Rapid Convergence of the Unadjusted Langevin Algorithm: Isoperimetry Suffices

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Abstract

We study the Unadjusted Langevin Algorithm (ULA) for sampling from a probability distribution \( \nu = e^{-f} \) on \( \mathbb{R}^n \). We prove a convergence guarantee in Kullback-Leibler (KL) divergence assuming \( \nu \) satisfies a log-Sobolev inequality and the Hessian of \( f \) is bounded. Notably, we do not assume convexity or bounds on higher derivatives. We prove convergence guarantees in Rényi divergence of order \( q > 1 \) assuming the limit of ULA satisfies isoperimetry, namely either the log-Sobolev or Poincaré inequality. We also prove a bound on the bias of the limiting distribution of ULA assuming third-order smoothness of \( f \), without requiring isoperimetry.

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1 Introduction

Sampling is a fundamental algorithmic task. Many applications require sampling from probability distributions in high-dimensional spaces, and in modern applications the probability distributions are complicated and non-logconcave. While the setting of logconcave functions is well-studied, it is important to have efficient sampling algorithms with good convergence guarantees beyond the logconcavity assumption. There is a close interplay between sampling and optimization, either via optimization as a limit of sampling (annealing) [43, 66], or via sampling as optimization in the space of distributions [46, 76]. Motivated by the widespread use of non-convex optimization and sampling, there is resurgent interest in understanding non-logconcave sampling.

In this paper we study a simple algorithm, the Unadjusted Langevin Algorithm (ULA), for sampling from a target probability distribution $\nu = e^{-f}$ on $\mathbb{R}^n$. ULA requires oracle access to the gradient $\nabla f$ of the log density $f = -\log \nu$. In particular, ULA does not require knowledge of $f$, which makes it applicable in practice where we often only know $\nu$ up to a normalizing constant.

As the step size $\eta \to 0$, ULA recovers the Langevin dynamics, which is a continuous-time stochastic process in $\mathbb{R}^n$ that converges to $\nu$. We recall the optimization interpretation of the Langevin dynamics for sampling as the gradient flow of the Kullback-Leibler (KL) divergence with respect to $\nu$ in the space of probability distributions with the Wasserstein metric [46]. When $\nu$ is strongly logconcave, the KL divergence is a strongly convex objective function, so the Langevin dynamics as gradient flow converges exponentially fast [6, 73]. From the classical theory of Markov chains and diffusion processes, there are several known conditions milder than logconcavity that are sufficient for rapid convergence in continuous time. These include isoperimetric inequalities such as Poincaré inequality or log-Sobolev inequality (LSI). Along the Langevin dynamics in continuous time, Poincaré inequality implies an exponential convergence rate in $L^2(\nu)$, while LSI—which is stronger—implies an exponential convergence rate in KL divergence (as well as in Rényi divergence).

However, in discrete time, sampling under Poincaré inequality or LSI is a more challenging problem. ULA is an inexact discretization of the Langevin dynamics, and it converges to a biased limit $\nu_\eta \neq \nu$. When $\nu$ is strongly logconcave and smooth, it is known how to control the bias and prove a convergence guarantee on KL divergence along ULA; see for example [19, 25, 26, 28]. When $\nu$ is strongly logconcave, there are many other sampling algorithms with provable rapid convergence; these include the ball walk and hit-and-run [47, 54, 55, 53] (which give truly polynomial algorithms), various discretizations of the overdamped or underdamped Langevin dynamics [25, 26, 28, 9, 30] (which have polynomial dependencies on smoothness parameters but low dependence on dimension), and more sophisticated methods such as the Hamiltonian Monte Carlo [58, 59, 29, 49, 18]. It is of great interest to extend these results to non-logconcave densities $\nu$, where existing results require strong assumptions with bounds that grow exponentially with the dimension or other parameters [2, 20, 56, 60]. There are also recent works that analyze convergence of sampling using various techniques such as reflection coupling [32], kernel methods [37], and higher-order integrators [51], albeit still under some strong conditions such as distant dissipativity, which is
similar to strong logconcavity outside a bounded domain.

In this paper we study the convergence along ULA under minimal (and necessary) isoperimetric assumptions, namely, LSI and Poincaré inequality. These are sufficient for fast convergence in continuous time; moreover, in the case of logconcave distribution, the log-Sobolev and Poincaré constants can be bounded and lead to convergence guarantees for efficient sampling in discrete time. However, do they suffice on their own without the assumption of logconcavity?

We note that LSI and Poincaré inequality apply to a wider class of measures than logconcave distributions. In particular, LSI and Poincaré inequality are preserved under bounded perturbation and Lipschitz mapping (see Lemma 16 and Lemma 19), whereas logconcavity would be destroyed. Given these properties, it is easy to exhibit examples of non-logconcave distributions satisfying LSI or Poincaré inequality. For example, we can take a small perturbation of a convex body to make it nonconvex but still satisfies isoperimetry; then the uniform probability distribution on the body (or a smooth approximation of it) is not logconcave but satisfies LSI or Poincaré inequality. Similarly, we can start with a strongly logconcave distribution such as a Gaussian, and subtract some small Gaussians from it; then the resulting (normalized) probability distribution is not logconcave, but it still satisfies LSI or Poincaré inequality as long as the Gaussians we subtract are small enough. See Figure 1 for an illustration.

![Figure 1: Illustrations of non-logconcave distributions satisfying LSI or Poincaré inequality: the uniform distribution on a nonconvex set (left), and a small perturbation of a logconcave distribution, e.g., Gaussian (right).](image)

We measure the mode of convergence using KL divergence and Rényi divergence of order $q \geq 1$, which is stronger. Our first main result says that the only further assumption we need is smoothness, i.e., the gradient of $f$ is Lipschitz (see Section 3.1). Here $H_\nu(\rho)$ is the KL divergence between $\rho$ and $\nu$. We say that $\nu = e^{-f}$ is $L$-smooth if $\nabla f$ is $L$-Lipschitz, or equivalently, $-LI \preceq \nabla^2 f(x) \preceq LI$ for all $x \in \mathbb{R}^n$.

**Theorem 1.** Assume $\nu = e^{-f}$ satisfies log-Sobolev inequality with constant $\alpha > 0$ and is $L$-smooth. ULA with step size $0 < \eta \leq \frac{\alpha}{4L^2}$ satisfies

$$H_\nu(\rho_k) \leq e^{-\alpha \eta k} H_\nu(\rho_0) + \frac{8\eta mL^2}{\alpha}.$$
In particular, for any $0 < \delta < 4n$, ULA with step size $\eta \leq \frac{\alpha \delta}{16L^2 n}$ reaches error $H_\nu(\rho_k) \leq \delta$ after $k \geq \frac{1}{\alpha \eta} \log \frac{2H_\nu(\rho_0)}{\delta}$ iterations.

For example, if we start with a Gaussian $\rho_0 = N(x^*, \frac{1}{\tau} I)$ where $x^*$ is a stationary point of $f$ (which we can find, e.g., via gradient descent), then $H_\nu(\rho_0) = O(n)$ (see Lemma 1), and Theorem 1 gives an iteration complexity of $k = \tilde{\Theta}\left(\frac{L^2 n}{\alpha^2 \delta}\right)$ to achieve $H_\nu(\rho_k) \leq \delta$ using ULA with step size $\eta = \Theta\left(\frac{\alpha \delta}{L^2 n}\right)$.

The result above matches previous known bounds for ULA when $\nu$ is strongly logconcave [19, 25, 26, 28]. Our result complements the work of Ma et al. [56] who study the underdamped version of the Langevin dynamics under LSI and show an iteration complexity for the discrete-time algorithm that has better dependence on the dimension ($\sqrt{\frac{n}{\delta}}$ in place of $\frac{n}{\delta}$ above for ULA), but under an additional smoothness assumption ($f$ has bounded third derivatives) and with higher polynomial dependence on other parameters. Our result also complements the work of Mangoubi and Vishnoi [60] who study the Metropolis-adjusted version of ULA (MALA) for non-logconcave $\nu$ and show a $\log(\frac{1}{\delta})$ iteration complexity from a warm start, under the additional assumption that $f$ has bounded third and fourth derivatives in an appropriate $\infty$-norm.

