Generative Modeling with Denoising Auto-Encoders and Langevin Sampling

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Abstract

We study convergence of a generative modeling method that first estimates the score function of the distribution using Denoising Auto-Encoders (DAE) or Denoising Score Matching (DSM) and then employs Langevin diffusion for sampling. We show that both DAE and DSM provide estimates of the score of the Gaussian smoothed population density, allowing us to apply the machinery of Empirical Processes. We overcome the challenge of relying only on $L^2$ bounds on the score estimation error and provide finite-sample bounds in the Wasserstein distance between the law of the population distribution and the law of this sampling scheme. We then apply our results to the homotopy method of [SE19] and provide theoretical justification for its empirical success.

1 Introduction

Recent empirical successes of generative modeling range from high-fidelity image generation with Generative Adversarial Networks (GANs) [GPAM+14] to protein folding with differentiable simulators [SEJ+20, IRSM19]. GANs are implicit likelihood models, in the sense that they do not directly model the likelihood. On the other hand, explicit generative models directly estimate the likelihood or the score function (the gradient of the log likelihood). Recent works, including [SE19, NCB+17, GWJ+19], show that successful image generation can be achieved by estimating the score function from data (using Denoising Score Matching, Denoising Auto-Encoders, and pre-trained classifiers respectively) and by using Langevin dynamics for sampling. Conditional text generation, as well as protein folding can be accomplished using a similar approach, see e.g [DML+19] for text generation and [IRSM19] for learning 3D protein structures from sequences. Motivated by the recent resurgence of those explicit methods and their empirical success in wide range of applications we focus on this family of explicit generative models and address their theoretical properties.

Formally, we consider the problem of data generation from an unknown distribution. The algorithm we consider is in two parts. In the first part, we estimate the score of the data using a Denoising Auto-Encoder (DAE), while in the second part we plug our estimate of the score of the data into a discretized approximation to the Langevin dynamics stochastic differential equation, generating a sample. In this paper we bound the Wasserstein 2-distance between the law of our sampling algorithm and the population law. The algorithm is a variation on the method of [SE19], which produced state-of-the-art results on standard vision datasets.

If we consider a distribution with density $p$ with respect to the Lebesgue measure, then Langevin Dynamics provide a well-known and much studied way to sample from this distribution. Supposing that $\nabla \log p$ is $\frac{M}{2}$-Lipschitz, we note that under mild conditions, the Langevin diffusion given by

$$dW(t) = \nabla \log p(W(t))dt + \sqrt{2}dB_t$$

where $B_t$ is a standard Brownian motion in $\mathbb{R}^d$, converges in law as $t \to \infty$ to the population distribution $p$. We consider the setting where $p$ is unknown, but we have access to $n$ i.i.d. samples $X_1, \ldots, X_n \sim p$. In this case, $\nabla \log p$, often called the score of the distribution, must be estimated. We build on the observations of [Vin11, AB14] and show that DAEs trained on the sample provide estimators of the score of a smoothed distribution that are close in the sense of $L^2$. We then show that this estimate suffices to bring the Langevin process associated to our estimate
close to the Langevin process that is actually associated with the population distribution. Finally we note that our error decomposition lends itself naturally to the homotopy method used in [SE19] and we show that this approach significantly helps the sampling scheme with respect to Wasserstein-2 distance. The new contributions are as follows:

- We show that an estimator of score that is close in the $L^2$ sense still furnishes us with a Langevin diffusion whose law at a fixed time $t > 0$ remains close in the sense of Wasserstein to the law of the Langevin diffusion driven by the score of the population distribution. In particular, many statistical estimators are only guaranteed to have small $L^2$ error, rather than small uniform error, and so the ability to provide estimates of Wasserstein distance for a Langevin sample using such estimates has the potential for significant general application. While the theory is more straightforward for an estimator that is uniformly close, a case that is studied in [RRT17], to our knowledge this is the first theoretical justification for the $L^2$-close regime.

- We exhibit a decomposition of the error between the law of our sampling algorithm and the law of the population distribution that makes the benefits of a homotopy method explicit, thereby providing the first rigorous, theoretical justification that we know of for the success realized by the algorithm in [SE19].

- We shed new light on what the Denoising Auto-Encoder learns from a distribution, showing that optimizing DAE loss is equivalent to optimizing Denoising score-matching (DSM) loss, which then implies that the population level DAE provides an unbiased estimator of the score of the population distribution convolved with a Gaussian. Moreover we provide a condition to guarantee that the convolved distribution satisfies a log-Sobolev inequality, the first such result of which we know.

- We use our connection between DAE and DSM losses to provide finite sample, high probability estimates of the error of a DAE. To our knowledge, these are the first such finite sample bounds.

We consider a sampling scheme where we fix in advance a sequence $(\eta_i, \sigma_i^2)$ with both $\eta_i$ and $\sigma_i^2$ non-increasing, $1 \leq i \leq N$. We then consider a sequence of DAEs $\tilde{f}_1, \ldots, \tilde{f}_N$ trained on the data with the variance parameter of $\tilde{f}_i$ equal to $\sigma_i^2$. Let $\tilde{f}_i(x) = \frac{1}{\sigma_i^2}(\tilde{f}_i(x) - x)$. Then we apply a homotopy method of discrete Langevin sampling with warm restarts where on the $i^{th}$ leg of the homotopy, we use $\tilde{f}_i$ as an estimate of score and a step length of $\eta_i$. This is the identical algorithm proposed by [SE19], up to the fact that we consider the DAE criterion, while they consider the DSM criterion.

### 2 Notation and Preliminaries

There are two steps to our sampling scheme: the estimation of the score and the Langevin sampling. For the first, we have

**Definition 1.** If $p$ is a density on $\mathbb{R}^d$, we call $\nabla \log p$ the score of the distribution. We let $g_{\sigma^2}$ denote the density of a centred Gaussian with variance $\sigma^2$ and let $p_{\sigma^2} = p * g_{\sigma^2}$ denote the convolved distribution. If $r : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a function, we denote the DAE error by

$$L_{DAE}(r) = \mathbb{E}_{X \sim p \epsilon \sim g_{\sigma^2}} [||r(X + \epsilon) - X|||^2] \quad (2)$$

We add a hat to indicate that we are considering the empirical distribution:

$$\hat{L}(r) = \frac{1}{n} \sum_{i=1}^{n} ||r(X_i + \epsilon_i) - X_i||^2 \quad (3)$$

where $\epsilon_i$ are i.i.d. centred Gaussians of variance $\sigma^2$. We define the Denoising Score-Matching (DSM) loss as

$$L_{DSM}(s) = \mathbb{E}_{X \sim p_{\sigma^2}} [||s(X) - \nabla \log p_{\sigma^2}(X)|||^2] \quad (4)$$

For the entirety of the paper, we assume that $\nabla \log p$ is $\frac{M}{\sigma^2}$-Lipschitz. Regarding the Langevin process, we have
Definition 2. We define the Langevin diffusion started at some distribution $\mu_0$ as the (guaranteed unique by say [KS91]) solution $W_{\sigma^2}(t)$ to
\[
dW_{\sigma^2}(t) = \nabla \log p_{\sigma^2}(W_{\sigma^2}(t)) dt + \sqrt{2} dB_t
\]
where we drop the $\sigma^2$ when context allows. If $\hat{f}$ is an $M^2$-Lipschitz estimate of $\nabla \log p_{\sigma^2}$, then we let $\hat{W}(t)$ be the unique solution to
\[
d\hat{W}(t) = \hat{f}(\hat{W}(t)) dt + \sqrt{2} dB_t
\]
For a fixed small step length $\eta > 0$, we define
\[
W_{k+1} = \eta \hat{f}(W_k) + \sqrt{2\eta} \xi_k
\]
where $\xi_k$ are i.i.d. standard Gaussians in $\mathbb{R}^d$.

We make use of the following definition

Definition 3. For constants $m, b > 0$, we say that a vector field $f : \mathbb{R}^d \to \mathbb{R}^d$ is $(m, b)$-dissipative if for all $x \in \mathbb{R}^d$, we have
\[
\langle f(x), x \rangle \geq m ||x||^2 - b
\]
We also introduce some of the notation related to the theory of empirical processes.

Definition 4. Let $\mathcal{G}$ be a class of real valued functions on $\mathbb{R}^d$ and let $S = (X_1, \ldots, X_n)$ be $n$ samples from $\mathbb{R}^d$. We define the Rademacher average with respect to the sample as
\[
\hat{\mathcal{R}}_n(\mathcal{G}, S) = \mathbb{E}_\varepsilon \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \varepsilon_i g(X_i) \right]
\]
where $\varepsilon_i$ are i.i.d random variables taking values $\{\pm 1\}$ with probability $\frac{1}{2}$ each. We define the Rademacher complexity of the function class $\mathcal{G}$ as
\[
\mathcal{R}_n(\mathcal{G}) = \sup_{S \subset (\mathbb{R}^d)^n} \hat{\mathcal{R}}_n(\mathcal{G}, S).
\]
For a class of $\mathbb{R}^k$-valued functions $\mathcal{G}$, we denote by $\mathcal{R}_n(\mathcal{G}) = \sum_{i=1}^{k} \mathcal{R}_n(\mathcal{G}_i)$ where $\mathcal{G}_i$ is the restriction of $\mathcal{G}$ to the $i$-th coordinate.

We make use of the following assumptions on the population distribution:

Assumption 1. The density $p$ is positive everywhere on $\mathbb{R}^d$.

Assumption 2. The vector field $\nabla \log p$ is $M$ Lipschitz for some $M > 0$ and there exist $\widetilde{\sigma}_{\max}^2, M > 0$ such that for all $0 \leq \sigma^2 \leq \widetilde{\sigma}_{\max}^2$, the vector field $\nabla \log \frac{p_{\sigma^2}}{p}$ is $\sigma^2 M^2$-Lipschitz.

Assumption 3. The vector field $-\nabla \log p$ is $(m, b)$-dissipative for some positive constants $m, b$.

