\|^2 \mathrm{d}s \right]. \tag{8}
$$

216 217 218 219 220 221 222 223 The mutual information computed by [Equation \(8\)](#page-3-5) is composed by two elements: first, the mutual information between the initial measurements Y_0 and ϕ , which is typically zero by construction. The second term quantifies how much the best prediction of the observation function H is influenced by the extra knowledge of ϕ , in addition to the measurement history $Y_{0 \le s \le t}$. By adhering to the premise that the conditional expectation of a stochastic variable constitutes the optimal estimator given the conditioning information, the integral on the r.h.s quantifies the expected square difference between predictions, having access to measurements only $(\mathbb{E}_{P}[\cdot | \mathcal{F}_{t}^{Y}])$ and those incorporating additional information $(\mathbb{E}_{P}[\cdot | \mathcal{R}_t]).$

224 225 226 227 228 229 230 231 232 233 Even though a precise characterization for general observation functions and and variables ϕ is typically out of reach, a **qualitative** analysis is possible. First, the mutual information between ϕ and the measurements depends on *i*) how much the amplitude of H is impacted by knowledge of ϕ and *ii*) the *number* of elements of H which are impacted (informally, how much localized vs global is the impact of ϕ). Second, it is possible to define a hierarchical interpretation about the emergence of the various latent factors: a variable with a local impact can "*appear*", in an information theoretic sense, only if the impact of other global variables is resolved, otherwise the remaining uncertainty of the global variables makes knowledge of the local variable irrelevant. In classical diffusion models, this is empirically known [\(Chen et al., 2023;](#page-10-3) [Linhardt et al., 2024;](#page-12-3) [Tang et al., 2023\)](#page-13-3), and corresponds to the phenomenon where *semantics emerges before details* (global vs local details in our language).

234 235 236 237 238 239 240 241 Now, consider any \mathcal{F}^Y_t measurable random variable \tilde{Y}_t , defined as a mapping to a generic measurable space (Ψ, B(Ψ)), which means it can also be seen as a process. The *data processing inequality* states that the mutual information between such Y and ϕ will be smaller than the mutual information between the original measurement process and ϕ . However, it can be shown that all the relevant information about the random variable ϕ contained in \mathcal{F}_t^Y is equivalently contained in the filtering process at time instant t, that is π_t . This is not trivial, since π_t is a \mathcal{F}_t^Y -measurable quantity, i.e., $\sigma(\pi_t) \subset \mathcal{F}_t^Y$. In other words, we show that π_t is a **sufficient statistic** for any $\sigma(X)$ measurable random variable when starting from the measurement process.

242 243 Theorem 6. [\[Proof\]](#page-18-0) For any \mathcal{F}_t^Y measurable random variable $\tilde{Y}_t : \Omega \to \Psi$, the following inequality *holds:*

$$
\mathcal{I}(\tilde{Y};\phi) \le \mathcal{I}(Y_{0 \le s \le t};\phi). \tag{9}
$$

245 246 247 248 *For a given* $t \geq 0$ *, the measurement process* $Y_{0 \leq s \leq t}$ *and* X *are conditionally-independent given* π_t *. This implies that* $P(A | \sigma(\pi_t)) = P(A | \mathcal{F}_t^Y)$, $\forall A \in \sigma(X)$ *. Then* $\mathcal{I}(Y_{0 \le s \le t}; \phi) = \mathcal{I}(\pi_t; \phi)$ *(i.e.*) *[Equation](#page-4-2)* (9) *is attained with equality).*

249 250 251 252 253 While π_t contains all the relevant information about ϕ , the same cannot be said about the conditional expectation, i.e. the particular case $Y = \langle \pi_t, \phi \rangle$. Indeed, from [Equation \(2\),](#page-2-2) $\langle \pi_t, \phi \rangle$ is obtained as a *transformation* of π_t and thus can be interpreted as a \mathcal{F}_t^Y measurable quantity subject to the constraint of [Equation \(9\).](#page-4-2) As a particular case, the quantity $\langle \pi_t, H \rangle$, of central importance in the construction of generative models [§ 3,](#page-4-1) carries in general less information about ϕ than the un-projected π_t .

3 GENERATIVE MODELLING

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We are interested in **generative models** for a given $\sigma(X)$ -measurable random variable V.

258 259 260 261 262 263 264 An intuitive illustration of how data generation works according to our framework is as follows. Consider, for example, the image domain, and the availability of a rendering engine that takes as an input a computer program describing a scene (coordinates of objects, textures, light sources, auxiliary labels, etc ...) and that produces an output image of the scene. In a similar vein, a generative model learns how to use latent variables (which are not explicitly provided in input, but rather implicitly learned through training) to generate an image. For such model to work, one valid strategy is to consider an SDE in the form of Equation (1) (1) (1) where the following holds¹.

265 Assumption 1. *The stochastic process* Y_t *satisfies* $Y_T = V$, $P - a.s$.

266 267 268 Then, we could numerically simulate the dynamics of Equation (1) until time T. Indeed, starting from initial conditions Y_0 , we could obtain Y_T that, under [Assumption 1,](#page-4-4) is precisely V. Unfortunately,

¹ From a strict technical point of view, [Assumption 1](#page-4-4) might be incompatible with other assumptions in [Appendix A,](#page-14-0) or proving compatibility could require particular effort. Such details are discussed in [Appendix G.](#page-19-1)

270 271 272 273 274 such a simple idea requires *explicit access* to X, as it is evident from [Equation \(1\).](#page-1-1) In mathematical terms, [Equation \(1\)](#page-1-1) is adapted to the filtration $\mathcal{F}_t^{Y,X}$. However, we have shown how to reduce the available information to account only for historical values of Y_t . Then, we can combine the result in [Theorem 4](#page-3-1) with [Theorem 2](#page-2-0) and re-interpret [Equation \(4\),](#page-3-3) which is a valid generative model, as

$$
\begin{cases} \pi_t = \pi_0 + \int_0^t \pi_s \left(H - \langle \pi_s, H \rangle \right) (\mathrm{d}Y_s - \langle \pi_s, H \rangle \mathrm{d}s), \\ Y_t = Y_0 + \int_0^t \langle \pi_s, H \rangle \mathrm{d}s + W_t^{\mathcal{F}^Y}, \end{cases}
$$

277 278 279 280 where H denotes $H(Y_s, \cdot, s)$. Explicit simulation of [Equation \(10\)](#page-5-0) only requires knowledge of the whole history of the measurement process: provided [Assumption 1](#page-4-4) holds, it allows generation of a sample of the random variable V.

281 282 283 284 285 Although the discussion in this work includes a large class of observation functions, we focus on the particular case of generative diffusion models [\(Song et al., 2021\)](#page-13-2). Typically, such models are presented through the lenses of a forward noising process and backward (in time) SDEs, following the intuition of [Anderson](#page-10-12) [\(1982\)](#page-10-12). Next, according to the framework we introduce in this work, we reinterpret such models under the perspective of enlargement of filtrations.

Consider the *reversed* process $\hat{Y}_t \stackrel{\text{def}}{=} Y_{T-t}$ defined on (Ω, \mathcal{F}, P) and the corresponding filtration $\mathcal{F}_t^{\hat{Y}} \stackrel{\text{def}}{=} \sigma(\hat{Y}_{0 \le s \le t})$. The measure P is selected such that the process \hat{Y}_t has $\mathcal{F}_t^{\hat{Y}}$ -adapted expression

$$
\hat{Y}_t = V + \int_0^t F(\hat{Y}_s, s)ds + \hat{W}_t,
$$
\n(11)

(10)

where $\{\hat{W}_t, \mathcal{F}_t^{\hat{Y}}\}$ is a Brownian motion. Then, [Assumption 1](#page-4-4) is valid since $Y_T = \hat{Y}_0 = V$. Note that [Equation \(11\),](#page-5-2) albeit with a different notation, is reminiscent of the forward SDE that is typically used as the starting point to illustrate score-based generative models [\(Song et al., 2021\)](#page-13-2). In particular, $F(\cdot)$ corresponds to the drift term of such a diffusion SDE.

[Equation \(11\)](#page-5-2) is equivalent to $Y_t = V + \int_0^T$ $\int_t^{\tau} F(Y_s, T - s) ds + \hat{W}_{T-t}$, which is an expression for the

process Y_t , which is adapted to $\mathcal{F}^{\hat{Y}}$. This constitutes the first step to derive an equivalent backward (generative) process according to the traditional framework of score-based diffusion models. Note that such an equivalent representation is not useful for simulation purposes: the goals of the next steps is to transform it such that it is adapted to \mathcal{F}^Y . Indeed, using simple algebra, it holds that

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$$
Y_t = Y_0 - \int_0^t F(Y_s, T - s) \mathrm{d} s + \left(-Y_0 + V + \int_0^T F(Y_s, T - s) \mathrm{d} s + \hat{W}_{T-t} \right),
$$

308 309 where the last term in the parentheses is equal to $-\hat{W}_T + \hat{W}_{T-t}$.

310 311 312 313 Note that $\mathcal{F}_t^Y = \sigma(\hat{Y}_{T-t \leq s \leq T})$. Since $\sigma(\hat{Y}_{T-t \leq s \leq T}) = \sigma(\hat{W}_{T-t \leq s \leq T}) \cup \sigma(\hat{Y}_{T-t})$, we can apply the result in [\(Pardoux, 2006\)](#page-12-11) (Thm 2.2) to claim the following: $-\hat{W}_T + \overline{\hat{W}}_{T-t} - \int_0^t \nabla \log \hat{p}(Y_s, T-s) ds$ is a Brownian motion adapted to \mathcal{F}_t^Y , where this time $P(\hat{Y}_t \in dy) = \hat{p}(y, t)dy$. Then [\(Pardoux,](#page-12-11) [2006\)](#page-12-11)

314 315 Theorem 7. *Consider the stochastic process* Y_t *which solves [Equation](#page-5-2)* (11)*. The same stochastic* process also admits a \mathcal{F}^Y_t –adapted representation

$$
Y_t = Y_0 + \int_0^t \underbrace{-F(Y_s, T-s) + \nabla \log \hat{p}(Y_s, T-s)}_{\text{In Theorem 8, we call this } F'(Y_s, s)} ds + W_t. \tag{12}
$$

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320 321 322 [Equation \(12\)](#page-5-3) corresponds to the backward diffusion process from [\(Song et al., 2021\)](#page-13-2) and, because it is adapted to the filtration \mathcal{F}^Y , it represents a valid, and easy to simulate, measurement process.