We note that in general some isoperimetry condition is needed for rapid mixing of Markov chains (such as the Langevin dynamics and ULA), otherwise there are bad regions in the state space from which the chains take arbitrarily long to escape. Smoothness or bounded Hessian is a common assumption that seems to be needed for the analysis of discrete-time algorithms (such as gradient descent or ULA above).

In the second part of this paper, we study the convergence of Rényi divergence of order $q > 1$ along ULA. Rényi divergence is a family of generalizations of KL divergence [67, 70, 12], which becomes stronger as the order $q$ increases. There are physical and operational interpretations of Rényi divergence [39, 3]. Rényi divergence has been useful in many applications, including for the exponential mechanism in differential privacy [31, 1, 13, 63], lattice-based cryptography [4], information-theoretic encryption [44], variational inference [52], machine learning [41, 61], information theory and statistics [24, 64], and black hole physics [27].

Our second main result proves a convergence bound for the Rényi divergence of order $q > 1$. While this is a stronger measure of convergence than KL divergence, the situation here is more complicated. First, we can only hope to converge to the target for finite $q$ for any step-size $\eta$ (as we illustrate with an example). Second, it is unclear how to bound the Rényi divergence between the biased limit $\nu_\eta$ and $\nu$. We first show the convergence of Rényi divergence along Langevin dynamics in continuous time under LSI; see Theorem 2 in Section 4.2. Here $R_{q,\nu}(\rho)$ is the Rényi divergence of order $q$ between $\rho$ and $\nu$.

**Theorem 2.** Suppose $\nu$ satisfies LSI with constant $\alpha > 0$. Let $q \geq 1$. Along the Langevin dynamics,

$$R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha t}{\delta}} R_{q,\nu}(\rho_0).$$
We also have the following convergence of Rényi divergence along Langevin dynamics under Poincaré inequality; see Theorem 3 in Section 6.1.

**Theorem 3.** Suppose \( \nu \) satisfies Poincaré inequality with constant \( \alpha > 0 \). Let \( q \geq 2 \). Along the Langevin dynamics,

\[
R_{q,\nu}(\rho_t) \leq \begin{cases} 
R_{q,\nu}(\rho_0) - \frac{2\alpha t}{q} & \text{if } R_{q,\nu}(\rho_0) \geq 1 \text{ and as long as } R_{q,\nu}(\rho_t) \geq 1, \\
e^{-\frac{2\alpha t}{q}}R_{q,\nu}(\rho_0) & \text{if } R_{q,\nu}(\rho_0) \leq 1.
\end{cases}
\]

The reader will notice that under Poincaré inequality, compared to LSI, the convergence is slower in the beginning before it becomes exponential. For a reasonable starting distribution (such as a Gaussian centered at a stationary point), this leads to an extra factor of \( n \) compared to the convergence under LSI.

We then turn to the discrete-time algorithm and show that ULA converges in Rényi divergence to the biased limit \( \nu_\eta \) under the assumption that \( \nu_\eta \) itself satisfies either LSI or Poincaré inequality. We combine this with a decomposition result on Rényi divergence to derive a convergence guarantee in Rényi divergence to \( \nu \); see Theorem 5 in Section 5.3 and Theorem 6 in Section 6.3.

Finally, we show some properties on the biased limit of ULA. We bound the bias in relative Fisher information assuming third-order smoothness (without isoperimetry); see Theorem 7. We also show the biased limit satisfies LSI if the original target is smooth and strongly log-concave; see Theorem 8.

In what follows, we review KL divergence and its properties along the Langevin dynamics in Section 2, and prove a convergence guarantee for KL divergence along ULA under LSI in Section 3. We provide a review of Rényi divergence and its properties along the Langevin dynamics in Section 4. We then prove the convergence guarantee for Rényi divergence along ULA under LSI in Section 5, and under Poincaré inequality in Section 6. We show properties on the biased limit of ULA in Section 7. We provide all proofs and details in Section 8. We conclude with a discussion in Section 9, including subsequent work that used some of the analysis techniques from this paper.

## 2 Review of KL divergence along Langevin dynamics

In this section we review the definition of Kullback-Leibler (KL) divergence, log-Sobolev inequality, and the convergence of KL divergence along the Langevin dynamics in continuous time under log-Sobolev inequality. See Appendix A.1 for a review on notation.

### 2.1 KL divergence

Let \( \rho, \nu \) be probability distributions on \( \mathbb{R}^n \), represented via their probability density functions with respect to the Lebesgue measure on \( \mathbb{R}^n \). We assume \( \rho, \nu \) have full support and smooth densities.
Recall the **Kullback-Leibler (KL) divergence** of $\rho$ with respect to $\nu$ is

$$H_\nu(\rho) = \int_{\mathbb{R}^n} \rho(x) \log \frac{\rho(x)}{\nu(x)} \, dx.$$

KL divergence is the relative form of Shannon entropy $H(\rho) = -\int_{\mathbb{R}^n} \rho(x) \log \rho(x) \, dx$. Whereas Shannon entropy can be positive or negative, KL divergence is nonnegative and minimized at $\nu$: $H_\nu(\rho) \geq 0$ for all $\rho$, and $H_\nu(\rho) = 0$ if and only if $\rho = \nu$. Therefore, KL divergence serves as a measure of (albeit asymmetric) “distance” of a probability distribution $\rho$ from a base distribution $\nu$. KL divergence is a relatively strong measure of distance; for example, Pinsker’s inequality implies that KL divergence controls total variation distance. Furthermore, under log-Sobolev (or Talagrand) inequality, KL divergence also controls the quadratic Wasserstein $W_2$ distance, as we review below.

We say $\nu = e^{-f}$ is **L-smooth** if $f$ has bounded Hessian: $-LI \preceq \nabla^2 f(x) \preceq LI$ for all $x \in \mathbb{R}^n$.

**Lemma 1.** Suppose $\nu = e^{-f}$ is L-smooth. Let $\rho = \mathcal{N}(x^*, \frac{1}{L} I)$ where $x^*$ is a stationary point of $f$. Then $H_\nu(\rho) \leq f(x^*) + \frac{n}{2} \log \frac{L}{2\pi}$.

We provide the proof of Lemma 1 in Section 8.1.1.

### 2.2 Log-Sobolev inequality

Recall we say $\nu$ satisfies the **log-Sobolev inequality (LSI)** with a constant $\alpha > 0$ if for all smooth function $g : \mathbb{R}^n \to \mathbb{R}$ with $\mathbb{E}_\nu[g^2] < \infty,

$$\mathbb{E}_\nu[g^2 \log g^2] - \mathbb{E}_\nu[g^2] \log \mathbb{E}_\nu[g^2] \leq \frac{2}{\alpha} \mathbb{E}_\nu[\|\nabla g\|^2].$$

(2)

Recall the relative Fisher information of $\rho$ with respect to $\nu$ is

$$J_\nu(\rho) = \int_{\mathbb{R}^n} \rho(x) \left\| \nabla \log \frac{\rho(x)}{\nu(x)} \right\|^2 \, dx.$$

(3)

LSI is equivalent to the following relation between KL divergence and Fisher information for all $\rho$:

$$H_\nu(\rho) \leq \frac{1}{2\alpha} J_\nu(\rho).$$

(4)

Indeed, to obtain (4) we choose $g^2 = \frac{\rho}{\nu}$ in (2); conversely, to obtain (2) we choose $\rho = \frac{g^2 \nu}{\mathbb{E}_\nu[|g|^2]}$ in (4).