The first two assumptions are standard and are used to ensure that there exists a unique strong solution to the Langevin diffusion. The last assumption has seen increased use in recent work to bound the log-Sobolev constant of $p$ when $-\log p$ is not strongly convex, as in, for example, [RRT17] (although note that as they are considering the optimization instead of the sampling regime, they consider $\nabla \log p$ to be dissipative as opposed to assuming the dissipativity of $-\nabla \log p$ as in this work). Note that the third condition coupled with the fundamental theorem of calculus implies that $p$ is $\frac{M}{2}$-sub-Gaussian, as per Lemma 38.
3 Estimating the Score

Our first result connects the DAE to Denoising Score-Matching (DSM), showing that the objectives are equivalent up to an affine transformation, a variant on a result in [Vin11]; while [Vin11] proves the following for a particular DAE parameterization, we show that the below is true in general:

**Proposition 5.** Let $p$ be a differentiable density. Then the DAE loss

$$L_{DAE}(r) = \mathbb{E}_{x \sim p}[|r(x + \epsilon) - x|^2]$$

and the DSM loss

$$L_{DSM}(s) = \mathbb{E}_{p_{\sigma^2}}[|s(x) - \nabla \log p_{\sigma^2}(x)|^2]$$

with

$$s(x) = \frac{r(x) - x}{\sigma^2}$$

are equivalent up to a term that does not depend on $r$ or $s$.

The proof of Proposition 5 is a simple application of the divergence theorem and Stein’s lemma (Lemma 39) and can be found in Appendix D.

An easy corollary of Proposition 5 is similar to a result in [AB14], which relates the population DAE to the score of the population distribution. Instead, we consider the score of the population distribution smoothed by the addition of Gaussian noise; obviously, without knowledge of $p$, the DSM loss cannot be explicitly evaluated, so this equivalence allows for a loss that can be evaluated in practice. Below, we establish Corollary 6 using Proposition 5; an alternate, direct proof, is included in Appendix D for those interested.

**Corollary 6.** Let $p$ be a population density with respect to the Lebesgue measure. Let $r_{\sigma^2}(x)$ denote the optimal DAE with Gaussian noise of variance $\sigma^2$. Then

$$r_{\sigma^2}(x) = x + \sigma^2 \nabla \log p_{\sigma^2}(x)$$

**Proof.** Clearly $s(x) = \nabla \log p_{\sigma^2}(x)$ minimizes the $L_{DSM}$ loss. Note that, by Proposition 5, we have that $r(x) = x + \sigma^2 s(x)$ then minimizes $L_{DAE}$, the DAE loss. The result follows.

Later, in our analysis of the Langevin dynamics, we will need to assume dissipative conditions not just on the score of the population distribution $p$, but also on the score of the smoothed distribution $p_{\sigma^2}$; in particular, we will need to establish a log-Sobolev inequality for the smoothed distribution. For reasons to become clear below, we define

$$\sigma_{max}^2 = \frac{m}{2M} \land \sigma_{max}^2$$

where $\sigma_{max}^2$ is as appears in Assumption 2. Then we have

**Proposition 7.** Suppose that $-\nabla \log p$ is $\frac{M}{\sigma^2}$-Lipschitz and $(m, b)$-dissipative. Then for $\sigma^2 \leq \sigma_{max}^2$, there is a constant $B$ such that $-\nabla \log p_{\sigma^2}$ is $(m_{\sigma^2}, b_{\sigma^2})$-dissipative where

$$m_{\sigma^2} = \frac{m - \sigma^2 M}{2}, \quad b_{\sigma^2} = b + \frac{B^2}{2(m - \sigma^2 M)}$$

**Remark 8.** Note that as $\sigma_{max}^2 \leq \frac{m}{2M}$, we can bound the dissipativity constants to say that $-\nabla \log p_{\sigma^2}$ is $(m, b + \frac{B^2}{4m^2})$-dissipative uniformly in $\sigma^2 \leq \sigma_{max}^2$.

The proposition follows from applying Cauchy-Schwarz and the definition of dissipativity, along with Assumption 2; details are provided in Appendix D. Both Assumption 2 and Proposition 7 are necessary for the analysis in Section 4, the first to show the existence of the Langevin diffusion and the second to show exponential convergence to the stationary distribution.

The above analysis deals with the population risk, but in reality we are only given $n$ i.i.d samples from $p$. We have the following result:
Theorem 9. Let $\mathcal{F}$ be a class of $\mathbb{R}^d$-valued functions, all of which are $\frac{M}{R}$-Lipschitz, bounded coordinate wise by $R > 0$, containing arbitrarily good uniform approximations of $\nabla \log p_{\sigma^2}$ on the ball of radius $R$. Let $\sigma^2 < \sigma^2_{\max}$ and suppose we have $n$ i.i.d samples from $p_{\sigma^2}$, $X_1, \ldots, X_n$. Let

$$\hat{s} \in \arg\min_{s \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} |s(X_i) - \nabla \log p_{\sigma^2}(X_i)|$$

(17)

Then with probability at least $1 - 4\delta - C\alpha e^{-\frac{\tilde{R}^2}{m_{\sigma^2}}}$ on the randomness due to the sample,

$$\mathbb{E}_{X \sim p_{\sigma^2}} \left[ \left| \hat{s}(X) - \nabla \log p_{\sigma^2}(X) \right|^2 \right] \leq C(MR + B)^2 \left( \log^3 n \cdot \mathfrak{R}^2_n(\mathcal{F}) + \beta_n d \right)$$

(18)

where $C$ is a universal constant, $m_{\sigma^2}$ can be found in Proposition 7, and

$$\beta_n = \frac{\log \frac{1}{\delta} + \log \log n}{n}$$

(19)

Remark 10. In order to have a high probability estimate, we need $C\alpha e^{-\frac{\tilde{R}^2}{m_{\sigma^2}}}$ to be small; as such we see that $R^2 = \Omega(\log n)$. Thus, up to factors polynomial in $\log n$, we see that the $L^2$ error of the estimate is $\tilde{O}(\mathfrak{R}^2_n(\mathcal{F}))$.

From the equivalence between DSM and DAE loss, we have as an immediate corollary

Corollary 11. Suppose we are in the setting of Theorem 9. Let

$$\hat{r} \in \arg\min_{r \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \left| r(X_i + \sigma \xi_i) - X_i \right|^2$$

(20)

where $\xi_i$ are iid standard Gaussians. Then with probability at least $1 - 4\delta - C\alpha e^{-\frac{\tilde{R}^2}{m_{\sigma^2}}}$

$$\mathbb{E}_{X \sim p_{\sigma^2}} \left[ \left| \hat{r}(X) - X - \nabla \log p_{\sigma^2}(X) \right|^2 \right] \leq \frac{1}{\sigma^4} C(MR + B)^2 \left( \log^3 n \cdot \mathfrak{R}^2_n(\mathcal{F}) + \beta_n d \right)$$

(21)

where the notation is as in Theorem 9.

Proof. Let $r^*(x) = x + \sigma^2 \nabla \log p_{\sigma^2}(x)$ be the population optimal DAE. Using the identical analysis as in Theorem 9, we get that

$$\mathbb{E}_{X \sim p_{\sigma^2}} \left[ \left| \hat{r}(X) - X - \sigma^2 \nabla \log p_{\sigma^2}(X) \right|^2 \right] \leq C(MR + B)^2 \left( \log^3 n \cdot \mathfrak{R}^2_n(\mathcal{F}) + \beta_n d \right)$$

(22)

Dividing by $\sigma^4 > 0$ on both sides of the above inequality concludes the proof.

The proof of Theorem 9 is an application of a result on lower isometry in [RST17]. We provide a sketch below, with full details appearing in Appendix A.

Proof. (Sketch of Theorem 9) By the fundamental theorem of calculus and the dissipativity assumption, we have that $p$ has Gaussian tails, as proved in Lemma 38. Thus with probability at least $1 - C\alpha e^{-\frac{\tilde{R}^2}{m_{\sigma^2}}}$ all the samples fall in a ball of radius $R$. Then the minimizer of the population DSM loss is given by $\nabla \log p_{\sigma^2}$ and we are in the well-specified case. Breaking the error up coordinate-wise, we bound the squared error by the product of the dimension and the largest coordinate-wise error. Applying [RST17, Lemmas 8, 9] to this coordinate concludes the proof.

The generality of Theorem 9 with regard to the function class is potentially helpful in fine-grained analysis of how DAEs are used in practice: usually $\mathcal{F}$ is a class of neural networks; combining known results on the complexity of such classes with Corollary 21 gives high-probability bounds on the DAE error. If we consider the special case where $\mathcal{F}$ is the class of Lipschitz functions bounded by $R$ in each coordinate, then we can apply known results on the complexity of this class [Tik93, Theorem XIII] to get a rate of $\tilde{O} \left( n^{-\frac{3}{2}} \right)$, ignoring factors polynomial in $\log n$. On the other hand, norm-based bounds for Rademacher averages of neural networks in [BFT17, GRS17, NTS15] can imply the faster $n^{-1}$ rate, as long as the empirical error in Equation (20) is small.
4 The Langevin Process: Approximation and Convergence

In this section, we analyze one section of the homotopy method described above. As such, we fix an $\eta$ and a $\sigma^2$ and bound $W_2(\mu_k,p)$, where we recall that $\mu_k$ is the law of $W_t$, the $k^{th}$ iterate in the discrete Langevin sampling scheme described in the introduction. We have the following theorem:

**Theorem 12.** Suppose that $-\nabla \log p$ is $\frac{M}{2}$-Lipschitz and $(m, b)$-dissipative. Suppose that $\hat{f}$ is an estimate of $\nabla \log p_{\sigma^2}$ that has the same Lipschitz constant and whose squared error is bounded by $\varepsilon^2$:

$$\mathbb{E}_{X \sim p_{\sigma^2}} \left[ \left\| \hat{f}(X) - \nabla \log p_{\sigma^2}(X) \right\| \right] \leq \varepsilon^2$$  \hspace{1cm} (23)

If we initialize $W_0$ according to a distribution $\mu_0$ such that $W_2(\mu_0, p_{\sigma^2}) < \infty$ and $\mu_0$ is concentrated in high probability on a ball of radius $R$, and we let $\mu_k$ denote the law of a discrete Langevin sampling scheme with constant step size $\eta$ run for $k$ iterations with score estimate $\hat{f}$, then with high probability with respect to the initialization for some small $\delta > 0$ with $\tau = k\eta$, we have

$$W_2(\mu_k, p) \leq \sigma \sqrt{d} + A_{M,d,B}(\eta, \tau) + W_2(\mu_0, p_{\sigma^2}) e^{-2\varepsilon_{LS}(\sigma^2)} + C_{\sigma^2, M, R, B, d}(\tau, \varepsilon)$$ \hspace{1cm} (24)

where $c_{LS}(\sigma^2)$ can be found in Proposition 17.

$$A_{M,d,B}(\eta, \tau) = M^2 \eta \left( 4d + M^2 \left( 2d \tau + B^2 \tau \right) e^{M^2 \tau} \right) e^{M^2 \tau}$$ \hspace{1cm} (25)

and $C_{\sigma^2, M, R, B, d}(\tau, \varepsilon)$ is given by

$$\sqrt{c_{LS}(\sigma^2)} \left( \varepsilon_\tau + \left( 16M^4 \tau \left( 2d \tau^2 + B^4 \tau \right) e^{M^4 \tau} + B^4 \tau \right) \tau e^{M^2 \tau} e^{MR-B} \frac{\Gamma\left( \frac{d}{2} - 1 \right)}{2\pi^{\frac{d}{2}}} \delta^{2-d\varepsilon} \right)$$ \hspace{1cm} (26)

where $B$ is a constant from Lemma 34.