323 By now, it is clear how to go from an $\mathcal{F}^{Y,X}$ –adapted filtration to a \mathcal{F}^Y –adapted one. We also showed that a \mathcal{F}^Y -adapted filtration can be linked to the reverse, $\mathcal{F}^{\hat{Y}}$ -adapted process induced by a forward

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324 325 326 327 328 diffusion SDE. What remains to be discussed is the connection that exists between the \mathcal{F}^Y -adapted filtration, and its *enlarged* version $\mathcal{F}^{Y,X}$. In other words, we have shown that a forward, diffusion SDE admits a backward process which is compatible with our generative model that simulates a NLF process having access only to measurements, but we need to make sure that such process admits a formulation that is compatible the standard NLF framework in which latent abstractions are available.

329 330 331 332 333 334 To do this, we can leverage existing results about Markovian bridges [\(Rogers & Williams, 2000;](#page-12-12) [Ye et al., 2022\)](#page-13-4) (and further work [\(Aksamit et al., 2017;](#page-10-13) [Ouwehand, 2022;](#page-12-13) [Grigorian & Jarrow,](#page-10-14) [2023;](#page-10-14) C[etin & Danilova, 2016\)](#page-13-7) on filtration enlargement). This requires assumptions about the existence and well-behavedness of densities $p(y, t)$ of the SDE process, defined by the logarithm of the Radon-Nikodym derivative of the instantaneous measure $P(Y_t \in dy)$ w.r.t. the Lebesgue measure in \mathbb{R}^N , $P(Y_t \in dy) = p(y, t) dy^2$ $P(Y_t \in dy) = p(y, t) dy^2$.

Theorem 8. *Suppose that on* (Ω, \mathcal{F}, P) *the Markov stochastic process* Y_t *satisfies*

$$
Y_t = Y_0 + \int_0^t F'(Y_s, s) \, \mathrm{d} s + W_t,\tag{13}
$$

339 340 341 where $\{W_{0\leq t\leq T},\mathcal{F}_{0\leq t\leq T}^{Y}\}$ is a Brownian motion and F satisfies the requirements for existence and *well definition of the stochastic integral [\(Shreve, 2004\)](#page-12-14). Moreover, let [Assumption 1](#page-4-4) hold. Then, the same process admits* $\mathcal{R}_t = \sigma(Y_{0 \leq s \leq t}, Y_T)$ –*adapted representation*

$$
Y_t = Y_0 + \int_0^t F'(Y_s, s) + \nabla_{Y_s} \log p(Y_T | Y_s) \mathrm{d} s + \beta_t,\tag{14}
$$

345 346 *where* $p(Y_T | Y_s)$ *is the density w.r.t the Lebesgue measure of the probability* $P(Y_T | \sigma(Y_s))$ *, and* $\{\beta_{0\leq t\leq T}, \mathcal{R}_{0\leq t\leq T}\}\$ is a Brownian motion.

347 348 349 350 The connection between time reversal of diffusion processes and enlarged filtrations is finalized with the result of [Al-Hussaini & Elliott](#page-10-15) [\(1987\)](#page-10-15), Thm. 3.3, where it is proved how the β_t term of [Equation \(14\)](#page-6-2) is a Brownian motion, using the techniques of time reversals of SDEs.

Since
$$
\hat{p}(y, T - t) = p(y, t)
$$
, the enlarged filtration version of Equation (12) reads

$$
Y_t = Y_0 + \int_0^t -F(Y_s, T - s) + \nabla_V \log p(Y_s | Y_T) \, ds + W_t.
$$

$$
Y_t = Y_0 + \int_0^{\cdot} \underbrace{-F(Y_s, T - s) + \nabla_{Y_s} \log p(Y_s | Y_T) \mathrm{d}s}_{\text{Equivalent to } H(Y_t, X, t) = -F(Y_s, T - s) + \nabla_{Y_s} \log p(Y_s | g(X))} + W_t. \tag{15}
$$

Note that the dependence of Y_t on the latent abstractions X is implicitly defined by conditioning the score term $\nabla_{Y_s} \log p(Y_s | Y_T)$ by Y_T , which is the "rendering" of X into the observable data domain.

358 359 360 361 Clearly, [Equation \(15\)](#page-6-3) can be reverted to the starting generative [Equation \(12\)](#page-5-3) by mimicking the results which allowed us to go from [Equation \(1\)](#page-1-1) to [Equation \(4\),](#page-3-3) by noticing that $\mathbb{E}_{P}[\nabla_{Y_s} \log p(Y_T | Y_s) | \mathcal{F}_t^Y] = 0$ (informally, this is obtained since $\int \nabla_{y_s} \log p(y_t | y_s) p(y_t | y_s) dy_t = \int \nabla_{y_s} p(y_t | y_s) dy_t = 0.$

It is also important to notice that we can derive the expression for the mutual information between the measurement process and a sample from the data distribution, as follows

$$
\mathcal{I}(Y_{0\leq s\leq t};V) = \mathcal{I}(Y_0;V) + \frac{1}{2}\mathbb{E}_{P}\left[\int_0^t \left\|\nabla_{Y_s}\log p(Y_s) - \nabla_{Y_s}\log p(Y_s \,|\, Y_T)\right\|^2\mathrm{d}s\right].\tag{16}
$$

Mutual information is tightly related to the classical loss function of generative diffusion models.

368 369 370 Furthermore, by casting the result of [Equation \(8\)](#page-3-5) according to the forms of [Equations \(12\)](#page-5-3) and [\(15\),](#page-6-3) we obtain the simple and elegant expression

$$
\mathcal{I}(Y_{0\leq s\leq t};V) = \mathcal{I}(Y_0;V) + \frac{1}{2}\mathbb{E}_{P}\left[\int_0^t \|\nabla_{Y_s}\log p(Y_T\,|\,Y_s)\|^2 ds\right].\tag{17}
$$

In [Appendix H,](#page-19-0) we present a specialization of our framework for the particular case of linear diffusion models, recovering the expressions for the variance-preserving and variance-exploding SDEs that are the foundations of score-based generative models [\(Song et al., 2021\)](#page-13-2).

²Similarly to what discussed in footnote 1, the analysis of the existence of the process adapted to \mathcal{F}_t^Y is considered in the time interval $[0, T)$ [\(Haussmann & Pardoux, 1986\)](#page-11-10). See also [Appendix G.](#page-19-1)

Figure 1: Graphical intuition for our results: nonlinear filtering (left) and generative modelling (right).

AN INFORMAL SUMMARY OF THE RESULTS

396 397 398 399 We shall now take a step back from the rigour of this work, and provide an intuitive summary of our results, using [Figure 1](#page-7-1) as a reference. We begin with an illustration of NLF, shown on the left of the figure. We consider an observable latent abstraction X and the measurement process Y_t , which for ease of illustration we consider evolving in discrete time, i.e. Y_0, Y_1, \ldots , and whose joint evolution is described by [Equation \(1\).](#page-1-1) Such interaction is shown in blue: Y_3 depends on its immediate past Y_2 and the latent abstraction X.

402 403 404 405 406 407 408 The a-posteriori measure process π_t is updated in an iterative fashion, by integrating the flux of information. We show this in green: π_1 is obtained by updating π_0 with $Y_1 - Y_0$ (the equivalent of dY_t). This evolution is described by Kushner's equation, which has been derived informally from the result of [Equation \(6\).](#page-3-4) The a-posteriori process is a sufficient statistic for the latent abstraction X : for example, π_3 contains the same information about ϕ as the whole Y_0, \ldots, Y_3 (red boxes). Instead, in general, a projected statistic $\langle \pi_t, \phi \rangle$ contains less information than the whole measurement process (this is shown in orange, for time instant 2). The mutual information between all these variables is proven in [Theorem 6,](#page-4-0) whereas the actual value of $\mathcal{I}(Y_{0 \leq s \leq t}; \phi)$ is shown in [Theorem 5.](#page-3-2)

409 410 411 412 413 414 Next, we focus on generative modelling. As by our definition, any stochastic process satisfying [Assumption 1](#page-4-4) ($Y_3 = V$, in the figure) can be used for generative purposes. Since the latent abstraction is by definition not available, it is not possible to simulate directly the dynamics using [Equation \(1\)](#page-1-1) (dashed lines from X to Y_t). Instead, we derive a version of the process adapted to the history of Y_t alone, together with the update of the projection $\langle \pi_t, H \rangle$, which amounts to simulating [Equation \(10\).](#page-5-0)

415 416 417 418 419 420 The update of the upper part of [Equation \(10\),](#page-5-0) which is a particular case of [Equation \(6\),](#page-3-4) can be interpreted as the composition of two steps: 1) (green) the update of the a-posteriori measure given new available measurements, and, 2) (orange) the projection of the whole π_t into the statistic of interest. The update of the measurement process, i.e. the lower part of [Equation \(10\),](#page-5-0) is color-coded in blue. This is in stark contrast to the NLF case, as the update of e.g. $Y_3 = V$ does not depend directly on X . The system in [Equation \(10\)](#page-5-0) and its simulation describes the emergence of latent world representations in SDE-based generative models:

We interpret the \mathcal{F}_t^Y measurable quantity $\langle \pi_t, H \rangle$ as the cascade of mappings trough the spaces $\langle \pi_t, H \rangle: \; \; \mathcal{C}([0,t],\mathbb{R}^N) \to \mathcal{P}(\mathcal{S}) \times \mathbb{R}^N \to \mathbb{R}^N$ $Y_{0\leq s\leq t}\to (\pi_t,Y_t)\to \langle \pi_t,H\rangle$ We consider it as a mapping that **first** transforms the whole $Y_{0 \le s \le t}$ into the *condensed* (in terms of sufficient statistics [Theorem 6\)](#page-4-0) π_t , keep also Y_t , and **second** uses these two to construct $\langle \pi_t, H \rangle$.