LSI is a strong isoperimetry statement and implies, among others, concentration of measure and sub-Gaussian tail property [48]. LSI was first shown by Gross [38] for the case of Gaussian $\nu$. It was extended by Bakry and Émery [6] to strongly log-concave $\nu$; namely, when $f = -\log \nu$ is $\alpha$-strongly convex, then $\nu$ satisfies LSI with constant $\alpha$. However, LSI applies more generally. For example, the classical perturbation result by Holley and Stroock [42] states that LSI is stable under bounded
perturbation. Furthermore, LSI is preserved under a Lipschitz mapping. In one dimension, there is an exact characterization of when a probability distribution on \( \mathbb{R} \) satisfies LSI \[10\]. Moreover, LSI satisfies a tensorization property \[48\]: If \( \nu_1, \nu_2 \) satisfy LSI with constants \( \alpha_1, \alpha_2 > 0 \), respectively, then \( \nu_1 \otimes \nu_2 \) satisfies LSI with constant \( \min\{\alpha_1, \alpha_2\} > 0 \). Thus, there are many examples of non-logconcave distributions \( \nu \) on \( \mathbb{R}^n \) satisfying LSI (with a constant independent of dimension). There are also Lyapunov function criteria and exponential integrability conditions that can be used to verify when a probability distribution satisfies LSI; see for example \[15, 16, 62, 74, 8\].

### 2.2.1 Talagrand inequality

Recall the **Wasserstein distance** between \( \rho \) and \( \nu \) is

\[
W_2(\rho, \nu) = \inf_{\Pi} \mathbb{E}_{\Pi}[\|X - Y\|^2]^{\frac{1}{2}}
\]

where the infimum is over joint distributions \( \Pi \) of \((X, Y)\) with the correct marginals \( X \sim \rho, Y \sim \nu \).

Recall we say \( \nu \) satisfies **Talagrand inequality** with a constant \( \alpha > 0 \) if for all \( \rho \):

\[
\frac{\alpha}{2} W_2(\rho, \nu)^2 \leq H_\nu(\rho).
\]

Talagrand’s inequality implies concentration of measure of Gaussian type. It was first studied by Talagrand \[69\] for Gaussian \( \nu \), and extended by Otto and Villani \[65\] to all \( \nu \) satisfying LSI; namely, if \( \nu \) satisfies LSI with constant \( \alpha > 0 \), then \( \nu \) also satisfies Talagrand’s inequality with the same constant \[65, \text{Theorem 1}\]. Therefore, under LSI, KL divergence controls the Wasserstein distance. Moreover, when \( \nu \) is log-concave, LSI and Talagrand’s inequality are equivalent \[65, \text{Corollary 3.1}\].

We recall the geometric interpretation of LSI and Talagrand’s inequality from \[65\]. In the space of probability distributions with the Riemannian metric defined by the Wasserstein \( W_2 \) distance, the relative Fisher information \(3\) is the squared norm of the gradient of KL divergence \(1\). Therefore, LSI \(4\) is the gradient dominated condition (also known as the Polyak-Lojacewicz (PL) inequality) for KL divergence. On the other hand, Talagrand’s inequality \(6\) is the quadratic growth condition for KL divergence. In general, the gradient dominated condition implies the quadratic growth condition \[65, \text{Proposition 1'}\]; therefore, LSI implies Talagrand’s inequality.

### 2.3 Langevin dynamics

The **Langevin dynamics** for target distribution \( \nu = e^{-f} \) is a continuous-time stochastic process \((X_t)_{t \geq 0}\) in \( \mathbb{R}^n \) that evolves following the stochastic differential equation:

\[
dX_t = -\nabla f(X_t) \, dt + \sqrt{2} \, dW_t
\]

where \((W_t)_{t \geq 0}\) is the standard Brownian motion in \( \mathbb{R}^n \) with \( W_0 = 0 \).
If \((X_t)_{t \geq 0}\) evolves following the Langevin dynamics (7), then their probability density function \((\rho_t)_{t \geq 0}\) evolves following the Fokker-Planck equation:

\[
\frac{\partial \rho_t}{\partial t} = \nabla \cdot (\rho_t \nabla f) + \Delta \rho_t = \nabla \cdot \left( \rho_t \nabla \log \frac{\rho_t}{\nu} \right).
\]

(8)

Here \(\nabla \cdot\) is the divergence and \(\Delta\) is the Laplacian operator. We provide a derivation in Appendix A.2. From (8), if \(\rho_t = \nu\), then \(\frac{\partial \rho_t}{\partial t} = 0\), so \(\nu\) is the stationary distribution for the Langevin dynamics (7). Moreover, the Langevin dynamics brings any distribution \(X_t \sim \rho_t\) closer to the target distribution \(\nu\), as the following lemma shows.

**Lemma 2.** Along the Langevin dynamics (7) (or equivalently, the Fokker-Planck equation (8)),

\[
\frac{d}{dt} H_\nu(\rho_t) = -J_\nu(\rho_t).
\]

(9)

We provide the proof of Lemma 2 in Section 8.1.2. Since \(J_\nu(\rho) \geq 0\), the identity (9) shows that KL divergence with respect to \(\nu\) is decreasing along the Langevin dynamics, so indeed the distribution \(\rho_t\) converges to \(\nu\).

### 2.3.1 Exponential convergence of KL divergence along Langevin dynamics under LSI

When \(\nu\) satisfies LSI, KL divergence converges exponentially fast along the Langevin dynamics.

**Theorem 4.** Suppose \(\nu\) satisfies LSI with constant \(\alpha > 0\). Along the Langevin dynamics (7),

\[
H_\nu(\rho_t) \leq e^{-2\alpha t} H_\nu(\rho_0).
\]

(10)

Furthermore, \(W_2(\rho_t, \nu) \leq \sqrt{\frac{2}{\alpha} H_\nu(\rho_0)} e^{-\alpha t}\).

We provide the proof of Theorem 4 in Section 8.1.3. We also recall the optimization interpretation of Langevin dynamics as the gradient flow of KL divergence in the space of distributions with the Wasserstein metric [46, 73, 65]. Then the exponential convergence rate in Theorem 4 is a manifestation of the general fact that gradient flow converges exponentially fast under gradient domination condition. This provides a justification for using the Langevin dynamics for sampling from \(\nu\), as a natural steepest descent flow that minimizes the KL divergence \(H_\nu\).

### 3 Unadjusted Langevin Algorithm

In this section we study the behavior of KL divergence along the Unadjusted Langevin Algorithm (ULA) in discrete time under log-Sobolev inequality assumption.

Suppose we wish to sample from a smooth target probability distribution \(\nu = e^{-f}\) in \(\mathbb{R}^n\). The Unadjusted Langevin Algorithm (ULA) with step size \(\eta > 0\) is the discrete-time algorithm

\[
x_{k+1} = x_k - \eta \nabla f(x_k) + \sqrt{2\eta} z_k
\]

(11)
where \( z_k \sim \mathcal{N}(0, I) \) is an independent standard Gaussian random variable in \( \mathbb{R}^n \). Let \( \rho_k \) denote the probability distribution of \( x_k \) that evolves following ULA.

As \( \eta \to 0 \), ULA recovers the Langevin dynamics (7) in continuous-time. However, for fixed \( \eta > 0 \), ULA converges to a biased limiting distribution \( \nu_\eta \neq \nu \). Therefore, KL divergence \( H_\nu(\rho_k) \) does not tend to 0 along ULA, as it has an asymptotic bias \( H_\nu(\nu_\eta) > 0 \).

**Example 1.** Let \( \nu = \mathcal{N}(0, \frac{1}{\alpha} I) \). The ULA iteration is \( x_{k+1} = (1 - \eta \alpha) x_k + \sqrt{2\eta} z_k \), \( z_k \sim \mathcal{N}(0, I) \). For \( 0 < \eta < \frac{2}{\alpha} \), the limit is \( \nu_\eta = \mathcal{N} \left( 0, \frac{1}{\alpha(1 - \frac{\alpha \eta}{2})} \right) \), and the bias is \( H_\nu(\nu_\eta) = \frac{n}{2} \left( \frac{\alpha}{2(1 - \frac{\alpha \eta}{2})} + \log \left( 1 - \frac{\alpha \eta}{2} \right) \right) \).