**Remark 13.** The $\varepsilon$ in Equation (23) above is controlled in high probability by Theorem 9 or Corollary 11 as rates depending on the number of samples and the complexity of the function class over which we are optimizing. Thus, combining Theorem 9 instantiated on a given function class and Theorem 12 gives explicit high probability bounds on how well the Langevin sampling algorithm with an estimate trained on $n$ samples approximates the population distribution.

**Remark 14.** While the exponential dependence on $\tau$ in the second and last terms of Equation (24) may seem bad, note that the exponential convergence in the third term tells us that if we want to get $\delta$-close in Wasserstein distance, then $\tau$ needs only be $O\left( \log \frac{1}{\delta} \right)$ and so the exponential dependence on $\tau$ is only a polynomial dependence on error.

The exponential growth with respect to dimension is a touch more serious. If we make more than a Lipschitz assumption on the score function and assume moreover that $|\Delta \log p| \leq C$ then $M \sqrt{d}$ can be replaced by $C$ in the factor under the square root above. While we leave to future work the job of determining if the $\Gamma\left( \frac{d}{2} - 1 \right)$ factor is tight, we suspect that, without further assumptions, an exponential dependence on dimension cannot be avoided. In similar work that makes no assumption of convexity, such as [RRT17], polynomial dependence on dimension is not achieved and there is reason to believe that it cannot be true in general. Regarding sample complexity, minimax results on Wasserstein estimation (see e.g. [NWR19, GGPW19]) suggest that exponential dependence in dimension cannot be improved without further assumptions.

The remainder of this section is devoted to a sketch of the proof of Theorem 12; the rigorous proof is relegated to the appendices. With respect to the approximation of the continuous Langevin diffusion by a discrete process, we adapt an argument using Girsanov’s theorem from [BEL18, RRT17]; in contradistinction to these papers, where they work with the population score and a uniformly close estimate of the population score respectively, we assume that we have access only to an estimate of the score that is $L^2(p)$-close, significantly increasing the difficulty of proving the bound.

In order to prove Theorem 12, we consider several intermediate measures. Let $\nu_t$ be the law of $W(t)$ and $\tilde{\nu}_t$ the law of $\tilde{W}(t)$ at a fixed time $t$. Then by the triangle inequality we can decompose

$$W_2(\mu_k, p) \leq W_2(\mu_k, \tilde{\nu}_t) + W_2(\tilde{\nu}_t, \nu_\tau) + W_2(\nu_\tau, \nu_\infty) + W_2(\nu_\infty, p)$$ \hspace{1cm} (27)

Note that $\nu_\infty = p_{\sigma^2}$ and so the last error term is controlled by
Lemma 15. Let \( p \) be a measure on \( \mathbb{R}^d \). Then
\[
W_2(p, p_{\sigma^2}) \leq \sigma \sqrt{d}
\] (28)

Proof. This is a special case of [AS05, Lemma 7.1.10] with \( \rho = g_1 \). The variance of \( g_1 \) is \( d \) so the result follows. \( \blacksquare \)

We now bound the other three terms.

The first term in Equation (27) comes from the error introduced by the fact that our sampling algorithm is only an approximation of the continuous Langevin process. We have as a standard result, with proof in Appendix D:

Proposition 16. With the notation as above and \( \hat{f} \frac{M}{2} \)-Lipschitz, we have
\[
W_2(\mu_k, \nu_\tau)^2 \leq M^2 \eta \left( 4d + M^2 (2d\tau + B^2\tau) e^{M^2\tau} \right) e^{M^2\tau}
\]

Having dispensed with the first and last terms in Equation (27), we are now ready to tackle the middle terms, the error due to the difference between the estimated and population Langevin diffusions and the error due to the lack of convergence to the stationary distribution.

4.1 Log-Sobolev Inequalities and Exponential Convergence in Wasserstein Distance

In order to deal with convergence in Wasserstein distance to the stationary distribution, we show that for sufficiently small \( \sigma^2 \geq 0 \), \( p_{\sigma^2} \) satisfies a log-Sobolev inequality. This will also be helpful in bounding the second term in Equation (27), as we shall see in the following section. We will use the Lyaponov function criterion as proved in [CGW09]. The key result is the proof that if \( -\nabla \log p \) is \((m, b)\)-dissipative, then \( p \) satisfies a log-Sobolev inequality with a constant bounded in terms of \( m \) and \( b \), a result proved in [RRT17]. We have as a translation of Proposition 3.2 from [RRT17]:

Proposition 17. Let \( -\nabla \log p \) be \( \frac{M}{2} \)-Lipschitz and \((m, b)\)-dissipative. Then for \( 0 \leq \sigma^2 \leq \sigma_{max}^2 \), the smoothed distribution \( p_{\sigma^2} \) satisfies a log-Sobolev inequality with constant
\[
c_{LS}(\sigma^2) \leq \frac{8M}{m_{\sigma^2}^2} + \frac{2}{M} + c_P \left( 2 + \frac{8M}{m_{\sigma^2}^2} \left( m_{\sigma^2} \left( d + \frac{b}{2} \right) + \frac{m_{\sigma^2}(b + d)}{4} \right) \right)
\] (29)

Where \( m_{\sigma^2} \) is the constant appearing in Proposition 7 and
\[
c_P(\sigma^2) \leq \frac{1}{m_{\sigma^2}(2d + b)} \left( 1 + C \left( d + \frac{b}{2} \right) (d + b)e^{\frac{8(M + B)(d + b)}{m_{\sigma^2}}} \right)
\] (30)

where the constant \( B \) appears in Lemma 34.

We replicate the proof used in [RRT17] in detail, in Appendix B. With the log-Sobolev constant established, the convergence in Wasserstein distance is immediate:

Proposition 18. Let \( -\nabla \log p \) be \( \frac{M}{2} \)-Lipschitz and \((m, b)\)-dissipative. Then for \( 0 \leq \sigma^2 \leq \frac{m_{\sigma^2}^{-1}}{M} \), if \( \nu_\tau \) is the law of \( W(t) \), then
\[
W_2(\nu_\tau, p_{\sigma^2}) \leq W_2(\nu_0, p_{\sigma^2}) e^{-\frac{2M}{c_{LS}(\sigma^2)}}
\] (31)

The proof of this result is well known; see [BL14] for details.

4.2 Running a Langevin Diffusion with a Score Estimator

The second term in Equation (27) is the error due to the difference between running a continuous Langevin diffusion with drift \( \hat{f} \) and that with drift \( \nabla \log p_{\sigma^2} \). The details are in Appendix C, but a sketch of the argument is below. Let \( \tilde{\nu}_t \) be the law of \( \tilde{W}(t) \) and let \( \nu_t \) be the law of \( W(t) \) at a fixed time \( t \). We recall that the classic theorem of Otto and Villani (found in [OV00]) tells us that
\[
W_2(\tilde{\nu}_t, \nu_t) \leq \sqrt{2c_{LS}(\sigma^2)KL(\tilde{\nu}_t, \nu_t)}
\] (32)
where

$$KL(\tilde{\nu}_t, \nu_t) = \mathbb{E}_{\tilde{\nu}_t} \left[ \log \frac{d\tilde{\nu}_t}{d\nu_t} \right]$$

(33)

is the relative entropy.

In order to compute the relative entropy between the laws of two diffusions with the same noise but different drifts, we can apply Girsanov’s theorem and take expectations, as in [BEL18, RRT17]. In particular, this tells us that

**Proposition 19.** Let \( W(t), \tilde{W}(t) \) be as above and assume that \( \tilde{f}, \nabla \log p_{\sigma^2} \) is \( \frac{M}{2} \)-Lipschitz. Then

$$KL(\tilde{\nu}_t, \nu_t) = \mathbb{E} \left[ \frac{1}{2} \int_0^t \left\| \nabla \log p_{\sigma^2} (W(s)) - \tilde{f}(W(s)) \right\|^2 ds \right]$$

(34)

Thus it suffices to control this last quantity. If we had that \( \tilde{f} \) were uniformly close to \( \nabla \log p \) or even that we were close in the \( L^2(W(t)) \) sense, we would be done; unfortunately, we only have that the estimate and the score are close in the sense of \( L^2(p_{\sigma^2}) \) and so it is not a priori obvious that the above integral can be controlled. In order to get around this, we use the concept of local time and expected occupation density, as seen in [KS91, GH80], as well as bounds on the transition density of a diffusion.

**Proposition 20.** Let \( \tilde{f} \) be an estimator of \( \nabla \log p_{\sigma^2} \) such that both the estimator and the score are \( \frac{M}{2} \)-Lipschitz and the error is bounded:

$$\mathbb{E}_{X \sim p_{\sigma^2}} \left[ \left\| \tilde{f}(X) - \nabla \log p_{\sigma^2}(X) \right\| \right] \leq \varepsilon^2$$

(35)

Suppose we initialize \( W(0) \sim \mu_0 \) which is concentrated in high probability on a ball of radius \( R \). Then with high probability under the randomness due to initialization at \( x \),

$$\mathbb{E}_x \left[ \int_0^t \left\| \nabla \log p(W(s)) - \tilde{f}(W(s)) \right\|^2 ds \right] \leq \varepsilon t + \sqrt{\left(16M^4 t \left((2dt)^2 + B^4 t \right) e^{M^4 t} + B^4 t \right) t e^{\frac{M^2 t}{2}} e^{MR-B} \frac{\Gamma \left( \frac{d}{2} - 1 \right)}{2\pi^{\frac{d}{2}}} \delta^2 \varepsilon}$$

(36)

for some small \( \delta > 0 \).

A full proof can be found in Appendix C, but we provide a sketch without details.