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⁴²⁹ 430 431 The theory developed in this work guarantees that the mutual information between measurements and any statistics ϕ , grows as described by [Theorem 5.](#page-3-2) Our framework offers a new perspective, according to which, the dynamics of SDE-based generative models [\(Song et al., 2021\)](#page-13-2) implicitly mimic the two steps procedure described in the box above. We claim that this is the reason why

432 433 434 435 it is possible to dissect the parametric drift of such generative models and find a *representation* of the abstract state distribution π_t , encoded into their activations. Next, we set to root our theoretical findings in experimental evidence.

5 EMPIRICAL EVIDENCE

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438 439 440 441 442 We complement existing empirical studies [\(Park et al., 2023;](#page-12-6) [Kwon et al., 2023;](#page-11-9) [Chen et al., 2023;](#page-10-3) [Linhardt et al., 2024;](#page-12-3) [Tang et al., 2023;](#page-13-3) [Xiang et al., 2023;](#page-13-6) [Haas et al., 2024;](#page-10-8) [Sclocchi et al., 2024\)](#page-12-7) that first measured the interactions between the generative process of diffusion models and latent abstractions, by focusing on a particular dataset that allows for a fine grained assessment of the influence of latent factors.

443 444 445 446 447 448 Dataset. We use the Shapes3D [\(Kim & Mnih, 2018\)](#page-11-11) dataset, which is a collection of 64×64 raytracing generated images, depicting simple 3D-scenes, with an object (a sphere, cube, ...) placed in a space, described by several attributes (color, size, orientation). Attributes have been derived from the computer program that the ray-tracing software executed to generate the scene: these are transformed into labels associated to each image. In our experiments, such labels are the materialization of the latent abstractions X we consider in this work (see [Appendix J.1](#page-21-0) for details).

449 450 451 452 453 454 455 456 457 Measurement Protocols. For our experiments, we use the base NCSPP model described by [Song](#page-13-2) [et al.](#page-13-2) [\(2021\)](#page-13-2): specifically, our denoising score network corresponds to a U-NET [\(Ronneberger et al.,](#page-12-15) [2015\)](#page-12-15). We train the unconditional version of this model from scratch, using score-matching objective. Detailed hyper-parameters and training settings are provided in [Appendix J.2.](#page-21-1) Next, we summarize three techniques to measure the emergence of latent abstractions through the lenses of the labels associated to each image in our dataset. For all such techniques, we use a specific "measurement" subset of our dataset, which we partition in 246 training, 150 validation, and 371 test examples. We use a multi-label stratification algorithm [\(Sechidis et al., 2011;](#page-12-16) Szymański & Kajdanowicz, 2017) to guarantee a balanced distribution of labels across all dataset splits.

Figure 2: Versions of an image corrupted by different values of noise for different times τ .

465 466 467 468 469 470 471 472 473 474 475 476 *Linear probing*. Each image in the measurement subset is perturbed with noise, using a variance-exploding schedule [\(Song et al., 2021\)](#page-13-2), with noise levels decreasing from $\tau = 0$ to $\tau = 1.0$ in steps of 0.1, as shown in [Figure 2.](#page-8-1) Intuitively, each time value τ can be linked to a different Signal to Noise Ratio (SNR), ranging from $SNR(\tau = 1) = \infty$ to $SNR(\tau = 0) \approx 0$. We extract several feature maps from all the linear and convolutional layers of the denoising score network, for each perturbed image, resulting in a total of 162 feature map sets for each noise level. This process yields 11 different datasets per layer, which we use to train a linear classifier (our probe) for each of these datasets, using the training subset. In these experiments, we use a batch size of 64 and adjust the learning rate based on the noise level (see [Appendix J.3\)](#page-22-0). Classifier performance is optimized by selecting models based on their log-probability accuracy observed on the validation subset. The final evaluation of each classifier is conducted on the test subset. Classification accuracy, measured by the model log likelihood, is a proxy of latent abstraction emergence [\(Chen et al., 2023\)](#page-10-3).

477 478 479 480 481 482 483 *Mutual information estimation*. We estimate mutual information between the labels and the outputs of the diffusion model across varying diffusion times, using [Equation \(39\)](#page-20-1) (which is a specialized version of our theory for linear diffusion models, see [Appendix H\)](#page-19-0) and adopt the same methodology discussed by [Franzese et al.](#page-10-16) [\(2024\)](#page-10-16) to learn conditional and unconditional score functions, and to approximate the mutual information. The training process uses a randomized conditioning scheme: 33% of training instances are conditioned on all labels, 33% on a single label, and the remaining 33% are trained unconditionally. See [Appendix J.4](#page-22-1) for additional details.

484 485 *Forking*. We propose a new technique to measure at which stage of the generative process, image features described by our labels emerge. Given an initial noise sample, we proceed with numerical integration of the backward SDE [\(Song et al., 2021\)](#page-13-2) up to time τ . At this point, we fork k replicas **490 494** of the backward process, and continue the k generative pathways independently until numerical integration concludes. We use a simple classifier (a pre-trained ResNet50 [\(He et al., 2016\)](#page-11-12) with an additional linear layer trained from scratch) to verify that labels are coherent across the k forks. Coherency is measured using the entropy of the label distribution output by our simple classifier on each latent factor for all the k forks. Intuitively: if we fork the process at time $\tau = 0.6$, and the k forks all end up displaying a cube in the image (entropy equals 0), this implies that the object shape is a latent abstraction that has already emerged by time τ . Conversely, lack of coherence implies that such a latent factor has not yet influenced the generative process. Details of the classifier training and sampling procedure are provided in [Appendix J.5.](#page-22-2)

Figure 3: Mutual information, Entropy across forked generative pathways, and Probing results as functions of τ .

510 511 512 513 514 515 516 517 518 519 520 Results. We present our results in [Figure 3.](#page-9-0) We note that some attributes like *floor hue*, *wall hue* and *shape* emerge earlier than others, which corroborates the hierarchical nature of latent abstractions, a phenomenon that is related to the spatial extent of each attribute in pixel space. This is evident from the results of linear probing, where we evaluate the performance of linear probes trained on features maps extracted from the denoiser network, and from the mutual information measurement strategy and the measured entropy of the predicted labels across forked generative pathways. Entropy decreases with τ , which marks the moment in which the generative process proceeds along k forks. When generative pathways converge to a unique scene with identical predicted labels (entropy reaches zero), this means that the model has committed to a specific set of latent factors. This coincides with the same noise level corresponding to high accuracy for the linear probe, and high-values of mutual information. Further ablation experiments are presented in [Appendix J.6.](#page-24-0)

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6 CONCLUSION

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524 525 526 527 528 Despite their tremendous success in many practical applications, a deep understanding of how SDE-based generative models operate remained elusive. A particularly intriguing aspect of several empirical work was to uncover the capacity of generative models to create entirely new data by combining latent factors learned from examples. To the best of our knowledge, there exist no theoretical framework that attempted at describing such phenomenon.

529 530 531 532 533 534 In this work, we closed this gap, and presented a novel theory — that builds on the framework of NLF — to describe the implicit dynamics allowing SDE-based generative models to tap into latent abstractions and guide the generative process. Our theory, that required advancing the standard NLF formulation, culminates in a new system of joint SDEs that fully describe the iterative process of data generation. Furthermore, we derived an information-theoretic measure to study the influence of latent abstractions, which provides a concrete understanding of the joint dynamics.

535 536 537 538 539 To root our theory into concrete examples, we collected experimental evidence by means of novel (and established) measurement strategies, that corroborates our understanding of diffusion models. Latent abstractions emerge according to an implicitly learned hierarchy, and can appear early on in the data generation process, much earlier than what is visible in the data domain. Our theory is especially useful as it allows analyses and measurements of generative pathways, opening up opportunities for a variety of applications, including image editing, and improved conditional generation.

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756 757 A ASSUMPTIONS

Assumption 2. *Whenever we mention a filtration, we assume as usual that it is augmented with the* P− *null sets, i.e. if the set* N *is such that* P(N) = 0*, then all* A ⊆ N *should be in the filtration.* Assumption 3.

$$
\mathbb{E}_{\mathcal{P}}\left[\int_0^t \|H(Y_s, X, s)\| \mathrm{d}s\right] < \infty. \tag{18}
$$

Assumption 4.

$$
P(\int_0^t \left\| \mathbb{E}_{P}[H(Y_s, X, s) \, | \, \mathcal{F}_s^Y] \right\|^2 ds < \infty) = 1. \tag{19}
$$

Eq 2.5 Fundamentals of Stochastic Filtering. Necessary for validity of [Equation \(3\).](#page-2-3) Assumption 5.

$$
\mathbb{E}_{\mathcal{P}}\left[\int_0^t \|H(Y_s, X, s)\|^2 \mathrm{d}s\right] < \infty. \tag{20}
$$

771 772 773 *Note: this assumption implies [Assumption 3](#page-14-2) and [Assumption 4.](#page-14-3) Despite it is more restrictive, it turns out that it is often easier to check.*

774 Eq 3.19 Fundamentals of Stochastic Filtering. Necessary for validity of [Theorem 3.](#page-3-0)

775 Assumption 6.

$$
\mathbb{E}_{\mathcal{P}}[\exp\left\{\frac{1}{2}\int_0^t \|H(Y_s, X, s)\|^2 \mathrm{d}s\right\}] < \infty,
$$
\n(21)

778 *and*

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$$
\mathbb{E}_{P}[\exp\left\{\frac{1}{2}\int_{0}^{t} \|\mathbb{E}_{P}[H(Y_{s}, X, s) \mid \mathcal{R}_{s}]\|^{2} \mathrm{d}s\right\}] < \infty, \tag{22}
$$

Note: [Assumption 6,](#page-14-4) as well as [Assumption 5,](#page-14-5) are trivially verified when H is bounded.