In particular, \( H_\nu(\nu_\eta) \leq \frac{\eta \alpha^2 n^2}{16(1 - \frac{\alpha \eta}{2})} = O(\eta^2) \).

### 3.1 Convergence of KL divergence along ULA under LSI

When the true target distribution \( \nu \) satisfies LSI and a smoothness condition, we can prove a convergence guarantee in KL divergence along ULA. Recall we say \( \nu = e^{-f} \) is \( L \)-smooth, \( 0 < L < \infty \), if \( -LI \preceq \nabla^2 f(x) \preceq LI \) for all \( x \in \mathbb{R}^n \).

A key part in our analysis is the following lemma which bounds the decrease in KL divergence along one iteration of ULA. Here \( x_{k+1} \sim \rho_{k+1} \) is the output of one step of ULA (11) from \( x_k \sim \rho_k \).

**Lemma 3.** Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \) and is \( L \)-smooth. If \( 0 < \eta \leq \frac{\alpha}{4L^2} \), then along each step of ULA (11),

\[
H_\nu(\rho_{k+1}) \leq e^{-\alpha \eta} H_\nu(\rho_k) + 6\eta^2 nL^2.
\]

(12)

We provide the proof of Lemma 3 in Section 8.2.1. The proof of Lemma 3 compares the evolution of KL divergence along one step of ULA with the evolution along the Langevin dynamics in continuous time (which converges exponentially fast under LSI), and bounds the discretization error; see Figure 2 for an illustration. This high-level comparison technique has been used in many papers. Our proof structure is similar to that of Cheng and Bartlett [19], whose analysis needs \( \nu \) to be strongly log-concave.

With Lemma 3, we can prove our main result on the convergence rate of ULA under LSI.

**Theorem 1.** Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \) and is \( L \)-smooth. For any \( x_0 \sim \rho_0 \) with \( H_\nu(\rho_0) < \infty \), the iterates \( x_k \sim \rho_k \) of ULA (11) with step size \( 0 < \eta \leq \frac{\alpha}{4L^2} \) satisfy

\[
H_\nu(\rho_k) \leq e^{-\alpha \eta k} H_\nu(\rho_0) + \frac{8\eta nL^2}{\alpha}.
\]

(13)

Thus, for any \( \delta > 0 \), to achieve \( H_\nu(\rho_k) < \delta \), it suffices to run ULA with step size \( \eta \leq \frac{\alpha}{4L^2} \min\{1, \frac{\delta}{4n}\} \) for \( k \geq \frac{1}{\alpha \eta} \log \frac{2H_\nu(\rho_0)}{\delta} \) iterations.
We provide the proof of Theorem 1 in Section 8.2.2.

In particular, suppose \( \delta < 4n \) and we choose the largest permissible step size \( \eta = \Theta \left( \frac{\alpha \delta}{L^2 n} \right) \). Suppose we start with a Gaussian \( \rho_0 = \mathcal{N}(x^*, \frac{1}{L} I) \), where \( x^* \) is a stationary point of \( f \) (which we can find, e.g., via gradient descent), so \( H_\nu(\rho_0) \leq f(x^*) + \frac{n}{2} \log \frac{L}{2\pi} = \tilde{O}(n) \) by Lemma 1. Therefore, Theorem 1 states that to achieve \( H_\nu(\rho_k) \leq \delta \), ULA has iteration complexity \( k = \tilde{\Theta} \left( \frac{L^2 n}{\alpha \delta} \right) \). Since LSI implies Talagrand’s inequality, Theorem 1 also yields a convergence guarantee in Wasserstein distance.

As \( k \to \infty \), Theorem 1 implies the following bound on the bias between \( \nu_\eta \) and \( \nu \) under LSI. However, note that the bound in Corollary 1 is \( H_\nu(\nu_\eta) = O(\eta) \), while from Example 1 we see that \( H_\nu(\nu_\eta) = O(\eta^2) \) in the Gaussian case.

**Corollary 1.** Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \) and is \( L \)-smooth. For \( 0 < \eta \leq \frac{\alpha}{4L} \), the biased limit \( \nu_\eta \) of ULA with step size \( \eta \) satisfies \( H_\nu(\nu_\eta) \leq \frac{8nL^2 \eta}{\alpha} \) and \( W_2(\nu, \nu_\eta)^2 \leq \frac{16nL^2 \eta}{\alpha^2} \).

**Remark 1.** If \( f \) satisfies a third-order smoothness condition (without isoperimetry), then we can show a bound on the bias in relative Fisher information; see Section 7.1.

### 4 Review of Rényi divergence along Langevin dynamics

In this section we review the definition of Rényi divergence and the exponential convergence of Rényi divergence along the Langevin dynamics under LSI.
4.1 Rényi divergence

Rényi divergence [67] is a family of generalizations of KL divergence. We refer to [70, 12] for basic properties of Rényi divergence.

For $q > 0$, $q \neq 1$, the **Rényi divergence** of order $q$ of a probability distribution $\rho$ with respect to $\nu$ is

$$ R_{q,\nu}(\rho) = \frac{1}{q - 1} \log F_{q,\nu}(\rho) $$

where

$$ F_{q,\nu}(\rho) = \mathbb{E}_\nu \left[ \left( \frac{\rho}{\nu} \right)^q \right] = \int_{\mathbb{R}^n} \nu(x) \frac{\rho(x)^q}{\nu(x)^q} \, dx = \int_{\mathbb{R}^n} \frac{\rho(x)^q}{\nu(x)^{q-1}} \, dx. $$

Rényi divergence is the relative form of Rényi entropy [67]: $H_q(\rho) = \frac{1}{q - 1} \log \int \rho(x)^q \, dx$. The case $q = 1$ is defined via limit, and recovers the KL divergence (1):

$$ R_{1,\nu}(\rho) = \lim_{q \to 1} R_{q,\nu}(\rho) = \mathbb{E}_\nu \left[ \frac{\rho}{\nu} \log \frac{\rho}{\nu} \right] = \mathbb{E}_\rho \left[ \log \frac{\rho}{\nu} \right] = H(\nu). $$

Rényi divergence has the property that $R_{q,\nu}(\rho) \geq 0$ for all $\rho$, and $R_{q,\nu}(\rho) = 0$ if and only if $\rho = \nu$. Furthermore, the map $q \mapsto R_{q,\nu}(\rho)$ is increasing (see Section 8.3.1). Therefore, Rényi divergence provides an alternative measure of “distance” of $\rho$ from $\nu$, which becomes stronger as $q$ increases. In particular, $R_{\infty,\nu}(\rho) = \log \left\| \frac{\rho}{\nu} \right\|_\infty = \log \sup_x \frac{\rho(x)}{\nu(x)}$ is finite if and only if $\rho$ is warm relative to $\nu$. It is possible that $R_{q,\nu}(\rho) = \infty$ for large enough $q$, as the following example shows.

**Example 2.** Let $\rho = \mathcal{N}(0, \sigma^2 I)$ and $\nu = \mathcal{N}(0, \lambda^2 I)$. If $\sigma^2 > \lambda^2$ and $q \geq \frac{\sigma^2}{\sigma^2 - \lambda^2}$, then $R_{q,\nu}(\rho) = \infty$. Otherwise, $R_{q,\nu}(\rho) = \frac{n}{2} \log \frac{\lambda^2}{\sigma^2} - \frac{n}{2(q-1)} \log \left( q - (q-1) \frac{\sigma^2}{\lambda^2} \right)$.

Analogous to Lemma 1, we have the following estimate of the Rényi divergence of a Gaussian.

**Lemma 4.** Suppose $\nu = e^{-f}$ is $L$-smooth. Let $\rho = \mathcal{N}(x^*, \frac{1}{L} I)$ where $x^*$ is a stationary point of $f$. Then for all $q \geq 1$, $R_{q,\nu}(\rho) \leq f(x^*) + \frac{n}{2} \log \frac{L}{2\pi}.$

We provide the proof of Lemma 4 in Section 8.3.2.