**Proof.** (Sketch) In order to bound the desired expected value, we consider the set \( U \subset \mathbb{R}^d \) where \( \left\| \tilde{f}(x) - \nabla \log p_{\sigma^2}(x) \right\| > \varepsilon \). We can break the integral into the times when \( W(s) \in U \) and the times when \( W(s) \notin U \). In the latter case we can apply a uniform bound of \( \varepsilon t \). In the former case, we can apply Cauchy-Schwarz to bound this term by the square root of the product of the fourth moment of \( \left\| \tilde{f}(W(s)) - \nabla \log p_{\sigma^2}(W(s)) \right\| \) and the expected amount of time that \( W(s) \) spends in \( U \). The former follows easily from the Lipschitz bounds of Lemma 34 and the moment bound of Lemma 35. The second comes from a bound on expected occupation times, which are time integrals of the transition density of the Langevin diffusion. We bound the Radon-Nikodym derivative of these transition densities with respect to the population distribution with the Girsanov theorem, and then integrate with respect to time, giving the result. ■

Combining Proposition 20 with the Otto-Villani theorem and Proposition 18 yields

**Corollary 21.** Let \( \tilde{f} \) be an estimator of \( \nabla \log p_{\sigma^2} \) such that both the estimator and the score are \( \frac{M}{2} \)-Lipschitz and the error is bounded:

$$\mathbb{E}_{X \sim p_{\sigma^2}} \left[ \left\| \tilde{f}(X) - \nabla \log p_{\sigma^2}(X) \right\| \right] \leq \varepsilon^2$$

(38)

Suppose we initialize \( W(0) \sim \mu_0 \) which is concentrated in high probability on a ball of radius \( R \). Then with high probability under the randomness due to initialization at \( x \), we have that \( \mathcal{W}_2(\tilde{\nu}_t, \nu_t) \) is bounded by

$$\sqrt{c_{LS}(\sigma^2) \left( \varepsilon t + \sqrt{\left(16M^4 t \left((2dt)^2 + B^4 t \right) e^{M^4 t} + B^4 t \right) t e^{\frac{M^2 t}{2}} e^{MR-B} \frac{\Gamma \left( \frac{d}{2} - 1 \right)}{2\pi^{\frac{d}{2}}} \delta^2 \varepsilon} \right)}$$

(39)

for some small \( \delta > 0 \), where \( c_{LS}(\sigma^2) \) is given in Proposition 17.
We are finally ready to prove Theorem 12:

Proof. (Proof of Theorem 12) Using the triangle inequality, we need to bound each of the four terms in Equation (27). These terms are bounded in Proposition 16, Corollary 21, Proposition 18, and Lemma 15. Combining these concludes the proof.

5 Homotopy and Annealing

The above section and the discussion surrounding Theorem 12 focuses on one leg of the homotopy; this section uses Theorem 12 to analyze the effect that the homotopy method and annealing the DAE has on the Wasserstein distance between the sample and the population distribution.

We consider the following sampling scheme. For fixed \( k \), we fix a sequence \( \{ (\eta_i, \sigma_i^2) | 1 \leq i \leq N \} \) where \( \eta_i, \sigma_i^2 \) are both decreasing in \( i \). We train a DAE with variance parameter \( \sigma_i^2, \tau_i \), and set \( s_i(x) = \frac{1}{\sigma_i^2}(r_i(x) - x) \) Then we initialize \( W^{(1)} = \mu_0 \) and evolve with \( \tilde{f} = s_1 \) with step size \( \eta_1 \) for \( k \) iterations. Then, we use warm restarts and for \( 2 \leq i \leq N \), we evolve a Langevin sampling scheme \( W^{(i)} \) with \( \tilde{f} = s_i \), step size \( \eta_i \), and \( W_0^{(i)} = W_k^{(i-1)} \). Our final sample, then is \( W_k^{(N)} \).

The decomposition in Equation (27) provides clues as to why the homotopy method described above speeds up the Langevin sampling. Consider, first, the effect that \( \eta \) has on the decomposition. According to Theorem 12, we have that the error is bounded by

\[
W_2(\mu_k, p_{\sigma^2}) \leq \sigma \sqrt{d} + A_{M,d,B}(\eta, \tau) + W_2(\mu_0, p_{\sigma^2}) e^{-\frac{2\tau}{c_{LS}(\sigma^2)}} + C_{\sigma^2,M,R,B,d}(\tau, \varepsilon)
\]

As \( \eta \) increases, since \( \tau = k \eta \), we see that \( \tau \) increases and we note that both \( A(\eta, \tau) \) and \( C(\tau, \varepsilon) \) increase, but \( W_2(\mu_0, p_{\sigma^2}) e^{-\frac{2\tau}{c_{LS}(\sigma^2)}} \) decreases. Thus with all other constants fixed, the optimal \( \eta \) can be determined as \( \eta_{opt} > 0 \).

With regard to score estimation, the greater value of \( \sigma^2 \) makes it easier to estimate the score. Consider that, in our regime, we are training a DAE and then using the transformation in Corollary 21 to plug the score estimate into Theorem 12. With a fixed number of samples, doing the proof of Corollary 11 in reverse, we note that if the DAE has squared error \( \varepsilon^2 \), then the score estimate has squared error \( \frac{1}{\tau \varepsilon^2} \). Thus, if we fix \( \varepsilon^2 \) as the achievable error of a DAE trained on \( n \) samples, then as \( \sigma^2 \) increases, \( \varepsilon^2 \) decreases and thus so, too, does \( C_{\sigma^2,M,R,B,d}(\tau, \varepsilon) \).

The effect of \( \sigma^2 \) on the log-Sobolev constant remains a bit more mysterious from a rigorous point of view. While Proposition 7 provides a bound on \( c_{LS}(\sigma^2) \), it is likely not tight, as it amounts to a ‘worst-case’ analysis of the effect that the Gaussian smoothing has on the population distribution, using a crude argument involving Cauchy-Schwarz. If we make further assumptions, these results can be tightened. For example, if we suppose that \( \rho \) has compact support, then [BGMZ15] gives a bound on the log-Sobolev constant of the smoothed distribution that decreases with larger variance, thereby accelerating the convergence of the Langevin diffusion to its stationary distribution; while their bound is dimension-dependent, they suggest that future work may lose this handicap. Thus, in this case, just as there exists an \( \eta_{opt} \) that minimizes the right hand side of Equation (40), there is too such a \( \sigma_{opt}^2 \). We leave to future work the task of better controlling \( c_{LS}(\sigma^2) \) in the general case. Thus the annealing and the homotopy method combine to provide a form of dynamic optimization of the upper bound of Theorem 12, significantly decreasing the error and simultaneously speeding up the naive Langevin sampling that does not involve homotopy or annealing. The above is empirically indicated by the success of the annealed score matching in [SE19]; as we saw in Proposition 5, though, the annealed score matching is equivalent to DAE loss, so the empirical success in one area transfers to the other mutatis mutandis.

6 Conclusion and Further Directions

We have provided rigorous justification above for two empirical approaches that have recently generated excitement: the use of score estimators to run Langevin sampling and the homotopy method method [SE19]. While the bounds in Theorems 9 and 12 allow for high probability guarantees with finite samples, there is a question of tightness. First, the dependence on the dimension of the bound in eq. (24) is probably not optimal, especially the \( \Gamma \left( \frac{d}{2} - 1 \right) \) factor. It is very possible that a more detailed analysis of the argument proving Proposition 20 would substantially improve this dependence on the dimension. Second, while we have proved that the smoothed distribution \( p_{\sigma^2} \) satisfies a log-Sobolev inequality, we almost certainly do not have the optimal log-Sobolev constant. In fact, as discussed in the
above section, while our bound on this constant gets worse with more noise, it is likely that the log-Sobolev constant actually improves with increased variance, which would explain fully the benefits of the annealing of DSM estimators that is so successful in [SE19]. Third, we could likely improve the algorithm by using lower variance estimators of the score function and a higher-order method for approximating the continuous Langevin diffusion. There has been some recent theoretical work in this direction (see, for example, [LWME19]) and we suspect that, especially in practical application, this would considerably accelerate the algorithm.

While the unconditional generative modeling studied in this work is certainly interesting in its own right, practitioners tend to focus on the benefits of conditional generative modeling, i.e., where there are two variables $x, y$ and we wish to input $y$ and generate samples from the conditional distribution $p(x|y)$. It is highly likely that, given the right conditions on the joint distribution of $x$ and $y$ to ensure a uniformity in $y$ to the dissipativity and Lipschitz nature of the conditional distribution, many of the results above could be extended to this regime.

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A Empirical Processes and Proving Theorem 9

We briefly sketch a few definitions from the theory of empirical processes. Denote by $\mathbb{E}$ as expectation with respect to $p_{n^2}$ and by $\overline{\mathbb{E}}$ as expectation with respect to the empirical measure. We have already defined the Rademacher complexity above. Given an $r > 0$, a function class $\mathcal{F}$, and a sample of $n$ points $X_1, \ldots, X_n \in \mathbb{R}^d$, we let

$$\mathcal{F}[r, S] = \left\{ f \in \mathcal{F} : \frac{1}{n} \sum_{i=1}^{n} f(X_i) \leq r \right\}$$  \hspace{1cm} (41)

We call a function $\phi_n : [0, \infty) \rightarrow \mathbb{R}_{\geq 0}$ an upper function for $\mathcal{F}$ if for all $r > 0$,

$$\sup_{S \subset (\mathbb{R}^d)^n} \overline{\mathbb{E}}_{n}(\mathcal{F}[r, S], S) \leq \phi_n(r)$$  \hspace{1cm} (42)

We define the (nonunique) localization radius $r^*$ as an upper bound on the maximal solution to the equation $\phi_n(r) = r$.

We recall two results:

Lemma 22. [RST17, Lemma 8.1] For any class $\mathcal{F}$ of real valued functions with image in the interval $[0, 1]$, with $n \geq 2$, we may take as localization radius of $\mathcal{G} = \{(f - f')^2 | f \in \mathcal{F}\}$

$$r^* = C \log^3(n) \mathcal{R}_n(\mathcal{F})^2$$  \hspace{1cm} (43)

Lemma 23. [RST17, Lemma 9] For any class $\mathcal{F}$ of real valued functions with image contained in the unit interval, and $\delta > 0$, with probability at least $1 - 4\delta$, if $X_1, \ldots, X_n \sim p$ i.i.d., for all $f, f' \in \mathcal{F}$

$$\mathbb{E}[(f - f')^2] \leq 2\overline{\mathbb{E}}(f - f')^2 + C(r^* + \beta)$$  \hspace{1cm} (44)

where $r^*$ is the localization radius of $\mathcal{G} = \{(f - f')^2 | f, f' \in \mathcal{F}\}$ and

$$\beta = \frac{\log \frac{1}{\delta} + \log \log n}{n}$$  \hspace{1cm} (45)

With these results, we can prove Theorem 9:

Proof. (Proof of Theorem 9) We prove for the case $\sigma^2 = 0$, as we rely only on the dissipativity and Lipschitz assumptions; thus Assumption 2 and Proposition 7 allow us to apply the same argument with slightly different constants.