B PROOF OF T[HEOREM](#page-2-0) 2

We start by combining [Equation \(3\)](#page-2-3) and [Equation \(1\)](#page-1-1)

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$$
W_t^{\mathcal{R}} = Y_0 + \int_0^t H(Y_s, X, s)ds + W_t - Y_0 - \int_0^t \mathbb{E}_{P}(H(Y_s, X, s) | \mathcal{R}_s)ds
$$

=
$$
\int_0^t H(Y_s, X, s)ds + W_t - \int_0^t \mathbb{E}_{P}(H(Y_s, X, s) | \mathcal{R}_s)ds.
$$

We begin by showing that it is a martingale. For any $0 \le \tau \le t$ it holds

$$
\mathbb{E}_{\mathcal{P}}[W_t^{\mathcal{R}} | \mathcal{R}_{\tau}] = \mathbb{E}_{\mathcal{P}}[\int_0^t H(Y_s, X, s) \mathrm{d}s |\mathcal{R}_{\tau}] + \mathbb{E}_{\mathcal{P}}[W_t | \mathcal{R}_{\tau}]
$$

\n
$$
- \mathbb{E}_{\mathcal{P}}[\int_0^t \mathbb{E}_{\mathcal{P}}(H(s, Y_s, X) | \mathcal{R}_s) \mathrm{d}s |\mathcal{R}_{\tau}]
$$

\n
$$
= \int_0^t \mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) | \mathcal{R}_{\tau}] \mathrm{d}s + \mathbb{E}_{\mathcal{P}}[\mathbb{E}_{\mathcal{P}}[W_t | \mathcal{F}_{\tau}^{Y, X}] | \mathcal{R}_{\tau}]
$$

\n
$$
- \int_0^{\tau} \mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) | \mathcal{R}_s] \mathrm{d}s - \int_{\tau}^t \mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) | \mathcal{R}_{\tau}] \mathrm{d}s
$$

\n
$$
= \int_0^{\tau} \mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) | \mathcal{R}_{\tau}] \mathrm{d}s + \mathbb{E}_{\mathcal{P}}[W_{\tau} | \mathcal{R}_{\tau}] + W_{\tau}^{\mathcal{R}} + Y_0 - Y_{\tau}
$$

\n
$$
= \mathbb{E}_{\mathcal{P}}[\int_0^{\tau} H(Y_s, X, s) \mathrm{d}s + W_{\tau} + Y_0 - Y_{\tau} | \mathcal{R}_{\tau}] + W_{\tau}^{\mathcal{R}} = W_{\tau}^{\mathcal{R}}.
$$

809 Moreover, it is easy to check that the cross-variation of W_t^R is the same as the one of W_t . Then, we can conclude the proof by Levy's characterization of Brownian motion ($W_0^R = 0$).

C PROOF OF T[HEOREM](#page-3-0) 3

First, by combining the definition of ψ_t^R and the fact that $dY_t = \mathbb{E}_{P}[H(Y_t, X, t) | \mathcal{R}_t] + dW_t^R$ we obtain

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$$
(\psi_t^{\mathcal{R}})^{-1} = \exp\biggl(-\int_0^t \mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) \mid \mathcal{R}_s] \mathrm{d}W_s^{\mathcal{R}} - \frac{1}{2} \int_0^t \|\mathbb{E}_{\mathcal{P}}[H(Y_s, X, s) \mid \mathcal{R}_s]\|^2 \mathrm{d}s\biggr). \tag{23}
$$

Notice that by [Assumption 6](#page-14-4) (which is actually the usual Novikov's condition), the local martingale $(\psi_t^R)^{-1}$ is a real-valued martingale starting from $(\psi_0^R)^{-1} = 1$. Then, we can apply Girsanov theorem and conclude that $dQ^{\mathcal{R}} = \psi_T^{\mathcal{R}} dP$ is a probability measure under which the process $\{\tilde{W}_{0\leq t\leq T}, \mathcal{R}_{0\leq t\leq T}\}$, with

$$
\tilde{W}_t = W_t^{\mathcal{R}} + \int_0^t \mathbb{E}_{\mathcal{P}}[H(Y_t, X, s) | \mathcal{R}_t] \mathrm{d}s,
$$

is a Brownian motion on the space $(\Omega, \mathcal{R}_T, \mathbb{Q}^{\mathcal{R}})$.

D PROOF OF T[HEOREM](#page-3-1) 4

First, let us give a precise meaning to being a weak solution of [Equation \(6\).](#page-3-4) We say that $\pi^\mathcal{R}_t$ solves [\(6\)](#page-3-4) in a weak sense in, for any for any $\phi : \mathcal{S} \to \mathbb{R}$ bounded and measurable, it holds

$$
\langle \pi_t^{\mathcal{R}}, \phi \rangle = \langle \pi_0^{\mathcal{R}}, \phi \rangle + \int_0^t \left(\langle \pi_s^{\mathcal{R}}, H(Y_s, \cdot, s) \phi \rangle - \langle \pi_s^{\mathcal{R}}, \phi \rangle \langle \pi_s^{\mathcal{R}}, H(Y_s, \cdot, s) \rangle \right) \left(dY_s - \langle \pi_s^{\mathcal{R}}, H(Y_s, \cdot, s) \rangle ds \right).
$$
\n(24)

Let us recall that, on (Ω, \mathcal{F}, P) , the process Y_t has the SDE representation [\(1\)](#page-1-1), where $\{W_{0\leq t\leq T}, \mathcal{F}_{0\leq t\leq T}^{Y,X}\}$ is a Brownian motion. Moreover, by [Theorem 3](#page-3-0) with $\mathcal{R}_t = \mathcal{F}_t^{Y,X}$, it holds that $\{(Y - Y_0)_{0 \le t \le T}, \mathcal{F}_{0 \le t \le T}^{Y, X}\}$ is a Brownian motion on the space $(\Omega, \mathcal{F}, \mathbf{Q}^{\mathcal{F}^{Y, X}})$, where $dQ^{\mathcal{F}^{Y,X}} = (\psi_T^{\mathcal{F}^{Y,X}})^{-1} dP$ and

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847

863

$$
\psi_t^{\mathcal{F}^{Y,X}} = \exp\biggl(\int_0^t H(Y_s, X, s) \mathrm{d}Y_s - \frac{1}{2} \int_0^t \|H(Y_s, X, s)\|^2 \mathrm{d}s\biggr). \tag{25}
$$

844 845 846 For notation simplicity, in this subsection $\psi_t^{\mathcal{F}^{Y,X}}$ and $Q^{\mathcal{F}^{Y,X}}$ are simply indicated as π_t , ψ_t and Q respectively.

848 Since we aim at showing that [\(24\)](#page-15-2) holds, let us fix ϕ and let us start from $\mathbb{E}_{P}[\phi(X) | \mathcal{R}_t] = \langle \pi_t^{\mathcal{R}}, \phi \rangle$. Bayes Theorem provides us with the following

$$
\langle \pi_t^{\mathcal{R}}, \phi \rangle = \mathbb{E}_{\mathcal{P}}[\phi(X) \mid \mathcal{R}_t] = \frac{\mathbb{E}_{\mathcal{Q}}[\frac{d\mathcal{P}}{d\mathcal{Q}}\phi(X) \mid \mathcal{R}_t]}{\mathbb{E}_{\mathcal{Q}}[\frac{d\mathcal{P}}{d\mathcal{Q}} \mid \mathcal{R}_t]} = \frac{\mathbb{E}_{\mathcal{Q}}[\psi_T \phi(X) \mid \mathcal{R}_t]}{\mathbb{E}_{\mathcal{Q}}[\psi_T \mid \mathcal{R}_t]} \stackrel{\text{def}}{=} \frac{\langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle}. \tag{26}
$$

Starting from the numerator $\langle \hat{\pi}_t^R, \phi \rangle$, we involve the tower property of conditional expectation and the fact that ψ_t is $\mathcal{F}^{Y,X}_t$ measurable to write

$$
\langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle = \mathbb{E}_{\mathcal{Q}}[\psi_T \phi(X) | \mathcal{R}_t] = \mathbb{E}_{\mathcal{Q}}\left[\mathbb{E}_{\mathcal{Q}}\left[\psi_T \phi(X) | \mathcal{F}_t^{Y,X}\right] | \mathcal{R}_t\right]
$$

$$
= \mathbb{E}_{\mathcal{Q}}\left[\mathbb{E}_{\mathcal{Q}}\left[\psi_T | \mathcal{F}_t^{Y,X}\right] \phi(X) | \mathcal{R}_t\right] = \mathbb{E}_{\mathcal{Q}}\left[\psi_t \phi(X) | \mathcal{R}_t\right].
$$
(27)

Recalling the definition of ψ_t (see [Equation \(25\)\)](#page-15-3), we have

$$
d\psi_t = \psi_t H(Y_t, X, t) dY_t,
$$
\n(28)

862 from which it follows

$$
\psi_t = 1 + \int_0^t \psi_s H(Y_s, X, s) \, dY_s. \tag{29}
$$

We continue processing [Equation \(27\),](#page-15-4) using [Equation \(29\),](#page-15-5) as

$$
\mathbb{E}_{\mathbf{Q}}\left[\psi_t\phi(X)\,|\,\mathcal{R}_s\right] = \mathbb{E}_{\mathbf{Q}}\left[\left(1 + \int_0^t \psi_s H(Y_s, X, s) \mathrm{d}Y_s\right) \phi(X)\,|\,\mathcal{R}_t\right]
$$

$$
= \mathbb{E}_{\mathbf{Q}} \left[\phi(X) \,|\, \mathcal{R}_t \right] + \mathbb{E}_{\mathbf{Q}} \left[\int_0^t \psi_s H(Y_s, X, s) \phi(X) \mathrm{d}Y_s \,|\, \mathcal{R}_t \right]
$$