4.1.1 Log-Sobolev inequality

For $q > 0$, we define the **Rényi information** of order $q$ of $\rho$ with respect to $\nu$ as

$$ G_{q,\nu}(\rho) = \mathbb{E}_\nu \left[ \left( \frac{\rho}{\nu} \right)^q \left\| \nabla \log \frac{\rho}{\nu} \right\|^2 \right] = \mathbb{E}_\nu \left[ \left( \frac{\rho}{\nu} \right)^{q-2} \left\| \nabla \frac{\rho}{\nu} \right\|^2 \right] = \frac{4}{q^2} \mathbb{E}_\nu \left[ \left\| \nabla \left( \frac{\rho}{\nu} \right)^{\frac{2}{q}} \right\|^2 \right]. $$

The case $q = 1$ recovers relative Fisher information (3): $G_{1,\nu}(\rho) = \mathbb{E}_\nu \left[ \frac{\rho}{\nu} \left\| \nabla \log \frac{\rho}{\nu} \right\|^2 \right] = J(\nu).$ We have the following relation under log-Sobolev inequality. Note that the case $q = 1$ recovers LSI in the form (4) involving KL divergence and relative Fisher information.
Lemma 5. Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \). Let \( q \geq 1 \). For all \( \rho \),

\[
\frac{G_{q,\nu}(\rho)}{F_{q,\nu}(\rho)} \geq \frac{2\alpha}{q^2} R_{q,\nu}(\rho).
\]

(18)

We provide the proof of Lemma 5 in Section 8.3.3.

4.2 Langevin dynamics

Along the Langevin dynamics (7) for \( \nu \), we can compute the rate of change of the Rényi divergence.

Lemma 6. For all \( q > 0 \), along the Langevin dynamics (7),

\[
\frac{d}{dt} R_{q,\nu}(\rho_t) = -q \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)}.
\]

(19)

We provide the proof of Lemma 6 in Section 8.3.4. In particular, \( \frac{d}{dt} R_{q,\nu}(\rho_t) \leq 0 \), so Rényi divergence is always decreasing along the Langevin dynamics. Furthermore, analogous to how the Langevin dynamics is the gradient flow of KL divergence under the Wasserstein metric, one can also show that the Langevin dynamics is the the gradient flow of Rényi divergence with respect to a suitably defined metric (which depends on the target distribution \( \nu \)) on the space of distributions; see [14].

4.2.1 Convergence of Rényi divergence along Langevin dynamics under LSI

When \( \nu \) satisfies LSI, Rényi divergence converges exponentially fast along the Langevin dynamics. Note the case \( q = 1 \) recovers the exponential convergence rate of KL divergence from Theorem 4.

Theorem 2. Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \). Let \( q \geq 1 \). Along the Langevin dynamics (7),

\[
R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha t}{q^2}} R_{q,\nu}(\rho_0).
\]

(20)

We provide the proof of Theorem 2 in Section 8.3.5. Theorem 2 shows that if the initial Rényi divergence is finite, then it converges exponentially fast. However, even if initially the Rényi divergence of some order is infinite, it will be eventually finite along the Langevin dynamics, after which time Theorem 2 applies. This is because when \( \nu \) satisfies LSI, the Langevin dynamics satisfies a hypercontractivity property [38, 11, 73]; see Section 8.3.6. Furthermore, as shown in [14], we can combine the exponential convergence rate above with the hypercontractivity property to improve the exponential rate to be \( 2\alpha \), independent of \( q \), at the cost of some initial waiting time; here we leave the rate as above for simplicity.

Remark 2. When \( \nu \) satisfies Poincaré inequality, we can still prove the convergence of Rényi divergence along the Langevin dynamics. However, in this case, Rényi divergence initially decreases linearly, then exponentially once it is less than 1. See Section 6.1.
5 Rényi divergence along ULA

In this section we prove a convergence guarantee for Rényi divergence along ULA under the assumption that the biased limit satisfies LSI.

As before, let $\nu = e^{-f}$, and let $\nu_\eta$ denote the biased limit of ULA (11) with step size $\eta > 0$. We first note that the asymptotic bias $R_{q,\nu}(\nu_\eta)$ may be infinite for large enough $q$.

**Example 3.** As in Examples 1 and 2, let $\nu = N(0, \frac{1}{\alpha} I)$, so $\nu_\eta = N\left(0, \frac{1}{\alpha(1 - \frac{\eta\alpha}{2})} I\right)$. The bias is

$$R_{q,\nu}(\nu_\eta) = \begin{cases} \frac{n}{2(q-1)} \left(q \log\left(1 - \frac{\eta\alpha}{2}\right) - \log\left(1 - \frac{q\eta\alpha}{2}\right)\right) & \text{if } 1 < q < \frac{2}{\eta\alpha}, \\ \infty & \text{if } q \geq \frac{2}{\eta\alpha}. \end{cases}$$

For $1 < q < \frac{2}{\eta\alpha}$, we can bound $R_{q,\nu}(\nu_\eta) \leq \frac{n\alpha^2\eta^2\eta^2}{8(q-1)(1 - \frac{\eta\alpha}{2})}$.

Thus, for each fixed $q > 1$, there is an asymptotic bias $R_{q,\nu}(\nu_\eta)$ which is finite for small $\eta > 0$. In Example 3, we have $R_{q,\nu}(\nu_\eta) = O(\eta^2)$.

5.1 Decomposition of Rényi divergence

For order $q > 1$, we have the following decomposition of Rényi divergence.

**Lemma 7.** Let $q > 1$. For all probability distribution $\rho$,

$$R_{q,\nu}(\rho) \leq \left(\frac{q - \frac{1}{2}}{q - 1}\right) R_{2q,\nu_\eta}(\rho) + R_{2q-1,\nu}(\nu_\eta). \quad (21)$$

We provide the proof of Lemma 7 in Section 8.4.1. The first term in the bound above is the Rényi divergence with respect to the biased limit, which converges exponentially fast under LSI assumption (see Lemma 8). The second term in (21) is the asymptotic bias in Rényi divergence.

5.2 Rapid convergence of Rényi divergence to biased limit under LSI

We show that Rényi divergence with respect to the biased limit $\nu_\eta$ converges exponentially fast along ULA, assuming $\nu_\eta$ itself satisfies LSI.

**Assumption 1.** The probability distribution $\nu_\eta$ satisfies LSI with a constant $\beta \equiv \beta_\eta > 0$.

We can verify Assumption 1 in the Gaussian case. We can also verify Assumption 1 when $\nu$ is smooth and strongly log-concave; see Section 7.2. However, it is unclear how to verify Assumption 1 in general. One might hope to prove that if $\nu$ satisfies LSI, then Assumption 1 holds.

**Example 4.** Let $\nu = N(0, \frac{1}{\alpha} I)$, so $\nu_\eta = N\left(0, \frac{1}{\alpha(1 - \frac{\eta\alpha}{2})} I\right)$, which is strongly log-concave (and hence satisfies LSI) with parameter $\beta = \alpha \left(1 - \frac{\eta\alpha}{2}\right)$. In particular, $\beta \geq \frac{\alpha}{2}$ for $\eta \leq \frac{1}{\alpha}$.
Under Assumption 1, we can prove an exponential convergence rate to the biased limit $\nu_\eta$.

**Lemma 8.** Assume Assumption 1. Suppose $\nu = e^{-f}$ is $L$-smooth, and let $0 < \eta \leq \min \left\{ \frac{1}{3L}, \frac{1}{9\beta} \right\}$. For $q \geq 1$, along ULA (11),

$$R_{q,\nu_\eta}(\rho_k) \leq e^{-\frac{3qk}{\eta}} R_{q,\nu_\eta}(\rho_0). \quad (22)$$

We provide the proof of Lemma 8 in Section 8.4.2. In the proof of Lemma 8, we decompose each step of ULA as a sequence of two operations; see Figure 3 for an illustration. In the first part, we take a gradient step; this is a deterministic bijective map, so it preserves Rényi divergence. In the second part, we add an independent Gaussian; this is the result of evolution along the heat flow, and we can derive a formula on the decrease in Rényi divergence (which is similar to the formula (19) along the Langevin dynamics; see Section 8.4.2 for detail).