By the fundamental theorem of calculus and the dissipativity assumption, we may invoke Lemma 38 to get that for sufficiently large $R > 0$ that there is a constant $C$ such that the probability that $X \sim p$ has norm bigger than $R$ is bounded above by $Ce^{-\frac{R^2}{2\sigma^2}}$. By a union bound, with probability at least $1 - Cne^{-\frac{R^2}{2\sigma^2}}$ all of the samples lie in the ball bounded by $R$. On this event then, the norm of $\nabla \log p$ is bounded by $MR + B$ by Lemma 34. Thus up to a factor of $MR + B$ we are in the situation of Lemma 22 and Lemma 23 with $\nabla \log p 1_{||X|| \leq R} \in \mathcal{F}$. Let $s^* = \nabla \log p$ and

$$\tilde{s} \in \arg\min_{s \in \mathcal{F}} \overline{\mathbb{E}}[||s(X) - s^*(X)||^2]$$.  \hspace{1cm} (46)

Clearly,

$$\overline{\mathbb{E}}[||\tilde{s}(X) - s^*(X)||^2] = 0$$  \hspace{1cm} (47)

since $s^* \in \mathcal{F}$ gives that

$$0 \leq \overline{\mathbb{E}}[||\tilde{s}(X) - s^*(X)||^2] \leq \overline{\mathbb{E}}[||s(X) - s^*(X)||^2] = 0$$  \hspace{1cm} (48)

We have

$$\mathbb{E}[||\tilde{s}(X) - s^*(X)||^2] = \sum_{i=1}^{d} \mathbb{E}[||\tilde{s}(X)_i - s^*(X)_i||^2]$$  \hspace{1cm} (49)

where the subscript $i$ denotes coordinates. Applying Lemma 23 yields

$$\mathbb{E}[||\tilde{s}(X)_i - s^*(X)_i||^2] \leq 2\overline{\mathbb{E}}[||\tilde{s}(X)_i - s^*(X)_i||^2] + C(MR + B)(r^*_i + \beta)$$  \hspace{1cm} (50)

where $r^*_i$ is the localization radius for the coordinate restriction $\mathcal{F}_i$. Applying Lemma 22 to bound $\sum r^*_i$ and noting that we are off by a factor of $(MR + B)$ from the result in [RST17], gives that

$$\sum_{i=1}^{d} r^*_i \leq (MR + B)C \log^3(n) \cdot \sum_{i=1}^{d} \mathcal{R}_n(\mathcal{F}_i)^2 \leq (MR + B)C \log^3(n) \cdot \mathcal{R}_n(\mathcal{F})^2$$  \hspace{1cm} (51)

which concludes the proof.
B The log-Sobolev Constant and Convergence to the Stationary Distribution

Background on log-Sobolev inequalities can be found in [BL14]. Recall that the generator of the process $W(t)$ is given by a second order differential operator $L$ acting on a test function $u$ by

$$L u = \Delta u + \langle \nabla \log p_{\sigma^2}, \nabla u \rangle$$

We call the Dirichlet form evaluated on a function $f$:

$$\mathcal{E}(f) = \int ||\nabla f||^2 p_{\sigma^2} dx$$

Note that $W(t)$, if $\nabla \log p_{\sigma^2}$ is Lipschitz, has a unique invariant distribution of $p_{\sigma^2}$. We say that $p_{\sigma^2}$ satisfies a Poincaré inequality with constant $c_P$ if for all measures $\mu \ll p_{\sigma^2}$, we have

$$\int \left| \frac{d\mu}{dp_{\sigma^2}} - 1 \right| p_{\sigma^2} \leq c_P \mathcal{E}\left( \frac{d\mu}{dp_{\sigma^2}} \right)$$

We say that $p_{\sigma^2}$ satisfies a log-Sobolev inequality with constant $c_{LS}$ if for all $\mu \ll p_{\sigma^2}$, we have

$$KL(\mu, p_{\sigma^2}) \leq c_{LS} \mathcal{E}\left( \frac{d\mu}{dp_{\sigma^2}} \right)$$

where $KL(\mu, \nu) = \mathbb{E}_{\nu} \left[ \log \frac{d\mu}{d\nu} \right]$ is the relative entropy. If $p_{\sigma^2}$ satisfies a log-Sobolev inequality, then we have two results:

**Theorem 24.** ([OV00]) If $p_{\sigma^2}$ satisfies a log-Sobolev inequality with constant $c_{LS}$ then for all $\mu \ll p_{\sigma^2}$,

$$\mathcal{W}_2(\mu, p_{\sigma^2}) \leq \sqrt{2c_{LS} KL(\mu, p_{\sigma^2})}$$

and the classic theorem whose proof can be found in [BL14]:

**Theorem 25.** If $p_{\sigma^2}$ satisfies a log-Sobolev inequality, with constant $c_{LS}$, and $W(t)$ is a Markov diffusion with law $\nu_t$ with stationary distribution $p_{\sigma^2}$ such that $\mathcal{W}_2(\nu_0, p_{\sigma^2}) < \infty$, then

$$\mathcal{W}_2(\nu_t, p_{\sigma^2}) \leq \mathcal{W}_2(\nu_0, p_{\sigma^2}) e^{-t c_{LS}}$$

If $\nabla \log p$ were strongly convex, then there are well-known bounds on the log-Sobolev constant; as we assume no such convexity, we, as in [RRT17], use a dissipativity condition and the Lyaponov function criteria found in [BBCG08, CGW09], presented in the following two theorems:

**Theorem 26.** ([BBCG08]) Let $V : \mathbb{R}^d \rightarrow [1, \infty)$ be a real valued function, and let $\mathcal{L}$ be the generator of the diffusion $W$ with stationary distribution $p$. If there are constants $\lambda_1, \lambda_2, R > 0$ such that

$$\frac{\mathcal{L} V(x)}{V(x)} \leq -\lambda_1 + \lambda_2 1_{B_R}(x)$$

Then $p$ satisfies a Poincaré inequality with constant

$$c_P \leq \frac{1}{\lambda_1} \left( 1 + C \lambda_2 R^2 e^{osc_{R}(\log p)} \right)$$

where $C > 0$ is a universal constant and for a continuous, real-valued function $f$, we let $osc_R(f) = \max_{B_R} f - \min_{B_R} f$. 

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Theorem 27. ([CGW09]) Suppose that \( p \) is a measure such that \( \nabla^2 \log p \geq -K \mathbb{I}_d \) for \( K \geq 0 \) in the sense of matrices and that \( p \) satisfies a Poincaré inequality with constant \( c_p \). Further suppose that there is a Lyapunov function \( V : \mathbb{R}^d \rightarrow [1, \infty) \) such that
\[
\frac{\mathcal{L}V(x)}{V(x)} \leq \kappa - \sigma ||x||^2
\]
(60)
Then \( p \) satisfies a log-Sobolev inequality with constant
\[
c_{LS} \leq \frac{2K}{\gamma} + \frac{2}{K} + c_p \left( 2 + \frac{2K}{\gamma} \left( \kappa + \gamma \mathbb{E}_{X \sim p} \left[ ||X||^2 \right] \right) \right)
\]
(61)
Further discussion regarding both theorems can be found in the appendix of [RRT17]. In order to apply the above results, we present a uniform bound on the second moment of \( W(t) \):

Lemma 28. ([RRT17, Lemma 3.2]) Suppose \( -\nabla \log p \) is \((m, b)\)-dissipative and \( \frac{M}{2} \)-Lipschitz. Suppose \( W(0) \sim \mu_0 \) such that \( \log \mathbb{E}_{X \sim \mu_0} \left[ e^{||X||^2} \right] = \kappa_0 < \infty \). Then
\[
\mathbb{E}[||W(t)||^2] \leq \kappa_0 e^{-2mt} + \frac{b + \frac{d}{m}}{m} (1 - e^{-2mt}) \leq \kappa_0 + \frac{b + \frac{d}{m}}{m}
\]
(62)

Remark 29. Note that in [RRT17], the authors consider Langevin optimization, and so they have the hypothesis that \( \nabla \log p \) is dissipative and they consider the diffusion driven by the drift \( -\nabla \log p \). These sign changes cancel out, allowing us to apply the lemma.

With this in hand, we are ready to prove Proposition 17:

Proof. (Proof of Proposition 17) Given that we rely on the \((m, b)\)-dissipativity and the \( \frac{M}{2} \)-Lipschitz of \( p_\sigma \), it suffices to prove in the case of \( \sigma^2 = 0 \) and apply Proposition 7. We apply in sequence the theorems from [BBCG08, CGW09]. Consider the following Lyapunov function: \( V(x) = e^{m||x||^2} \). We compute:
\[
\frac{\mathcal{L}V}{V} = \Delta \left( \frac{m}{2} ||x||^2 \right) + \left| \left| \nabla \left( \frac{m}{2} ||x||^2 \right) \right| \right| + \left< \frac{m}{2} x, \nabla \log p(x) \right>
\]
(63)
\[
= md + \frac{m^2}{4} ||x||^2 - \frac{m}{2} < x, -\nabla \log p(x) >
\]
(64)
\[
\leq m \left( d + \frac{b}{2} \right) - \frac{m^2}{4} ||x||^2
\]
(65)
by the dissipativity assumption. Let
\[
R^2 = \frac{4 \left( d + \frac{b}{2} \right)}{m} \quad \lambda_1 = m(2d + b) \quad \lambda_2 = m \left( d + \frac{b}{2} \right)
\]
(66)
in the theorem of [BBCG08]. Then we see that by Lemma 34 and the fundamental theorem of calculus, we may choose \( B \) such that
\[
\text{osc}_R(\log p) \leq (M + B)R^2 + B
\]
(67)
Thus we have
\[
c_p \leq \frac{1}{m(2d + b)} \left( 1 + C \left( d + \frac{b}{2} \right) (d + b) e^{\frac{m(2d + b)(d + b)}{m}} \right)
\]
(68)
Now, we may apply the theorem of [CGW09] with the same Lyapunov function. Note that as \( \nabla \log p \) is \( \frac{M}{2} \)-Lipschitz, we have \( \nabla^2 \log p \geq -M \mathbb{I}_d \). Then if we set
\[
\kappa = m \left( d + \frac{b}{2} \right) \quad \gamma = \frac{m^2}{4}
\]
(69)
then the above computation with the Lyapunov function shows that the assumptions of the theorem of [CGW09] hold. In order to conclude, we need to bound \( \mathbb{E}_p[||X||^2] \). Let \( W(t) \) be the Langevin diffusion initialized on a measure supported on a compact set. Then by Theorem 25 and Lemma 28, we have
\[
\mathbb{E}_p[||X||^2] = \lim_{t \to \infty} \mathbb{E}[||W(t)||^2] \leq \lim_{t \to \infty} \kappa_0 e^{-2mt} + \frac{b + d}{m} (1 - e^{-2mt}) = \frac{b + d}{m}
\]
(70)
The result follows.
C Bounding the Distance between \( \hat{W}(t) \) and \( W(t) \)