=
$$
\mathbb{E}_{\mathbf{Q}} \left[\phi(X) \,|\, \mathcal{R}_t \right] + \int_0^t \mathbb{E}_{\mathbf{Q}} \left[\psi_s H(Y_s, X, s) \phi(X) \,|\, \mathcal{R}_s \right] \mathrm{d}Y_s,
$$

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> where to obtain the last equality we used Lemma 5.4 in [Xiong](#page-13-9) [\(2008\)](#page-13-9). We also recall that, under Q, the process $(Y_t - Y_0)$ is independent of X. Thus, since $\mathcal{R}_t = \sigma(\mathcal{R}_0 \cup \sigma(Y_{0 \le s \le t} - Y_0))$ and $\frac{dP}{dQ} \mid_{\mathcal{F}_0^{Y,X}} = 1$, we obtain $\mathbb{E}_Q [\phi(X) | \mathcal{R}_t] = \mathbb{E}_P [\phi(X) | \mathcal{R}_0]$. Concluding and rearranging:

$$
\langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle = \langle \hat{\pi}_0^{\mathcal{R}}, \phi \rangle + \int_0^t \langle \hat{\pi}_s^{\mathcal{R}}, \phi H(Y_s, \cdot, s) \rangle dY_s.
$$

Obviously by the same arguments $\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle = \mathbb{E}_{\mathbf{Q}}[\frac{\mathrm{dP}}{\mathrm{dQ}} | \mathcal{R}_t] = \mathbb{E}_{\mathbf{Q}}[\psi_t | \mathcal{R}_t]$, and

$$
\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle = 1 + \int_0^t \langle \hat{\pi}_s^{\mathcal{R}}, H(Y_s, \cdot, s) \rangle \mathrm{d}Y_s. \tag{30}
$$

From now on, for simplicity we assume that all the processes involved in our computations are 1-dimensional. The extension to the multidimensional case is trivial. First, let us notice that, by [\(30\)](#page-16-1) and Itô's lemma, it holds

$$
d\left(\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^{-1}\right) = -\frac{\langle \hat{\pi}_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^2} dY_s + \frac{\langle \hat{\pi}_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle^2}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^3} dt.
$$
 (31)

Then, by the stochastic product rule,

$$
d\langle \pi_t^{\mathcal{R}}, \psi \rangle = d\left(\langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle \langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^{-1} \right)
$$

\n
$$
= \langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle d\left(\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^{-1} \right) + \langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^{-1} d\langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle - \langle \hat{\pi}_t^{\mathcal{R}}, \phi H(Y_t, \cdot, t) \rangle \frac{\langle \hat{\pi}_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^2} dt
$$

\n
$$
= -\langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle \frac{\langle \hat{\pi}_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^2} dY_t + \langle \hat{\pi}_t^{\mathcal{R}}, \phi \rangle \frac{\langle \hat{\pi}_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle^2}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^3} dt
$$

\n
$$
+ \frac{\langle \hat{\pi}_t^{\mathcal{R}}, \phi H(Y_t, \cdot, t) \rangle}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle} dY_t - \langle \hat{\pi}_t^{\mathcal{R}}, \phi H(Y_t, \cdot, t) \rangle \frac{\langle \hat{\pi}_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle}{\langle \hat{\pi}_t^{\mathcal{R}}, 1 \rangle^2} dt.
$$

Recalling [\(26\)](#page-15-6) and rearranging the terms lead us to

$$
d\langle \pi_t^{\mathcal{R}}, \psi \rangle = -\langle \pi_t^{\mathcal{R}}, \phi \rangle \langle \pi_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle dY_t + \langle \pi_t^{\mathcal{R}}, \phi \rangle \langle \pi_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle^2 dt + \langle \pi_t^{\mathcal{R}}, \phi H(Y_t, \cdot, t) \rangle dY_t - \langle \pi_t^{\mathcal{R}}, \phi H(Y_t, \cdot, t) \rangle \langle \pi_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle dt = \left(\langle \pi_t^{\mathcal{R}}, \phi H(Y_t, \cdot, t) \rangle - \langle \pi_t^{\mathcal{R}}, \phi \rangle \langle \pi_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle \right) \left(dY_t - \langle \pi_t^{\mathcal{R}}, H(Y_t, \cdot, t) \rangle dt \right).
$$

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E PROOF OF T[HEOREM](#page-3-2) 5

910 911 912 913 The proof of this Theorem involves two separate parts. First, we should show the second equality in [Equation \(7\),](#page-3-6) i.e. $\int \log \frac{dP_{\# Y_{0\leq s\leq t},\phi}}{dP_{\# Y_{0\leq s\leq t}} dP_{\# Y_{0\leq s\leq t},\phi}} = \mathbb{E}_{P} \left[\log \frac{dP |_{\mathcal{R}_t}}{dP |_{\mathcal{F}_t^Y} dP |_{\sigma(\phi)}} \right]$. Then, we should prove that the r.h.s of [Equation \(7\)](#page-3-6) is equal to [Equation \(8\).](#page-3-5)

915 E.1 PART 1

917 We overload in this Section the notation adopted in the rest of the paper for sake of simplicity in exposition. A random variable X on a probability space (Ω, \mathcal{F}, P) is defined as a measurable **918 919 920 921 922 923 924** mapping $X : \Omega \to \Psi$, where the measure space (Ψ, \mathcal{G}) satisfies the usual assumptions. To be precise, X is measurable w.r.t. F if $\forall E \in \mathcal{G}, X^{-1}(E) \in \mathcal{F}$, where $X^{-1}(E) = \{ \omega \in \Omega : X(\omega) \in E \}.$ Equivalently, $\forall E \in \mathcal{G}, \exists S \in \mathcal{F} : X(S) = E$. Of all the possible sigma-algebras which allow measurability, the sigma algebra induced by the random variable, $\sigma(X)$, is the *smallest* one. It can be shown that $\sigma(X) = X^{-1}(\mathcal{G}) = \{A = X^{-1}(B)| B \in \mathcal{G}\}$. We also denote by $P_{\#}X: \mathcal{G} \to [0,1]$ the push-forward measure associated to X (i.e. the law), which is defined by the relation $P_{\#X}(E)$ = $P(X^{-1}(E))$ for any $E \in \mathcal{G}$. Moreover, for any \mathcal{G} -measurable ϕ , the following integration rule holds

$$
\int_{\Psi} \varphi(x) dP_{\#X}(x) = \int_{\Omega} \varphi(X(\omega)) dP(\omega).
$$
\n(32)

928 929 930 931 932 Let us focus on $(\Omega, \sigma(X), P)$ and let us consider a new measure Q absolutely continuous w.r.t. P. Radon-Nikodym theorem guarantees existence of a $\sigma(X)$ -measurable function $Z: \Omega \to [0, +\infty)$ (the "derivative" $\frac{dQ}{dP} = Z$) such that $Q(A) = \int_A Z dP$, for all $A \in \sigma(X)$. Moreover, by Doob's measurability criterion (see e.g. Lemma 1.13 in [Kallenberg](#page-11-13) [\(2002\)](#page-11-13)), there exists a G-measurable map $f: \Psi \to [0, +\infty)$ such that $Z = f(X)$. Then, for any $E \in \mathcal{G}$,

$$
Q_{\#X}(E) = Q(X^{-1}(E)) = \int_{X^{-1}(E)} f(X)dP(\omega) = \int_{\Omega} \mathbf{1}_{X^{-1}(E)}(\omega)f(X(\omega))dP(\omega)
$$

$$
= \int_{\Omega} \mathbf{1}_{E}(X(\omega))f(X(\omega))dP(\omega) = \int_{\Psi} \mathbf{1}_{E}(x)f(x)dP_{\#X}(x) = \int_{E} f(x)dP_{\#X}(x).
$$

In summary, we have that $\frac{dQ_{\#X}}{dP_{\#X}} = f$, with $f: \Psi \to [0, +\infty)$.

Finally, then,

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$$
\int_{\Psi} \log \left(\frac{dP_{\#X}}{dQ_{\#X}} \right) dP_{\#X} = -\int_{\Psi} \log(f) dP_{\#X} = -\int_{\Omega} \log(f(X)) dP = \int_{\Omega} \log \frac{dP}{dQ} dP = \mathbb{E}_{P} [\log \frac{dP}{dQ}].
$$
\n(33)

What discussed so far, allows to prove that $\int \log \frac{dP_{\#Y_{0\leq s\leq t},\phi}}{dP_{\#Y_{0\leq s\leq t}}dP_{\#Y_{0\leq s\leq t},\phi}}$ = $\mathbb{E}_{\mathrm{P}}\left[\log\frac{\mathrm{d}\mathrm{P}\mid_{\mathcal{R}_t}}{\mathrm{d}\mathrm{P}\mid_{\mathcal{F}_t^Y}\mathrm{d}\mathrm{P}\mid_{\sigma(\phi)}}\right]$. Indeed:

- Consider on the space $(\Omega, \mathcal{R}_t, P |_{\mathcal{R}_t})$ the random variable $T = (Y_{0 \le s \le t}, \phi)$. By construction, $\sigma(T) = \mathcal{R}_t$.
- Suppose that $P|_{\mathcal{R}_t}$ is absolutely continuous w.r.t $P|_{\mathcal{F}_t^Y} \times P|_{\sigma(\phi)}$ (proved in the next subsection).
- Then the desired equality follows from [Equation \(33\).](#page-17-0)

E.2 PART 2

Before proceeding, remember that the following holds: for all $\mathcal{R}'_t \subseteq \mathcal{R}_t$, $\mathbf{Q}^{\mathcal{R}} \mid_{\mathcal{R}'_t} = \mathbf{Q}^{\mathcal{R}'} \mid_{\mathcal{R}'_t}$. We restart from the r.h.s. of [Equation \(7\).](#page-3-6) Thanks to the chain rule for Radon-Nykodim derivatives

$$
\log \frac{dP|\pi_t}{dP|\mathcal{F}_t^Y dP|\sigma(\phi)} = \log \frac{dP|\pi_t}{dQ^{\mathcal{R}}|\pi_t} \frac{dQ^{\mathcal{R}}|\pi_t}{dP|\mathcal{F}_t^Y dP|\sigma(\phi)}
$$