![Figure 3: An illustration for the proof of Lemma 8. We decompose each step of ULA into two operations: (a) a deterministic gradient step, and (b) an evolution along the heat flow. If the current Rényi divergence is $R \equiv R_{q,\nu_\eta}(\rho_k)$, then the gradient step (a) does not change the Rényi divergence: $R_{q,\nu_\eta}(\tilde{\rho}_k) = R$, while the heat flow (b) decreases the Rényi divergence: $R_{q,\nu_\eta}(\rho_{k+1}) \leq e^{-\alpha\eta} R$.](attachment:image.png)

5.3 Convergence of Rényi divergence along ULA under LSI

We combine Lemma 7 and Lemma 8 to obtain the following characterization of the convergence of Rényi divergence along ULA under LSI.

**Theorem 5.** Assume Assumption 1. Suppose $\nu = e^{-f}$ is $L$-smooth, and let $0 < \eta \leq \min \left\{ \frac{1}{3L}, \frac{1}{9\beta} \right\}$. Let $q > 1$, and suppose $R_{2q,\nu_\eta}(\rho_0) < \infty$. Then along ULA (11),

$$R_{q,\nu}(\rho_k) \leq \left( \frac{q - \frac{1}{2}}{q - 1} \right) R_{2q,\nu_\eta}(\rho_0) e^{-\frac{qk}{2\eta}} + R_{2q-1,\nu}(\nu_\eta). \quad (23)$$

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We provide the proof of Theorem 5 in Section 8.4.3. For $\delta > 0$, let $\gamma_q(\delta) = \sup \{\eta > 0 : R_{q,\nu}(\rho_\eta) \leq \delta\}$. Theorem 5 states that to achieve $R_{q,\nu}(\rho_k) \leq \delta$, it suffices to run ULA with step size $\eta = \Theta\left(\frac{1}{\beta \gamma_q(\delta)}\right)$ for $k = \Theta\left(\frac{1}{\beta \gamma_q(\delta)}\right)$ iterations. Suppose $\delta$ is small enough that $\gamma_q(\delta) < \frac{1}{L}$. Note that $\nu_\eta$ is $\frac{1}{2\eta}$-smooth, so by choosing $\rho_0$ to be a Gaussian with covariance $2\eta I$, we have $R_{2q,\nu_\eta}(\rho_0) = \tilde{O}(n)$ by Lemma 4. Therefore, Theorem 5 yields an iteration complexity of $k = \tilde{O}\left(\frac{1}{\beta \gamma_q(\delta)}\right)$.

For example, if $R_{q,\nu}(\nu_\eta) = O(\eta)$, then $\gamma_q(\delta) = \Omega(\delta)$, so the iteration complexity is $k = \tilde{O}\left(\frac{1}{\delta^2}\right)$ with step size $\eta = \Theta(\delta)$. On the other hand, if $R_{q,\nu}(\eta) = O(\eta^2)$, as in Example 3, then $\gamma_q(\delta) = \Omega(\sqrt{\delta})$, so the iteration complexity is $k = \tilde{O}\left(\frac{1}{\beta \sqrt{\delta}}\right)$ with step size $\eta = \Theta(\sqrt{\delta})$.

**Remark 3.** Our result for Rényi divergence above involves the asymptotic bias, which we do not bound. Another approach to analyze ULA in Rényi divergence was proposed in [35] (and improved in [34]), albeit with a bound that does not provide an estimate of the Rényi bias. The work of [21] extended our one-step interpolation technique to show the convergence of ULA in Rényi divergence under LSI and smoothness, and provides an estimate on the Rényi bias.

### 6 Poincaré inequality

In this section we review the definition of Poincaré inequality and prove convergence guarantees for the Rényi divergence along the Langevin dynamics and ULA. As before, let $\rho, \nu$ be smooth probability distributions on $\mathbb{R}^n$.

Recall we say $\nu$ satisfies **Poincaré inequality (PI)** with a constant $\alpha > 0$ if for all smooth function $g : \mathbb{R}^n \to \mathbb{R}$,

$$\text{Var}_\nu(g) \leq \frac{1}{\alpha} \mathbb{E}_\nu[\|\nabla g\|^2]$$

(24)

where $\text{Var}_\nu(g) = \mathbb{E}_\nu[g^2] - \mathbb{E}_\nu[g]^2$ is the variance of $g$ under $\nu$. Poincaré inequality is an isoperimetric-type statement, but it is weaker than LSI. It is known that LSI implies PI with the same constant; in fact, PI is a linearization of LSI (4), i.e., when $\rho = (1 + \eta g)\nu$ as $\eta \to 0$ [68, 73]. Furthermore, it is also known that Talagrand’s inequality implies PI with the same constant, and in fact PI is also a linearization of Talagrand’s inequality [65]. Poincaré inequality is better behaved than LSI [16], and there are various Lyapunov function criteria and integrability conditions that can be used to verify when a probability distribution satisfies Poincaré inequality; see for example [5, 62, 23].

Under Poincaré inequality, we can prove the following bound on Rényi divergence, which is analogous to Lemma 5 under LSI. When $R_{q,\nu}(\rho)$ is small, the two bounds are approximately equivalent.
Lemma 9. Suppose $\nu$ satisfies Poincaré inequality with constant $\alpha > 0$. Let $q \geq 2$. For all $\rho$,

$$\frac{G_{q,\nu}(\rho)}{F_{q,\nu}(\rho)} \geq \frac{4\alpha}{q^2} \left(1 - e^{-R_{q,\nu}(\rho)}\right).$$

We provide the proof of Lemma 9 in Section 8.5.1.

6.1 Convergence of Rényi divergence along Langevin dynamics under Poincaré

When $\nu$ satisfies Poincaré inequality, Rényi divergence converges along the Langevin dynamics. The convergence is initially linear, then becomes exponential once the Rényi divergence falls below a constant.

Theorem 3. Suppose $\nu$ satisfies Poincaré inequality with constant $\alpha > 0$. Let $q \geq 2$. Along the Langevin dynamics (7),

$$R_{q,\nu}(\rho_t) \leq \begin{cases} R_{q,\nu}(\rho_0) - \frac{2\alpha t}{q} & \text{if } R_{q,\nu}(\rho_0) \geq 1 \text{ and as long as } R_{q,\nu}(\rho_t) \geq 1, \\ e^{-\frac{2\alpha t}{q} R_{q,\nu}(\rho_0)} & \text{if } R_{q,\nu}(\rho_0) \leq 1. \end{cases}$$

We provide the proof of Theorem 3 in Section 8.5.2. Theorem 3 states that starting from $R_{q,\nu}(\rho_0) \geq 1$, the Langevin dynamics reaches $R_{q,\nu}(\rho_t) \leq \delta$ in $t \leq O\left(\frac{q}{\alpha} \left(R_{q,\nu}(\rho_0) + \log \frac{1}{\delta}\right)\right)$ time.

6.2 Convergence of Rényi divergence to biased limit under Poincaré

We show that Rényi divergence with respect to the biased limit $\nu_\eta$ converges exponentially fast along ULA, assuming $\nu_\eta$ satisfies Poincaré inequality.

Assumption 2. The distribution $\nu_\eta$ satisfies Poincaré inequality with a constant $\beta \equiv \beta_\eta > 0$.

We can verify Assumption 2 in the Gaussian case, and when $\nu$ is smooth and strongly log-concave; see Section 7.2. However, it is unclear how to verify Assumption 2 in general. One might hope to prove that if $\nu$ satisfies Poincaré, then Assumption 2 holds.