In this appendix, we provide a detailed account of the results appearing in Section 4.2, in particular a proof of the key proposition, Proposition 20. We assume that \( \hat{f} \) is Lipschitz and, for the sake of convenience, we assume that \( \hat{f}, \nabla \log p_{\sigma^2} \) have the same Lipschitz constant \( M \). Again we let \( W(t) \) evolve according to the continuous Langevin process, and we consider the process \( \hat{W}(t) \), the unique solution

\[
d\hat{W}(t) = \hat{f}(\hat{W}(t)) \, dt + \sqrt{\frac{2}{\beta}} \, dB(t) \quad \quad \quad \quad \hat{W}(0) = W(0)
\]

In order to bound the distance between the law of \( \hat{W}(t) \) and that of \( W(t) \), we can apply the method used in [RRT17, BEL18] of the application of the Girsanov theorem. In particular, we restate and prove Proposition 19:

**Proposition 30.** Let \( W(t), \hat{W}(t) \) be as above and assume that \( \nabla \log p_{\sigma^2} \) is \( \frac{M}{2} \)-Lipschitz. Suppose further that \( W(0) = \hat{W}(0) \sim \mu_0 \) such that

\[
E_{X \sim \mu_0} \left[ e^\frac{M^2}{2} ||X||^2 \right] < \infty
\]

Then

\[
KL(\nu_t, \nu_{\hat{t}}) = E \left[ \frac{1}{2} \int_0^t \left| |\nabla \log p_{\sigma^2}(W(s)) - \hat{f}(W(s))|^2 \right| \right]
\]

**Proof.** We apply the version of Girsanov’s theorem found in Theorem 7.20 in [LS77]. Note that

\[
E \left[ \exp \left( \frac{1}{2} \int_0^t \left| \hat{f}(W(s)) - \nabla \log p_{\sigma^2}(W(s)) \right|^2 ds \right) \right] \leq E \left[ \exp \left( \frac{M^2}{2} \int_0^t \left| |W(t)|^2 \right| ds \right) \right] < \infty
\]

by Lemma 36. Thus by Girsanov’s theorem, we have that

\[
d\nu_{\hat{t}} = E \left[ \exp \left( \int_0^t (\hat{f}(W(s)) - \nabla \log p_{\sigma^2}(W(s))) dB_s + \frac{1}{2} \int_0^t |\hat{f}(W(s)) - \nabla \log p_{\sigma^2}(W(s))|^2 ds \right) \right] \frac{d\nu_t}{d\nu_{\hat{t}}}
\]

and so

\[
KL(\nu_t, \nu_{\hat{t}}) = E \left[ \log \frac{d\nu_{\hat{t}}}{d\nu_t} \right]
\]

\[
= E \left[ \int_0^t (\hat{f}(W(s)) - \nabla \log p_{\sigma^2}(W(s))) dB_s + \frac{1}{2} \int_0^t |\hat{f}(W(s)) - \nabla \log p_{\sigma^2}(W(s))|^2 ds \right]
\]

But the first term is a real martingale by Novikov’s condition so has expectation zero, yielding the result.

Thus it suffices to bound

\[
E \left[ \int_0^t \left| \hat{f}(W(s)) - \nabla \log p(W(s)) \right|^2 ds \right]
\]

We first need the following identity:

**Lemma 31.** Let \( U \subset \mathbb{R}^d \) be measurable and let \( W(s) \) be as above. Let \( \pi_s(x, y) \) be the transition density of \( W(s) \). Then if \( E_x[\cdot] \) denotes expectation with respect to the measure associated with \( W(s) \) started at \( W(0) = x \), then

\[
E_x \left[ \int_0^t 1_U(W(s)) \, ds \right] = \int_U \left( \int_0^t \pi_s(x, y) \, ds \right) \, dy
\]

**Proof.** Following the proof of [MP10, Theorem 3.32] and appealing to [GH80] for justification in the case that \( W(t) \) is not just Brownian motion, we have

\[
E_x \left[ \int_0^t 1_U(W(s)) \, ds \right] = \int_0^t E_x[1_U(W(s))] \, ds = \int_0^t \int_U \pi_s(x, y) \, dy \, ds = \int_A \left( \int_0^t \pi_s(x, y) \, ds \right) \, dy
\]

by Fubini’s theorem and the definition of the transition density.
In order to construct a bound on the relevant integral, we need a bound on $\pi_t(x, y)$. In order to construct a Gaussian bound, we adapt an argument of [Dow08]:

**Lemma 32.** For fixed $x$, let $W(t)$ evolve as above and let $W(0) = x$. If $\nabla \log p_{\sigma^2}$ is $\frac{M}{2}$-Lipschitz, $\pi_t(x, y)$ is the transition density of $W(t)$ for $y \in \mathbb{R}^d$, then we have

$$\pi_t(x, y) \leq \frac{p_{\sigma^2}(y)}{p_{\sigma^2}(x)} \cdot \Delta \log g_t(x, y) \quad \text{(79)}$$

where $g_t(x, y)$ is the standard Gaussian heat kernel.

**Proof.** We adapt a proof in [Dow08] to the case of higher dimensions. By the same argument as in the proof of Proposition 19, we may apply Girsanov’s theorem. Let $Q_x$ be a measure under which $W(t) = \tilde{B}_t$ is a $Q_x$ Brownian motion started at $x$. Let $P_x$ be the original measure pertaining to the Brownian motion $B_t$ that drives $W(t)$. Then by Girsanov’s theorem, we have

$$\begin{align*}
\left( \frac{dP_x}{dQ_x} \right)_t & = \mathbb{E}_x \left[ \exp \left( \int_0^t \nabla \log p_{\sigma^2}(W(s))dW(s) - \frac{1}{2} \int_0^t ||\nabla \log p_{\sigma^2}(W(s))||^2 ds \right) \right] \\
& = \mathbb{E}_x \left[ \exp \left( \int_0^t \nabla \log p_{\sigma^2}(W(s))d\tilde{B}_s - \frac{1}{2} \int_0^t ||\nabla \log p_{\sigma^2}(W(s))||^2 ds \right) \right]
\end{align*} \quad \text{(80)}$$

where $\mathbb{E}_x$ denotes expectation with respect to $Q_x$. Now, by Rademacher’s theorem we may apply Ito’s lemma to $\log p_{\sigma^2}()$, thus we get

$$\log p_{\sigma^2}(W(t)) - \log p_{\sigma^2}(W(0)) = \int_0^t \nabla \log p_{\sigma^2}(W(s))dW(s) + \frac{1}{2} \int_0^t \Delta \log p_{\sigma^2}(W(s))ds \quad \text{(82)}$$

Rearranging, we get that

$$\int_0^t \nabla \log p_{\sigma^2}(W(s))d\tilde{B}_s = \log \left( \frac{p_{\sigma^2}(W(t))}{p_{\sigma^2}(x)} \right) - \frac{1}{2} \int_0^t \Delta \log p_{\sigma^2}(W(s))ds \quad \text{(83)}$$

By the fact that $\nabla \log p_{\sigma^2}$ is $\frac{M}{2}$-Lipschitz, we have that $|\Delta \log p_{\sigma^2}(y)| \leq \sqrt{d}M$ for all $y \in \mathbb{R}^d$. Because $||\nabla \log p_{\sigma^2}(\cdot)||^2 \geq 0$, we have by the above work and the fact that the transition density of Brownian motion is $g_t(x, y)$, that

$$\pi_t(x, y) \leq \frac{p_{\sigma^2}(y)}{p_{\sigma^2}(x)} \cdot \Delta \log g_t(x, y) \quad \text{(84)}$$

as desired. 

This allows us to prove the following lemma:

**Lemma 33.** Let $\phi : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$ be measurable and $W(t)$ as above and suppose that $\mathbb{E}[\phi(X)] \leq \epsilon^2$, where $X$ is distributed according to $p_{\sigma^2}$. Let $x \in \mathbb{R}^d$. Then

$$\mathbb{E}_x \left[ \int_0^t \phi(W(s))ds \right] \leq \epsilon t + \sqrt{\left( \int_0^t \mathbb{E}_x[\phi(W(s))^2]ds \right) t \frac{\Delta \log g_t(x)}{p_{\sigma^2}(x)} \cdot \|\psi_t(x, \cdot)\|_{L^\infty(U)} \epsilon} \quad \text{(85)}$$

where $\mathbb{E}_x$ denotes expectation with respect to $W(t)$ started at $W(0) = x$ and

$$\psi_t(x, y) = \int_0^t g_s(x, y)ds \quad \text{(86)}$$

**Proof.** For the sake of simplicity, we assume that $\sigma^2 = 0$, as nothing in the proof changes except for the added notation if we lose this assumption.