\n
$$
= \log \frac{dP|\pi_t}{dQ^{\mathcal{R}}|\pi_t} \frac{dQ^{\mathcal{R}}|\mathcal{F}_t^Y}{dP|\mathcal{F}_t^Y} \frac{dQ^{\mathcal{R}}|\pi_t}{dQ^{\mathcal{R}}|\mathcal{F}_t^Y dP|\sigma(\phi)}
$$

\n
$$
= \log \frac{dP|\pi_t}{dQ^{\mathcal{R}}|\pi_t} \frac{dQ^{\mathcal{F}^Y}|\mathcal{F}_t^Y}{dP|\mathcal{F}_t^Y} \frac{dQ^{\mathcal{R}}|\pi_t}{dQ^{\mathcal{R}}|\mathcal{F}_t^Y dP|\sigma(\phi)}
$$

\n
$$
= \log \psi_t^{\mathcal{R}}(\psi_t^{\mathcal{F}^Y})^{-1} \frac{dQ^{\mathcal{R}}|\mathcal{F}_t^Y}{dQ^{\mathcal{R}}|\mathcal{F}_t^Y dP|\sigma(\phi)}
$$

$$
= \log \psi_t^{\mathcal{R}} - \log \psi_t^{\mathcal{F}^Y} + \log \frac{\mathrm{d} \mathrm{Q}^{\mathcal{R}} \mid_{\mathcal{R}_t}}{\mathrm{d} \mathrm{Q}^{\mathcal{R}} \mid_{\mathcal{F}_t^Y} \mathrm{d} \mathrm{Q}^{\mathcal{R}} \mid_{\sigma(\phi)}},
$$

972 973 974 where we used [Theorem 3](#page-3-0) to make $\psi_t^{\mathcal{R}}$ and $\psi_t^{\mathcal{F}^Y}$ appear, and the fact that $dQ^{\mathcal{R}}|_{\sigma(\phi)} = dP|_{\sigma(\phi)}$. Consequently

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$$
\mathbb{E}_{\mathcal{P}}\left[\log \frac{d\mathcal{P}|\mathcal{R}_{t}}{d\mathcal{P}|\mathcal{F}_{t}d\mathcal{P}|\sigma(\phi)}\right] = \mathbb{E}_{\mathcal{P}}\left[\log \psi_{t}^{\mathcal{R}} - \log \psi_{t}^{\mathcal{F}^{Y}}\right] + \mathcal{I}(Y_{0};\phi)
$$
\n
$$
= \mathbb{E}_{\mathcal{P}}\left[\int_{0}^{t} \mathbb{E}_{\mathcal{P}}[h(Y_{s}, X, s) | \mathcal{R}_{s}]dW_{s}^{\mathcal{R}} + \frac{1}{2}\int_{0}^{t} \|\mathbb{E}_{\mathcal{P}}[h(Y_{s}, X, s) | \mathcal{R}_{s}]\|^{2}ds\right]
$$
\n
$$
- \mathbb{E}_{\mathcal{P}}\left[\int_{0}^{t} \mathbb{E}_{\mathcal{P}}[h(Y_{s}, X, s) | \mathcal{F}_{s}^{Y}]dW_{s}^{\mathcal{F}^{Y}} + \frac{1}{2}\int_{0}^{t} \|\mathbb{E}_{\mathcal{P}}[h(Y_{s}, X, s) | \mathcal{F}_{s}^{Y}]\|^{2}ds\right] + \mathcal{I}(Y_{0};\phi)
$$
\n
$$
= \frac{1}{2} \mathbb{E}_{\mathcal{P}}\left[\int_{0}^{t} \|\mathbb{E}_{\mathcal{P}}[h(Y_{s}, X, s) | \mathcal{R}_{s}]\|^{2} - \|\mathbb{E}_{\mathcal{P}}[h(Y_{s}, X, s) | \mathcal{F}_{s}^{Y}]\|^{2}ds\right] + \mathcal{I}(Y_{0};\phi).
$$

Actually, the result in the main is in a slightly different form. To show equivalence, it is necessary to prove that

$$
\mathbb{E}_{P}\left[\left\|\mathbb{E}_{P}[h(Y_{s}, X, s) | \mathcal{F}_{s}^{Y}]\right\|^{2}\right] - 2\mathbb{E}_{P}\left[\mathbb{E}_{P}[h(Y_{s}, X, s) | \mathcal{F}_{s}^{Y}]\mathbb{E}_{P}[h(Y_{s}, X, s) | \mathcal{R}_{s}]\right]
$$

$$
= -\mathbb{E}_{P}\left[\left\|\mathbb{E}_{P}[h(Y_{s}, X, s) | \mathcal{F}_{s}^{Y}]\right\|^{2}\right]
$$

which is trivially true since $\mathbb{E}_{P}\left[\cdot | \mathcal{F}_{t}^{Y}\right] = \mathbb{E}_{P}\left[\mathbb{E}_{P}\left[\cdot | \mathcal{R}_{s}\right] | \mathcal{F}_{t}^{Y}\right]$.

F PROOF OF T[HEOREM](#page-4-0) 6

F.1 PROOF OF E[QUATION](#page-4-2) (9)

The inequality is proven considering that: i)

$$
\mathcal{I}(Y_{0 \le s \le t}; \phi) = \mathbb{E}_{P|_{\mathcal{F}_t^Y} \times P|_{\sigma(\phi)}} \left[\eta \left(\frac{\mathrm{d}P|_{\mathcal{R}_t}}{\mathrm{d}P|_{\mathcal{F}_t^Y} \mathrm{d}P|_{\sigma(\phi)}} \right) \right]
$$

and

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$$
\mathcal{I}(\tilde{Y}_t; \phi) = \mathbb{E}_{P|_{\sigma(\tilde{Y}_t)} \times P|_{\sigma(\phi)}} \left[\eta \left(\frac{dP|_{\sigma(\tilde{Y}_t, \phi)}}{dP|_{\sigma(\tilde{Y}_t)} dP|_{\sigma(\phi)}} \right) \right] = \mathbb{E}_{P|_{\mathcal{F}_t^Y} \times P|_{\sigma(\phi)}} \left[\eta \left(\frac{dP|_{\sigma(\tilde{Y}_t, \phi)}}{dP|_{\sigma(\tilde{Y}_t)} dP|_{\sigma(\phi)}} \right) \right],
$$

1007 1008 1009 with $\eta(x) = x \log x$, ii) that $\frac{dP|_{\sigma(\tilde{Y}_t, \phi)}}{dP|_{\sigma(\tilde{Y}_t)} dP|_{\sigma(\phi)}} = \mathbb{E}_{P|_{\mathcal{F}_t^Y} \times P|_{\sigma(\phi)}}$ $\left[\begin{array}{cc} dP & \pi_t \end{array}\right]$ $\frac{dP | \pi_t}{dP |_{\mathcal{F}_t^Y} dP |_{\sigma(\phi)}} | \sigma(\tilde{Y}_t, \phi)]$ and iii) that Jensen's inequality holds (η is convex on its domain)

1010 1011

$$
\mathbb{E}_{P|_{\mathcal{F}_{t}^{Y}} \times P|_{\sigma(\phi)}} \left[\eta \left(\frac{dP|_{\sigma(\tilde{Y}_{t}, \phi)}}{dP|_{\sigma(\tilde{Y}_{t})} dP|_{\sigma(\phi)}} \right) \right]
$$
\n
$$
= \mathbb{E}_{P|_{\mathcal{F}_{t}^{Y}} \times P|_{\sigma(\phi)}} \left[\eta \left(\mathbb{E}_{P|_{\mathcal{F}_{t}^{Y}} \times P|_{\sigma(\phi)}} \left[\frac{dP|_{\mathcal{R}_{t}}}{dP|_{\mathcal{F}_{t}^{Y}} dP|_{\sigma(\phi)}} | \sigma(\tilde{Y}_{t}, \phi) \right] \right) \right]
$$
\n
$$
\leq \mathbb{E}_{P|_{\mathcal{F}_{t}^{Y}} \times P|_{\sigma(\phi)}} \left[\mathbb{E}_{P|_{\mathcal{F}_{t}^{Y}} \times P|_{\sigma(\phi)}} \left[\eta \left(\frac{dP|_{\mathcal{R}_{t}}}{dP|_{\mathcal{F}_{t}^{Y}} dP|_{\sigma(\phi)}} \right) | \sigma(\tilde{Y}_{t}, \phi) \right] \right]
$$
\n
$$
= \mathbb{E}_{P|_{\mathcal{F}_{t}^{Y}} \times P|_{\sigma(\phi)}} \left[\eta \left(\frac{dP|_{\mathcal{R}_{t}}}{dP|_{\mathcal{F}_{t}^{Y}} dP|_{\sigma(\phi)}} \right) \right].
$$

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1023 F.2 PROOF OF CONDITIONAL INDEPENDENCE AND MUTUAL INFORMATION EQUALITY

1025 Formally the condition of conditional independence given π is satisfied if for any a_1, a_2 positive random variables which are respectively $\sigma(X)$ and \mathcal{F}_t^Y measurable, the following holds:

1026 1027 1028 $\mathbb{E}_{\mathrm{P}}[a_1a_2 | \sigma(\pi_t)] = \mathbb{E}_{\mathrm{P}}[a_1 | \sigma(\pi_t)] \mathbb{E}_{\mathrm{P}}[a_2 | \sigma(\pi_t)]$ (see for instance [Van Putten & van Schuppen](#page-13-10) [\(1985\)](#page-13-10)).