Analogous to Lemma 8, we have the following convergence to the biased limit in discrete time, at a rate which matches the continuous-time convergence in Theorem 6.

Lemma 10. Assume Assumption 2. Suppose $\nu = e^{-f}$ is $L$-smooth, and let $0 < \eta \leq \min\left\{\frac{1}{3L}, \frac{1}{9L}\right\}$. For $q \geq 2$, along ULA (11),

$$R_{q,\nu_\eta}(\rho_k) \leq \begin{cases} R_{q,\nu_\eta}(\rho_0) - \frac{\eta k}{q} & \text{if } R_{q,\nu_\eta}(\rho_0) \geq 1 \text{ and as long as } R_{q,\nu_\eta}(\rho_k) \geq 1, \\ e^{-\frac{\eta k}{q} R_{q,\nu_\eta}(\rho_0)} & \text{if } R_{q,\nu_\eta}(\rho_0) \leq 1. \end{cases}$$

(25)

We provide the proof of Lemma 10 in Section 8.5.3. Lemma 10 states that starting from $R_{q,\nu_\eta}(\rho_0) \geq 1$, ULA reaches $R_{q,\nu_\eta}(\rho_k) \leq \delta$ in $k \leq O\left(\frac{q}{\eta \beta} \left(R_{q,\nu_\eta}(\rho_0) + \log \frac{1}{\delta}\right)\right)$ iterations.

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6.3 Convergence of Rényi divergence along ULA under Poincaré

We combine Lemma 7 and Lemma 10 to obtain the following characterization of the convergence of Rényi divergence along ULA to the true target distribution under Poincaré inequality.

**Theorem 6.** Assume Assumption 2. Suppose $\nu = e^{-f}$ is $L$-smooth, and let $0 < \eta \leq \min \left\{ \frac{1}{3L}, \frac{1}{3\beta} \right\}$. Let $q > 1$, and suppose $1 \leq R_{2q,\nu}(\rho) < \infty$. Then along ULA (11), for $k \geq k_0 := \frac{2q}{\beta\eta}(R_{2q,\nu}(\rho) - 1)$,

$$R_{q,\nu}(\rho_k) \leq \left( \frac{q - 2}{q - 1} \right) e^{-\frac{\beta q (k - k_0)}{2q}} + R_{2q,\nu}(\nu). \quad (26)$$

We provide the proof of Theorem 6 in Section 8.5.4.

For $\delta > 0$, recall $\gamma_q(\delta) = \sup \{ \eta > 0 : R_{q,\nu}(\nu) \leq \delta \}$. Theorem 6 states that to achieve $R_{q,\nu}(\rho_k) \leq \delta$, it suffices to run ULA with step size $\eta = \Theta \left( \min \left\{ \frac{1}{L}, \gamma_{2q-1} \left( \frac{3}{2} \right) \right\} \right)$ for $k = \Theta \left( \frac{1}{\beta\eta} \right) (R_{2q,\nu}(\rho) + \log \frac{1}{\delta})$ iterations. Suppose $\delta$ is small enough that $\gamma_{2q-1} \left( \frac{3}{2} \right) < \frac{1}{2}$. Note that $\nu_q$ is $\frac{1}{2\eta}$-smooth, so by choosing $\rho_0$ to be a Gaussian with covariance $2\eta I$, we have $R_{2q,\nu}(\rho_0) = O(n)$ by Lemma 4. Therefore, Theorem 6 yields an iteration complexity of $k = \tilde{O} \left( \frac{n}{\beta\gamma_{2q-1} \left( \frac{3}{2} \right)} \right)$. Note the additional dependence on dimension, compared to the LSI case in Section 5.3.

For example, if $R_{q,\nu}(\nu_q) = O(n)$, then $\gamma_{q}(\delta) = \Omega(\delta)$, so the iteration complexity is $k = \tilde{O} \left( \frac{n}{\beta} \right)$ with step size $\eta = \Theta(\delta)$. On the other hand, if $R_{q,\nu}(\nu_q) = O(\eta^2)$, as in Example 3, then $\gamma_{q}(\delta) = \Omega(\sqrt{\delta})$, so the iteration complexity is $k = \tilde{O} \left( \frac{n}{\beta\sqrt{\delta}} \right)$ with step size $\eta = \Theta(\sqrt{\delta})$.

7 Properties of Biased Limit

7.1 Bound on bias under third-order smoothness

Let $\nu_\eta$ be the biased limit of ULA with step size $\eta > 0$. Let $\mu_\eta = (I - \eta \nabla f) \# \nu_\eta$, so $\nu_\eta$ satisfies

$$\nu_\eta = \mu_\eta \ast \mathcal{N}(0, 2\eta I).$$

We will bound bound the relative Fisher information $J_\nu(\nu_\eta)$ under third-order smoothness. We say $f$ is $(L, M)$-smooth if $f$ is $L$-smooth ($\nabla f$ is $L$-Lipschitz), and $\nabla^2 f$ is $M$-Lipschitz, or $\|\nabla^3 f\|_{op} \leq M$. We provide the proof of Theorem 7 in Sections 8.6.4 and 8.6.5.

**Theorem 7.** 1. If $f$ is $(L, M)$-smooth and $\eta \leq \frac{1}{2L}$, then:

$$J_\nu(\nu_\eta) \leq 2\eta n \left( L^2 + 2\sqrt{nLM} + 3nM^2 \right).$$

2. For any $f$ and $\eta > 0$ (such that $\nu_\eta$ exists and the quantities below are defined):

$$J_\nu(\nu_\eta) \geq \frac{\eta^2 \left( \mathbf{E}_{\nu_\eta} \|\nabla f\|^2 \right)^2}{4 \mathbf{Var}_{\nu_\eta}(X)}.$$
Note the dependence on $\eta$ in the upper bound above is $O(\eta^2)$, while the lower bound is $\Omega(\eta^2)$.

**Example 5.** Recall that if $\nu = \mathcal{N}(0, \frac{1}{\alpha} I)$, then $\nu_\eta = \mathcal{N}(0, \frac{1}{\alpha(1 - \eta^2)} I)$ for $\eta < \frac{2}{\alpha}$. Then\footnote{Recall for $\nu = \mathcal{N}(0, \frac{1}{\alpha} I)$ and $\rho = \mathcal{N}(0, \frac{1}{\beta} I)$, the relative Fisher information is $J_\nu(\rho) = \frac{\alpha}{\beta} (\beta - \alpha)^2$.}

$$J_\nu(\nu_\eta) = \frac{\eta^2}{4} \frac{n_\alpha^2}{(1 - \eta^2)^2} = \Theta(\eta^2 n_\alpha^2).$$  

(27)

So the lower bound in Theorem 7 has the right order of $\eta$, but not the upper bound.

**Remark 4.** Recall from Theorem 1 that under LSI and L-smoothness we have $H_\nu(\nu_\eta) \leq O(\eta n L^2)$. Under LSI, the upper bound in Theorem 7 implies $H_\nu(\nu_\eta) \leq O(\eta n (L^2 + \sqrt{nLM} + nM^2))$, which has an additional dependence on third-order smoothness, but without requiring isoperimetry.

However, we also note that in general, convergence in relative Fisher information does not necessarily imply convergence of the underlying distributions; see for example [7].

**Remark 5.** By examining the proof of the upper bound in Section 8.6.4, we can also conclude that $J_\nu(\nu_\eta) \leq \eta n L^2$ assuming $f$ is L-smooth and $\Delta \Delta f \geq 0$.

### 7.2 Isoperimetry of biased limit under strong log-concavity and smoothness

If $\nu$ is smooth and strongly log-concave, then the biased limit $\nu_\eta$ satisfies LSI (hence also Poincaré), so Assumptions 1 and 2 are satisfied. The authors thank Sinho Chewi for communicating the following result to us. We provide the proof of Theorem 8 in Section 8.6.6.

**Theorem 8.** If $\nu$ is $\alpha$-strongly log-concave and L-smooth, and $\eta \leq \frac{1}{L}$, then $\nu_\eta$ is $\beta$-LSI with $\beta \geq \frac{\alpha^2}{2}$.