Let $U = \{ y \in \mathbb{R}^d : \phi(y) > \epsilon \}$. Then we have

$$\int_0^t \phi(W(s))ds = \int_0^t \phi(W(s))1_{U^c}ds + \int_0^t \phi(W(s))1_Uds \leq \epsilon t + \int_0^t \phi(W(s))1_Uds \quad \text{(87)}$$
By Cauchy-Schwarz,
\[
\mathbb{E}_x \left[ \int_0^t \phi(W(s)) \mathbf{1}_U ds \right] \leq \sqrt{\int_0^t \mathbb{E}_x [\phi(W(s))^2] ds \int_0^t \mathbb{E}_x [\mathbf{1}_U] ds}
\] (88)

Now by Lemma 32 and Lemma 31, we have that
\[
\int_0^t \mathbb{E}_x [\mathbf{1}_U] ds = \int_U \int_0^t \pi_s(x, y) dy dx \leq e^{\frac{M^2 t}{4}} - \int_U \int_0^t p(y) g_s(x, y) dy dx = e^{\frac{M^2 t}{4}} - \int_U \psi_t(x, y) p(y) dy (89)
\]

By assumption, we have
\[
\varepsilon^2 \geq \mathbb{E}[\phi(X)] \geq \mathbb{E} [\phi(X) \mathbf{1}_U] \geq \varepsilon \int_U p(y) dy
\] (90)

Thus we have
\[
\int_0^t \mathbb{E}_x [\mathbf{1}_U (W(s))] ds \leq \frac{e^{\frac{M^2 t}{4}}}{p(x)} t \varepsilon \| \psi_t(x, \cdot) \|_{L^\infty(U)}
\]

Putting this altogether yields the result. ■

Finally, we are able to prove Proposition 20.

Proof. (Proof of Proposition 20) We apply Lemma 33 to \( \phi(x) = \| \nabla \log p(x) - \hat{f}(x) \|^2 \). By the Lipschitz condition and Lemma 34, we note that
\[
\phi(x)^2 \leq 16M^4 ||x||^4 + B^4
\] (91)

and by Lemma 35, we have then
\[
\int_0^t \mathbb{E}_x [\phi(W(s))^2] ds \leq 16M^4 t \left( (2 dt)^2 + B^4 t \right) e^{M^4 t} + B^4 t
\] (92)

Now, we note that
\[
\psi_t(x, y) \leq \int_0^\infty g_s(x, y) ds = \frac{\Gamma\left(\frac{d}{2} - 1\right)}{2\pi^d} ||x - y||^{2-d}
\] (93)

by, for instance, \([MP10, \text{Theorem 3.33}]\). By assumption and the Lipschitz nature of \( \phi \), we have that if \( y \in U \) from Lemma 33, then \( ||x - y|| \geq \delta \). Note that by Lemma 34 and the fact that \( \nabla \log p \) is Lipschitz, if our initial distribution is supported in a ball of radius \( R \), then we have a lower bound on \( p(x) \) of \( e^{B - MR} \). Thus with high probability, we have
\[
\mathbb{E}_x \left[ \left\| \nabla \log p(W(s)) - \hat{f}(W(s)) \right\|^2 ds \right] \leq \varepsilon t + \sqrt{\left( 16M^4 t \left( (2 dt)^2 + B^4 t \right) e^{M^4 t} + B^4 t \right) te^{\frac{M^2 t}{4}} t e^{M^4 t - B} \frac{\Gamma\left(\frac{d}{2} - 1\right)}{2\pi^d} \delta^{2-d} \varepsilon}
\] (94)

where \( \delta \) is chosen as
\[
\delta = \inf_{y \in U} ||x - y||
\] (96)
D Miscellaneous Proofs

Proof. (Proof of Proposition 5) Let $\epsilon \sim g_{\alpha^2}$ and $X \sim p$. Then we have, letting $y = x + \epsilon$,

$$L_{DAE}(r) = \mathbb{E}_X \mathbb{E}_\epsilon [||r(x + \epsilon) - x||^2] = \int \int ||r(y) - y + \epsilon||^2 p(y - \epsilon) g(\epsilon) dyd\epsilon$$

$$= \int \int ||r(y) - y||^2 p(y - \epsilon) g(\epsilon) dyd\epsilon + \int \int 2\epsilon, r(y) - y)p(y - \epsilon) g(\epsilon) dyd\epsilon + \int \int ||\epsilon||^2 p(y - \epsilon) g(\epsilon) dyd\epsilon$$

(97)

(98)

(99)

The last term above does not depend on $r$ and so we may ignore it. We focus now on the second term. Let $\xi \sim g_1$ be a standard Gaussian and let $s'(x) = r(x) - x$. By Lemma 39, we have that

$$\int \langle \epsilon, s'(x + \epsilon) \rangle g(\epsilon) d\epsilon = \sigma \int \langle \xi, s'(x + \sigma \xi) \rangle g_1(\xi) d\xi$$

$$= \sigma^2 \int \langle \xi, s'(x + \sigma \xi) \rangle g_1(\xi) d\xi$$

$$= \sigma^2 \int s'(x + \epsilon) g(\epsilon) d\epsilon$$

(100)

(101)

(102)

where we used Stein Gaussian identity above. Now, note that as we know that $p_{\alpha^2}$ is a density, it must tend to zero as $||x|| \to \infty$. Thus we may apply the divergence theorem to get

$$\int \int 2\langle \epsilon, r(y) - y \rangle p(y - \epsilon) g(\epsilon) dyd\epsilon = 2\sigma^2 \int p(x) \text{div} (\mathbb{E}_\epsilon [s'(x + \epsilon)]) dx$$

$$= 2\sigma^2 \int \text{div}(s'(y)) p_{\alpha^2}(y) dy$$

$$= -2\sigma^2 \int \left\langle s'(x), \frac{\nabla p_{\alpha^2}}{p_{\alpha^2}}(x) \right\rangle p_{\alpha^2} dx$$

(103)

(104)

(105)

Thus we have that

$$L_{DAE}(r) = \mathbb{E}_X \mathbb{E}_{p_{\alpha^2}} [||r(X) - X||^2 - 2\sigma^2 \langle s'(X), \nabla \log p_{\alpha^2}(X) \rangle] + C(p, \sigma^2)$$

$$= \mathbb{E}_X \mathbb{E}_{p_{\alpha^2}} [||s'(X) - \sigma^2 \nabla \log p_{\alpha^2}(X)||^2] + C(p, \sigma^2) - \sigma^4 \mathbb{E}_X \mathbb{E}_{p_{\alpha^2}} [||\nabla \log p_{\alpha^2}||^2]$$

$$= \mathbb{E}_X \mathbb{E}_{p_{\alpha^2}} [||s'(X) - \sigma^2 \nabla \log p_{\alpha^2}(X)||^2] + C'(p, \sigma^2)$$

(106)

(107)

(108)

where $C'(p, \sigma^2)$ does not depend on $r$. Dividing by $\sigma^2$ and setting $s(x) = \frac{s(x)}{\sigma^2}$ shows that

$$L_{DSM}(s) = \mathbb{E}_{p_{\alpha^2}} [||s(x) - \nabla \log p_{\alpha^2}||^2] = \frac{1}{\sigma^2} L_{DAE}(r) + C(p, \sigma^2)$$

(109)

Thus, the two losses are equivalent to minimize with respect to $r$ or $s$.

Proof. (Alternate proof of Corollary 6) For $y \in \mathbb{R}^d$, the loss of the DAE is given by

$$\int_{\mathbb{R}^d} \mathbb{E}_\epsilon [p(y)||r(y + \epsilon) - y||^2] dy = \int_{\mathbb{R}^d} \mathbb{E}_\epsilon [p(x - \epsilon)||r(x) - x + \epsilon||^2] dx$$

(110)

where we substituted $x = y + \epsilon$. Now by the calculus of variations, it suffices to minimize the integrand with respect to $r(x)$ for each $x \in \mathbb{R}^d$. Taking the derivative and setting it equal to zero gives

$$r_{\alpha^2}(x) = \frac{\mathbb{E}_\epsilon [p(x - \epsilon)(x - \epsilon)]}{\mathbb{E}_\epsilon [p(x - \epsilon)]}$$

(111)

the result given by [AB14, Theorem 1]. By linearity, then we have

$$r_{\alpha^2}(x) = \frac{\mathbb{E}_\epsilon [xp(x - \epsilon)]}{\mathbb{E}_\epsilon [p(x - \epsilon)]} - \frac{\mathbb{E}_\epsilon [lp(x - \epsilon)]}{\mathbb{E}_\epsilon [p(x - \epsilon)]} = x - \frac{\mathbb{E}_\epsilon [lp(x - \epsilon)]}{\mathbb{E}_\epsilon [p(x - \epsilon)]}$$

(112)
But we have
\[ \mathbb{E}_\epsilon [e^{p(x - \epsilon)}] = \int e^{p(x - \epsilon)} g_{\sigma^2}(\epsilon) d\epsilon = \sigma^2 \int \nabla g_{\sigma^2}(\epsilon) p(x - \epsilon) d\epsilon = -\sigma^2 \int g_{\sigma^2}(\epsilon) \nabla p(x - \epsilon) d\epsilon \] (113)
by lemma \ref{lem:iterate}. But then we have
\[ \frac{\mathbb{E}_\epsilon [e^{p(x - \epsilon)}]}{\mathbb{E}_\epsilon [p(x - \epsilon)]} = -\sigma^2 \frac{\mathbb{E}_\epsilon [-\nabla_x p(x - \epsilon)]}{\mathbb{E}_\epsilon [p(x - \epsilon)]} = \sigma^2 \frac{\nabla p * g_{\sigma^2}(x)}{p * g_{\sigma^2}(x)} = \sigma^2 \nabla \log p_{\sigma^2} \] (114)
Putting this together yields the result.