1029 1030 1031 1032 1033 1034 The sigma-algebra $\sigma(\pi_t)$ is by definition the smallest one that makes π_t measurable. Since π_t is \mathcal{F}_t^Y measurable, clearly $\sigma(\pi_t) \subseteq \mathcal{F}_t^Y$. By the very definition of conditional expectation, $\mathbb{E}_{P}[a_1 | \mathcal{F}_{t_1}^Y] = \langle \pi_t, a_1 \rangle$, which is an $\sigma(\pi_t)$ measurable quantity. Then $\mathbb{E}_{P}[a_1a_2 | \sigma(\pi_t)] =$ $\mathbb{E}_{\mathrm{P}}[\mathbb{E}_{\mathrm{P}}[a_1a_2\,|\,\mathcal{F}_t^Y]\,|\,\sigma(\pi_t)] \hspace{2mm} = \hspace{2mm} \mathbb{E}_{\mathrm{P}}[\mathbb{E}_{\mathrm{P}}[a_1\,|\,\mathcal{F}_t^Y]a_2\,|\,\sigma(\pi_t)] \hspace{2mm} = \hspace{2mm} \mathbb{E}_{\mathrm{P}}[\mathbb{E}_{\mathrm{P}}[\langle \pi_t, a_1\rangle a_2\,|\,\sigma(\pi_t)] \hspace{2mm} = \hspace{2mm}$ $\langle \pi_t, a_1 \rangle \mathbb{E}_P[a_2 | \sigma(\pi_t)].$ Since $\langle \pi_t, a_1 \rangle = \mathbb{E}_P[\langle \pi_t, a_1 \rangle | \sigma(\pi_t)] = \mathbb{E}_P[\mathbb{E}_P[a_1 | \mathcal{F}_t^{\bar{Y}}] | \sigma(\pi_t)] =$ $\mathbb{E}_{P}[a_1 | \sigma(\pi_t)]$, the proof of conditional independence is concluded.

1035 1036 1037 1038 1039 1040 1041 In summary, $\sigma(X)$ and \mathcal{F}^Y_t are conditionally independent given $\sigma(\pi_t) \subset \mathcal{F}^Y_t$. This implies that $P(A | \sigma(\pi_t)) = P(A | \mathcal{F}_t^Y)$, $\forall A \in \sigma(X)$, or equivalently $\mathbb{E}_P[\mathbf{1}(A) | \sigma(\pi_t)] =$ $\mathbb{E}_{\mathbb{P}}[1(A) | \mathcal{F}_t^Y].$ To prove this, it is sufficient to show that for any $B \in \mathcal{F}_t^Y$, $\mathbb{E}_{\mathrm{P}}[\mathbb{E}_{\mathrm{P}}[1(A)] \sigma(\pi_t)]1(B)] = \mathbb{E}_{\mathrm{P}}[1(A)1(B)].$ By standard properties of conditional expectation $\mathbb{E}_{P}[\mathbb{E}_{P}[1(A)|\sigma(\pi_{t})]1(B)] = \mathbb{E}_{P}[\mathbb{E}_{P}[1(A)|\sigma(\pi_{t})]\mathbb{E}_{P}[1(B)|\sigma(\pi_{t})]].$ Due to conditional independence $\mathbb{E}_{P}[\mathbf{1}(A)|\sigma(\pi_t)|\mathbb{E}_{P}[\mathbf{1}(B)|\sigma(\pi_t)]=\mathbb{E}_{P}[\mathbf{1}(A)\mathbf{1}(B)|\sigma(\pi_t)].$ Then, $\mathbb{E}_{\mathrm{P}}[\mathbb{E}_{\mathrm{P}}[1(A)\mid\sigma(\pi_t)|\mathbb{E}_{\mathrm{P}}[1(B)\mid\sigma(\pi_t)]] = \mathbb{E}_{\mathrm{P}}[\mathbb{E}_{\mathrm{P}}[1(A)1(B)\mid\sigma(\pi_t)]] = \mathbb{E}_{\mathrm{P}}[1(A)1(B)].$

1042 1043 1044 The mutual information equality is then proved considering that $\frac{dP |_{\mathcal{R}_t}}{dP |_{\mathcal{F}_t^Y} dP |_{\sigma(\phi)}} = \frac{dP(\omega^x | \mathcal{F}_t^Y)}{dP(\omega^x)}$ $\frac{(\omega + \mathcal{F}_t)}{dP(\omega^x)}$, since the conditional probabilities exist, and that $P(\omega^x | \mathcal{F}_t^Y) = P(\omega^x | \sigma(\pi_t)).$

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G A TECHNICAL NOTE

1048 1049 1050 1051 1052 1053 1054 1055 1056 1057 As anticipated in the main, [Assumption 1](#page-4-4) might be incompatible with the other technical assumptions in [Appendix A.](#page-14-0) The problem might arise for singularities in the drift term at time $t = T$, which are usually present in the construction of dynamics satisfying [Assumption 1](#page-4-4) like stochastic bridges. This mathematical subtlety can be more clearly interpreted by noticing that when [Assumption 1](#page-4-4) is satisfied the evolution of the posterior process π_t at time T can occupy a portion of the space of dimensionality lower than at any $T - \epsilon$, $\epsilon > 0$. Or, we can notice that if [Assumption 1](#page-4-4) is satisfied, $\mathcal{I}(Y_{0\leq s\leq T};V)=\mathcal{I}(V;V)$ which can be equal to infinity depending on the actual structure of S and the mapping V . In many cases, a simple technical solution is to consider in the analysis only dynamics of the process in the time interval $[0, T)^3$ $[0, T)^3$. In the reduced time interval $[0, T)$, the technical assumptions are generally shown to be satisfied. For the practical purposes explored in this work this restriction makes no difference, and consequently neglect it for the rest of our discussion.

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H LINEAR DIFFUSION MODELS

1061 1062 1063 1064 Consider the particular case of **linear** generative diffusion models [Song et al.](#page-13-2) [\(2021\)](#page-13-2), which are widely adopted in the literature and by practitioners. We consider the particular case of [Equation \(11\),](#page-5-2) where the function F has linear expression

$$
\hat{Y}_t = \hat{Y}_0 - \alpha \int_0^t \hat{Y}_s \, \mathrm{d}s + \hat{W}_t,\tag{34}
$$

1068 1069 1070 1071 1072 1073 for a given $\alpha \geq 0$. We assume of course again that [Assumption 1](#page-4-4) holds, which implies that we should select $\hat{Y}_0 = Y_T = V$. Now, α dictates the behavior of the SDE, which can be cast to the so called Variance-Preserving and Variance Exploding schedules of diffusion models [Song et al.](#page-13-2) [\(2021\)](#page-13-2). In diffusion models jargon, [Equation \(34\)](#page-19-3) is typically referred to as a *noising* process. Indeed, by analysing the evolution of [Equation \(34\),](#page-19-3) \hat{Y}_t evolves to a noisier and noisier version of V as t grows. In particular, it holds that

$$
\frac{1074}{1075}
$$

$$
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$$

 $\hat{Y}_t = \exp(-\alpha t)V + \exp(-\alpha t)\int_0^t$ 0 $\exp(\alpha s) \mathrm{d}\hat{W}_{s}.$

¹⁰⁷⁷ 1078 1079 ³This is akin to the discussion of *arbitrage* strategies in finance when the initial filtration is augmented with knowledge of the future value at certain time instants, and the fact that while the new process adapted w.r.t the new filtration is also a martingale w.r.t. a given new measure for all $t \in [0, T)$, it fails to do so for $t = T$ (thus giving an arbitrage opportunity).

1080 1081 The next result is a particular case of [Theorem 7.](#page-5-1)

1082 1083 Lemma 1. *Consider the stochastic process* Y_t *which solves [Equation](#page-19-3)* (34)*. The same stochastic* process also admits a \mathcal{F}^Y_t –adapted representation

$$
Y_t = Y_0 + \int_0^t \alpha Y_s + 2\alpha \frac{\exp(-\alpha(T-s))\mathbb{E}_{P}[V|\sigma(Y_s)] - Y_s}{1 - \exp(-2\alpha(T-s))}ds + W_t,
$$
 (35)

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1087 1088 1089 *where* $Y_0 = \exp(-\alpha T)V + \sqrt{\frac{1-\exp(-2\alpha T)}{2\alpha}}$ $\frac{2a-2\alpha+1}{2\alpha}$ *c*, with ϵ a standard Gaussian random variable indepen*dent of* V *and* W_t *.*

1090 1091 1092 1093 1094 1095 As discussed in the main paper, we can now show that the same generative dynamics can be obtained under the NLF framework we present in this work, without the need to explicitly defining a backward and a forward process. In particular, we can directly select a observation function that corresponds to an Orstein-Uhlenbeck bridge [\(Mazzolo, 2017;](#page-12-17) [Corlay, 2013\)](#page-10-17), consequently satisfying [Assumption 1,](#page-4-4) and obtain the generative dynamics of classical diffusion models. In particular we consider the following about H^4 H^4 :

1096 Assumption 7. *The function* H *in [Equation](#page-1-1)* (1) *is selected to be of the linear form*

$$
H(Y_t, X, t) = m_t V - \frac{\mathrm{d}\log m_t}{\mathrm{d}t} Y_t,\tag{36}
$$

1100 1101 1102 1103 with $m_t = \frac{\alpha}{\sinh{(\alpha(T-t))}}$, where $\alpha \ge 0$. When $\alpha = 0$, $m_t = \frac{d \log m_t}{dt} = \frac{1}{T-t}$. Furthermore, Y_0 is $s^{e}}$ *selected as in [Theorem 7.](#page-5-1) Under this assumption,* $Y_T = V$, $P - a.s.,$ *i.e. [Assumption 1](#page-4-4) is satisfied [\[Proof\].](#page-20-3)*

1104 1105 1106 In summary, the particular case of [Equation \(1\)](#page-1-1) (which is $\mathcal{F}^{Y,X}$ adapted) under [Assumption 7,](#page-20-4) can be transformed into a generative model leveraging [Theorem 2,](#page-2-0) since [Assumption 1](#page-4-4) holds. When doing so, we obtain that the process Y_t has \mathcal{F}^Y adapted representation equal to

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$$
Y_t = Y_0 + \int_0^t m_s \mathbb{E}_{\mathcal{P}}(V \, | \, \mathcal{F}_s^Y) \mathrm{d}s - \int_0^t \frac{\mathrm{d}\log m_s}{\mathrm{d}s} Y_s \mathrm{d}s + W_t^{\mathcal{F}^Y},\tag{37}
$$

1110 1111 1112 which is nothing but [Equation \(35\)](#page-20-5) after some simple algebraic manipulation. The only relevant detail worth deeper exposition is the clarification about the actual computation of expectation of interest. If P is selected such that \hat{Y}_t solves [Equation \(34\),](#page-19-3) we have that

$$
\mathbb{E}_{P}(V|\mathcal{F}_{t}^{Y}) = \mathbb{E}_{P}(Y_{T}|\sigma(Y_{0\leq s\leq t})) = \mathbb{E}_{P}(\hat{Y}_{0}|\sigma(\hat{Y}_{T-t\leq s\leq T})) = \mathbb{E}_{P}(\hat{Y}_{0}|\sigma(\hat{Y}_{T-t})) = \mathbb{E}_{P}(V|\sigma(Y_{t})),
$$
\n(38)

1116 where the second to last equality is due to the Markov nature of \hat{Y}_t .

1117 1118 1119 Moreover, in this particular case we can express the mutual information $\mathcal{I}(Y_{0 \le s \le t}; \phi) = \mathcal{I}(Y_t; \phi)$ (where we removed the past of Y since the following Markov chain holds $\phi \to \overline{\hat{Y}}_0 \to \hat{Y}_{t>0}$) can be expressed in the simpler form

$$
\mathcal{I}(Y_t; \phi) = \mathcal{I}(Y_0; \phi) + \frac{1}{2} \mathbb{E}_{P} \left[\int_0^t m_s^2 \|\mathbb{E}_{P}[V | \sigma(Y_s)] - \mathbb{E}_{P}[V | \sigma(Y_s, \phi)]\|^2 ds \right]
$$
(39)

1123 1124 matching the result described in [Franzese et al.](#page-10-18) [\(2023\)](#page-10-18), obtained with the formalism of time reversal of SDEs.

1126 1127 I DISCUSSION ABOUT A[SSUMPTION](#page-20-4) 7

This is easily checked thanks to the following equality

$$
Y_t = Y_0 \frac{m_0}{m_t} + V \frac{m_0}{m_{T-t}} + \int_0^t \frac{m_s}{m_t} dW_s.
$$
 (40)

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¹¹³³ ⁴Notice that with H selected as in [Assumption 7](#page-20-4) the validity of the theory considered is restricted to the time interval $[0, T)$, see also [Appendix G.](#page-19-1)

1134 1135 1136 1137 To avoid cluttering the notation, we define $f_t = \frac{d \log m_t}{dt}$. To show that [Equation \(40\)](#page-20-6) is true, it is sufficient to observe i) that initial conditions are met and ii) that the time differential of the process is the correct one. We proceed to show that indeed the second condition holds (the first one is trivially observed to be true).

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$$
dY_t = -\alpha Y_0 \frac{\cosh(\alpha(T-t))}{\sinh(\alpha T)} + \alpha r(X) \frac{\cosh(\alpha t)}{\sinh(\alpha T)} - \alpha \cosh(\alpha(T-t)) \int_0^t \frac{1}{\sinh(\alpha(T-s))} dW_s + dW_t
$$
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$$
1151 = -f_t Y_t + \alpha r(X) \left(\frac{\coth(\alpha(T-t)) \sinh(\alpha t) + \cosh(\alpha t)}{\sinh(\alpha T)} \right) + dW_t
$$

$$
1154 = -f_t Y_t + m_t r(X) + \mathrm{d}W_t
$$

where the result is obtained considering that

$$
\frac{\coth(\alpha(T-t))\sinh(\alpha t) + \cosh(\alpha t)}{\sinh(\alpha T)} = \frac{\frac{e^{\alpha(T-t)} + e^{-\alpha(T-t)}}{e^{\alpha(T-t)} - e^{-\alpha(T-t)}}(e^{\alpha t} - e^{-\alpha t}) + (e^{\alpha t} + e^{-\alpha t})}{e^{\alpha T} - e^{-\alpha T}}
$$

$$
= \frac{\frac{e^{\alpha T} + e^{-\alpha(T-2t)} - e^{\alpha(T-2t)} - e^{-\alpha T}}{e^{\alpha(T-t)} - e^{-\alpha(T-t)}} + (e^{\alpha t} + e^{-\alpha t})}{e^{\alpha T} - e^{-\alpha T}}
$$

$$
= \frac{e^{\alpha T} + e^{-\alpha (T - 2t)} - e^{\alpha (T - 2t)} - e^{-\alpha T} + e^{\alpha T} - e^{-\alpha (T - 2t)} + e^{\alpha (T - 2t)} - e^{-\alpha T}}{(e^{\alpha (T - t)} - e^{-\alpha (T - t)}) (e^{\alpha T} - e^{-\alpha T})}
$$

$$
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$$

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> $=\frac{2}{\sqrt{(T-t)}}$ $\frac{2}{e^{\alpha(T-t)}-e^{-\alpha(T-t)}}.$

1167 1168 J EXPERIMENTAL DETAILS

1169 1170 J.1 DATASET DETAILS

1171 1172 The Shapes3D dataset [\(Kim & Mnih, 2018\)](#page-11-11) includes the following attributes and the number of classes for each, as shown in Table [1.](#page-21-2)

Table 1: Attributes and class counts in the Shapes3D dataset.

1186 1187 We train the unconditional denoising score network using the NCSN++ architecture [\(Song et al.,](#page-13-2) [2021\)](#page-13-2), which corresponds to a U-NET [\(Ronneberger et al., 2015\)](#page-12-15). The model is trained from scratch using the score-matching objective. The training hyperparameters are summarized in Table [2.](#page-22-3)

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J.3 LINEAR PROBING EXPERIMENT DETAILS

1211 1212 1213 In the linear probing experiments, we train a linear classifier on the feature maps extracted from the denoising score network at various noise levels τ . The training details are provided in Table [3.](#page-22-4)

Table 3: Hyperparameters for linear probing experiments.

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1227 1228 J.4 MUTUAL INFORMATION ESTIMATION EXPERIMENT DETAILS

1229 1230 1231 1232 For mutual information estimation, we train a conditional diffusion model using the same NCSN++ architecture as before. The conditioning is incorporated by adding a distinct class embedding for each label present in the input image, added to the input embedding along with the timestep embedding. The hyperparameters are the same as those used for the unconditional diffusion model (see Table [2\)](#page-22-3).

1233 1234 1235 To calculate the mutual information, we use Equation [39,](#page-20-1) estimating the integral using the midpoint rule with 999 points uniformly spaced in $[0, T]$.

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1237 J.5 FORKING EXPERIMENT DETAILS

1238 1239 1240 1241 In the forking experiments, we use a ResNet50 [\(He et al., 2016\)](#page-11-12) model with an additional linear layer, trained from scratch, to classify the generated images and assess label coherence across forks. The training details for the classifier are summarized in Table [4.](#page-23-0)

During the sampling process of the forking experiment, we use the settings summarized in Table [5.](#page-23-1)

Figure 4: Visualization of the forking experiment with num forks $= 4$ and one initial seed. The image at time $\tau = 0.4$ is quite noisy. In the final generations after forking, the images exhibit coherence in the labels *shape*, *wall hue*, *floor hue*, and *object hue*. However, there is variation in *orientation* and *scale*.

Table 4: Hyperparameters for the classifier in forking experiments.

Table 5: Sampling settings for the forking experiments.

 J.6 LINEAR PROBING ON RAW DATA

 In [Figure 5,](#page-24-1) we evaluate the performance of linear probes trained on features maps extracted from the denoiser network, and show compare their log probability accuracy with a linear probe trained on the raw, noisy input and a random guesser. Throughout the generative process, linear probes obtain higher accuracy than the baselines: for large noise levels, a linear probe on raw input data fails, whereas the inner layers of the denoising network extract features that are sufficient to discern latent labels.

Figure 5: Log-probability accuracy of linear classifiers at τ . 'Feature map' classifiers are trained on network features; 'Noisy Image' trained on noisy images; 'Random Guess' is the baseline for random guessing.

J.7 ADDITIONAL EXPERIMENTS ON CELEBA DATASET

 We present our results conducted on the CelebA dataset [\(Liu et al., 2015\)](#page-12-19), consisting of over 200000 celebrity images with 40 binary attributes. Next, we focus our analysis on the attributes "Male" and "Eyeglasses" as these are i) among the most reliable and objectively labeled features in the CelebA dataset^{[5](#page-24-2)} and ii) significant examples of attributes which can be mapped to more global and local features respectively. The unconditional and conditional diffusion models were trained using the identical architectural, optimization, and training hyperparameters as in [Song et al.](#page-13-2) [\(2021\)](#page-13-2). Both models employed a variance-exploding diffusion process with a U-Net backbone for the denoising score network. Training details, including the learning rate, batch size, and noise schedules, are the same as of [Song et al.](#page-13-2) [\(2021\)](#page-13-2). We present a comprehensive analysis of the results derived from probing experiments, mutual information (MI) estimation, and the rate of increase of MI across the generative process.

Figure 6: Probing accuracy and mutual information (MI) as a function of the noise intensity parameter τ .

 Probing vs. MI. Our results, as shown in Figure [6,](#page-24-3) illustrate a coherent growth between classifier accuracy (probing performance) and mutual information as a function of the noise intensity parameter τ . For both attributes, probing accuracy increases steadily, mirroring the growth of MI.

 Mutual Information Across Labels Figure [7](#page-25-0) compares MI growth across the "Male" and "Eyeglasses" attributes. A key observation is that the MI for "Male" rises earlier than for "Eyeglasses", beginning at $\tau = 0.2$, compared to $\tau = 0.3$. This aligns with the intuition that some latent abstractions emerge earlier in the generative process than others, given that the average number of pixels impacted by the global features is larger than the local ones.

 $⁵$ This is supported by previous work, which highlights significant labeling issues for many other attributes,</sup> making them less suitable for consistent analysis [\(Lingenfelter et al., 2022\)](#page-11-15).