\textbf{Proof.} (Proof of Proposition 7) Let \( \sigma^2 \leq \sigma_{\text{max}}^2 \). Let \( \eta_{\sigma^2}(X) = \nabla \log p_{\sigma^2}(X) - \nabla \log p(X) \). By Assumption 2, \( \eta_{\sigma^2} \) is Lipschitz with constant \( \sigma^2 M^2 \). Thus, we have:
\[ \langle -\nabla \log p_{\sigma^2}(x), x \rangle = \langle -\nabla \log p(x), x \rangle - \langle \eta_{\sigma^2}(X), x \rangle \] (115)
By Lemma 34 we know that there is some constant, which, by raising \( B \) if necessary, we may take to be equal to \( B \), such that
\[ ||\eta_{\sigma^2}(x)|| \leq \sigma^2 M ||x|| + B \] (116)
By Cauchy-Schwarz,
\[ ||\eta_{\sigma^2}(X), x|| \leq ||\eta_{\sigma^2}(x)|| \cdot ||x|| \leq \sigma^2 M ||x||^2 + B ||x|| \] (117)
and thus
\[ \langle \eta_{\sigma^2}(X), x \rangle \geq -\sigma^2 M ||x||^2 - B ||x|| \] (118)
By the dissipativity assumption, we have
\[ \langle -\nabla \log p(x), x \rangle \geq m ||x||^2 - b \] (119)
Thus we have
\[ \langle -\nabla \log p_{\sigma^2}(x), x \rangle \geq (m - \sigma^2 M) ||x||^2 - b - B ||x|| \] (120)
\[ \geq \frac{m - \sigma^2 M}{2} ||x||^2 - b + \frac{m - \sigma^2 M}{2} ||x||^2 - B ||x|| \] (121)
\[ \geq \frac{m - \sigma^2 M}{2} ||x||^2 - b - \frac{B^2}{2(m - \sigma^2 M)} \] (122)
where the last inequality follows by the fact that
\[ \frac{m - \sigma^2 M}{2} ||x||^2 - B ||x|| = \frac{m - \sigma^2 M}{2} \left( ||x|| - \frac{B}{m - \sigma^2 M} \right)^2 - \frac{B^2}{2(m - \sigma^2 M)} \] (123)
\[ \geq -\frac{B^2}{2(m - \sigma^2 M)} \] (124)
\textbf{Proof.} (Proof of Proposition 16) Consider the coupling where the Brownian motion driving \( W(t) \) also generates the Gaussians in \( W_k \). Let \( \hat{W}(s) \) be the continuous time process such that \( \hat{W}(s) = W(\lfloor s \rfloor) \) and \( \hat{W}(0) = W(0) \). Then we can compute
\[ \mathbb{E} \left[ ||W(\tau) - W_{\tau}||^2 \right] = \mathbb{E} \left[ \left| \left| W(\tau) - \hat{W}(\tau) \right| \right|^2 \right] = \mathbb{E} \left[ \left| \left| \int_0^{\tau} \nabla \log p(W(s)) - \nabla \log p(\hat{W}(s))^2 ds \right| \right|^2 \right] \]
\[ \leq \int_0^{\tau} \mathbb{E} \left[ \left| \left| \nabla \log p(W(s)) - \nabla \log p(\hat{W}(s)) \right| \right|^2 \right] ds \]
\[ \leq M^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E} \left[ ||W(s) - W_j||^2 \right] ds \]
Now note that for $j\eta \leq s < (j+1)\eta$, we have
\[ E \left[ \|W(s) - W_j\|^2 \right] \leq 2E \left[ \|W(s) - W(j\eta)\|^2 \right] + 2E \left[ \|W(j\eta) - W_j\|^2 \right] \]

For the first term, we have
\[ E \left[ \|W(s) - W_j\|^2 \right] = E \left[ \left\| \int_{j\eta}^s \nabla \log p(W(u)) du + \sqrt{2} \int_{j\eta}^s dB_u \right\|^2 \right] \]
\[ \leq 2\eta M^2 E \left[ \|W(s)\|^2 \right] + 4d\eta \leq 2\eta M^2 E \left[ \|W(\tau)\|^2 \right] + 4d\eta \]

where we recall that $\tau = k\eta$. Plugging this last bound into our above inequality, we get
\[ E \left[ \|W(\tau) - W_\tau\|^2 \right] \leq M^2 \tau \left( 2\eta M^2 E \left[ \|W(\tau)\|^2 \right] + 4d\eta \right) + M^2 \sum_{j=0}^{k-1} E \left[ \|W(j\eta) - W_j\|^2 \right] \]

Applying the discrete Gronwall lemma, we have
\[ E \left[ \|W(\tau) - W_\tau\|^2 \right] \leq M^2 \tau \left( 2\eta M^2 E \left[ \|W(\tau)\|^2 \right] + 4d\eta \right) e^{M^2 \tau} \]

To conclude, we apply Lemma 35 to bound $E \left[ \|W(\tau)\|^2 \right]$ and the result follows from the fact that the Wasserstein distance is bounded by the above explicit coupling of the two laws $\mu_k$ and $\nu_\tau$.  

\[ \square \]

E Auxiliary Lemmata

**Lemma 34.** If $\nabla \log p$ is $M/2$-Lipschitz, then there is some constant $B$ such that
\[ \|\nabla \log p(x)\|^p \leq M^p \|x\|^p + B^p \]
for all $p \geq 1$.

**Proof.** By the definition of Lipschitz, we have that
\[ \|\nabla \log p(x)\| \leq \|\nabla \log p(x) - \nabla \log p(0)\| + \|\nabla \log p(0)\| \leq \frac{M}{2} \|x\| + \|\nabla \log p(0)\| \]

Applying Minkowski’s inequality concludes the proof.  

\[ \square \]

**Lemma 35.** For all $p > 1$ and all $t > 0$, we have that if $\nabla \log p$ is $\frac{M}{2}$ Lipschitz, then
\[ E \left[ \|W(t)\|^p \right] \leq \left( (2dt)^{\frac{p}{2}} + B^p t \right) e^{Mp t} \]
where $B$ is as appears in Lemma 34.

**Proof.** By the triangle inequality and Lemma 34, we have
\[ \|W(t)\|^p = \left\| \sqrt{2} B_t + \int_0^t \nabla \log p(W(s)) ds \right\|^p \leq 2\frac{p}{2} \|B_t\|^p + \int_0^t \|\nabla \log p(W(s))\|^p ds \]
\[ \leq 2\frac{p}{2} \|B_t\|^p + \int_0^t (Mp \|W(s)\|^p + B^p) ds \]

Taking expected values and applying Fubini, we get
\[ E \left[ \|W(t)\|^p \right] \leq 2\frac{p}{2} E \|B_t\|^p + \int_0^t (Mp E \|W(s)\|^p + B^p) ds \]
\[ \leq (2dt)^{\frac{p}{2}} + B^p t + Mp \int_0^t E \|W(s)\|^p ds \]

Applying Gronwall’s inequality finishes the proof.  

\[ \square \]
Lemma 36. Suppose that \( \nabla \log p \) is \( \frac{M}{2} \)-Lipschitz. If \( W(t) \) is a solution to the Langevin SDE, and \( W(0) \) distributed such that \( \mathbb{E} \left[ e^{\frac{c}{2} ||W(0)||^2} \right] \leq C \), then
\[
\mathbb{E} \left[ \exp \left( \frac{c}{2} ||W(t)||^2 \right) \right] \leq C \exp \left( c^2 \left( \frac{d}{2} t + B^2 t + M^2 (4d + B^2) t e^{M^2 t} \right) \right)
\]  
(133)

Proof. Let \( Y(t) = e^{\frac{c}{2} ||W(t)||^2} \). As multiplying by positive \( c > 0 \) only changes the computations by a factor of \( c^2 \), we assume that \( c = 1 \) below. We apply Itô’s lemma to get
\[
dY(t) = \frac{1}{2} (d + ||W(t)||^2) Y(t) dt + W(t)^* Y(t) dW(t)
\]
(134)
\[
dY(t) = \frac{1}{2} (d + ||W(t)||^2) Y(t) dt + \langle W(t), \nabla \log p(W(t)) \rangle Y(t) dt + \sqrt{2} Y(t) W(t)^* dB_t
\]
(135)

We cite without proof, as in [RRT17], that [WGD04, Corollary 4.1] gives \( \int_0^t \mathbb{E}[||Y(s)||^2] ds < \infty \). Thus the stochastic part of the integral is an actual martingale and has expectation 0. Thus, integrating and taking expectations gives,
\[
\mathbb{E}[Y(t)] = \mathbb{E}[Y(0)] + \int_0^t \left( \frac{d}{2} + \mathbb{E} \left[ \frac{1}{2} ||W(s)||^2 - \langle W(s), \nabla \log p(W(s)) \rangle \right] \right) ds
\]
(136)

Applying Gronwall’s inequality and using the assumption that \( \mathbb{E}[Y(0)] \leq C \), we have
\[
\mathbb{E}[Y(t)] \leq C \exp \left( \frac{d}{2} t + \int_0^t \left( \mathbb{E} \left[ \frac{1}{2} ||W(s)||^2 - \langle W(s), \nabla \log p(W(s)) \rangle \right] \right) ds \right)
\]
(137)

Now, by Cauchy-Schwarz and Lemma 34, we have
\[
||\langle W(s), \nabla \log p(W(s)) \rangle|| \leq ||W(s)|| ||\nabla \log p(W(s))|| \leq M^2 ||W(s)||^2 + B^2
\]
(138)

and thus
\[
\frac{1}{2} ||W(s)||^2 - \langle W(s), \nabla \log p(W(s)) \rangle \leq \left( \frac{1}{2} + M^2 \right) ||W(s)||^2 + B^2
\]
(139)

Applying Lemma 35 with \( p = 2 \) and plugging this into our expression above, we have
\[
\mathbb{E}[Y(t)] \leq C \exp \left( \frac{d}{2} t + B^2 t + M^2 (4d + B^2) t e^{M^2 t} \right)
\]
(140)

Lemma 37. Let \( -\nabla \log p \) be \((m, b)\)-dissipative. Then
\[
\log p(x) \leq -\frac{m}{4} ||x||^2 + \frac{2b^2}{m} + \log p(0)
\]
(141)

Proof. By the fundamental theorem of calculus,
\[
\log p(x) = \log p(0) + \int_0^1 \frac{d}{dt} (\log p(tx)) dt = \log p(0) + \int_0^1 \langle \nabla \log p(tx), x \rangle dt
\]
(142)
\[
\leq \log p(0) - \int_0^1 mt^2 ||x||^2 + b dt = \log p(0) + b - \frac{m}{2} ||x||^2
\]
(143)
\[
= -\frac{m}{4} ||x||^2 + \log p(0) - \frac{m}{4} ||x||^2 + b ||x||
\]
(144)

by the dissipativity assumption. Maximizing the last two terms with respect to \( ||x|| \) yields the result. □

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**Lemma 38.** Let $-\nabla \log p$ be $(m, b)$-dissipative. Then there is a constant $C$ such that for all $||x||$,

$$p(x) \leq Ce^{-\frac{4||x||^2}{m}}$$

(145)

In particular, $p$ is $\frac{m}{2}$-sub-Gaussian.

**Proof.** The first statement follows immediately from Lemma 37. The second follows from a Gaussian tail-bound. ■

**Lemma 39.** (Gaussian Stein Identity, [Ste81]) Let $\xi \sim N(0, I_d)$ and let $g : \mathbb{R}^d \to \mathbb{R}$ be an almost everywhere differentiable function with $E_{\xi}[||\nabla g(\xi)||] < \infty$. Then

$$E_{\xi}[g(\xi)\xi] = E_{\xi}[\nabla g(\xi)]$$

(146)