With Theorem 8, we know that for target distributions which are smooth and strongly log-concave, we have convergence of ULA in Rényi divergence to the biased limit, as in Theorem 5. However, the final bound is in terms of the bias in Rényi divergence, which we do not bound. (Under third-order smoothness, we can bound it in relative Fisher information as in Theorem 7, but it does not bound the Rényi divergence.) The work of [7] extends our interpolation technique to show the convergence in Rényi divergence under LSI as well as a general family of isoperimetric inequalities, and proves a bound on the Rényi bias under LSI and smoothness.

### 8 Proofs and details

#### 8.1 Proofs for §2: KL divergence along Langevin dynamics

**8.1.1 Proof of Lemma 1**

**Proof of Lemma 1.** Since $f$ is L-smooth and $\nabla f(x^*) = 0$, we have the bound

$$f(x) \leq f(x^*) + \langle \nabla f(x^*), x - x^* \rangle + \frac{L}{2} \|x - x^*\|^2 = f(x^*) + \frac{L}{2} \|x - x^*\|^2.$$
Let $X \sim \mathcal{N}(x^*, \frac{1}{L} I)$. Then

$$\mathbb{E}_\rho[f(X)] \leq f(x^*) + \frac{L}{2} \text{Var}_\rho(X) = f(x^*) + \frac{n}{2}. $$

Recall the entropy of $\rho$ is $H(\rho) = -\mathbb{E}_\rho[\log \rho(X)] = \frac{n}{2} \log \frac{2\pi e}{L}$. Therefore, the KL divergence is

$$H_\nu(\rho) = \mathbb{E}_\rho \left[ \log \rho + f \right] dx = -H(\rho) + \mathbb{E}_\rho[f] \leq f(x^*) + \frac{n}{2} \log \frac{L}{4\pi e}. $$

8.1.2 Proof of Lemma 2

Proof of Lemma 2. Recall the time derivative of KL divergence along any flow is given by

$$\frac{d}{dt} H_\nu(\rho_t) = \frac{d}{dt} \int_{\mathbb{R}^n} \rho_t \log \frac{\rho_t}{\nu} \, dx = \int_{\mathbb{R}^n} \frac{\partial \rho_t}{\partial t} \log \frac{\rho_t}{\nu} \, dx$$

since the second part of the chain rule is zero: $\int \rho_t \frac{\partial}{\partial t} \log \frac{\rho_t}{\nu} \, dx = \int \frac{\partial \rho_t}{\partial t} \, dx = \frac{d}{dt} \int \rho_t \, dx = 0$. Therefore, along the Fokker-Planck equation (8) for the Langevin dynamics (7),

$$\frac{d}{dt} H_\nu(\rho_t) = \int \nabla \cdot \left( \rho_t \nabla \log \frac{\rho_t}{\nu} \right) \log \frac{\rho_t}{\nu} \, dx$$

$$= -\int \rho_t \left\| \nabla \log \frac{\rho_t}{\nu} \right\|^2 \, dx$$

$$= -J_\nu(\rho_t)$$

where in the second equality we have applied integration by parts.

8.1.3 Proof of Theorem 4

Proof of Theorem 4. From Lemma 2 and the LSI assumption (4),

$$\frac{d}{dt} H_\nu(\rho_t) = -J_\nu(\rho_t) \leq -2\alpha H_\nu(\rho_t).$$

Integrating implies the desired bound $H_\nu(\rho_t) \leq e^{-2\alpha t} H_\nu(\rho_0)$.

Furthermore, since $\nu$ satisfies LSI with constant $\alpha$, it also satisfies Talagrand’s inequality (6) with constant $\alpha$ [65, Theorem 1]. Therefore, $W_2(\rho_t, \nu)^2 \leq \frac{2}{\alpha} H_\nu(\rho_t) \leq \frac{2}{\alpha} e^{-2\alpha t} H_\nu(\rho_0)$, as desired.

8.2 Proofs for §3: Unadjusted Langevin Algorithm

8.2.1 Proof of Lemma 3

We will use the following auxiliary results.
Lemma 11. Assume \( \nu = e^{-f} \) is \( L \)-smooth. Then
\[
\mathbb{E}_\nu[\|\nabla f\|^2] \leq nL.
\]

Proof. Since \( \nu = e^{-f} \), by integration by parts we can write
\[
\mathbb{E}_\nu[\|\nabla f\|^2] = \mathbb{E}_\nu[\Delta f].
\]

Since \( \nu \) is \( L \)-smooth, \( \nabla^2 f(x) \preceq LI \), so \( \Delta f(x) \leq nL \) for all \( x \in \mathbb{R}^n \). Therefore, \( \mathbb{E}_\nu[\|\nabla f\|^2] = \mathbb{E}_\nu[\Delta f] \leq nL \), as desired. \( \square \)

Lemma 12. Suppose \( \nu \) satisfies Talagrand’s inequality with constant \( \alpha > 0 \) and is \( L \)-smooth. For any \( \rho \),
\[
\mathbb{E}_\rho[\|\nabla f\|^2] \leq \frac{4L^2}{\alpha} H_\nu(\rho) + 2nL.
\]

Proof. Let \( x \sim \rho \) and \( x^* \sim \nu \) with an optimal coupling \((x, x^*)\) so that \( \mathbb{E}[\|x - x^*\|^2] = W_2(\rho, \nu)^2 \). Since \( \nu = e^{-f} \) is \( L \)-smooth, \( \nabla f \) is \( L \)-Lipschitz. By triangle inequality,
\[
\|\nabla f(x)\| \leq \|\nabla f(x) - \nabla f(x^*)\| + \|\nabla f(x^*)\| \\
\leq L\|x - x^*\| + \|\nabla f(x^*)\|.
\]

Squaring, using \((a + b)^2 \leq 2a^2 + 2b^2\), and taking expectation, we get
\[
\mathbb{E}_\rho[\|\nabla f(x)\|^2] \leq 2L^2 \mathbb{E}[\|x - x^*\|^2] + 2\mathbb{E}_\nu[\|\nabla f(x^*)\|^2] \\
= 2L^2 W_2(\rho, \nu)^2 + 2\mathbb{E}_\nu[\|\nabla f(x^*)\|^2].
\]

By Talagrand’s inequality (6), \( W_2(\rho, \nu)^2 \leq \frac{2}{\alpha} H_\nu(\rho) \). By Lemma 11 we have \( \mathbb{E}_\nu[\|\nabla f(x^*)\|^2] \leq nL \). Plugging these to the bound above gives the desired result. \( \square \)

We are now ready to prove Lemma 3.

Proof of Lemma 3. For simplicity suppose \( k = 0 \), so we start at \( x_0 \sim \rho_0 \). We write one step of ULA
\[
x_0 \mapsto x_0 - \eta \nabla f(x_0) + \sqrt{2\eta} z_0
\]
as the output at time \( \eta \) of the stochastic differential equation
\[
dx_t = -\nabla f(x_t) \, dt + \sqrt{2} \, dW_t
\]
\[
(28)
\]
where $W_t$ is the standard Brownian motion in $\mathbb{R}^n$ starting at $W_0 = 0$. Indeed, the solution to (28) at time $t = \eta$ is

$$x_\eta = x_0 - \eta \nabla f(x_0) + \sqrt{2}W_\eta$$

$$= x_0 - \eta \nabla f(x_0) + \sqrt{2\eta}z_0.$$  \hspace{1cm} (29)

where $z_0 \sim \mathcal{N}(0, I)$, which is identical to the ULA update.

We derive the continuity equation corresponding to (28) as follows. For each $t > 0$, let $\rho_{0t}(x_0, x_t)$ denote the joint distribution of $(x_0, x_t)$, which we write in terms of the conditionals and marginals as

$$\rho_{0t}(x_0, x_t) = \rho_0(x_0)\rho_{t|0}(x_t | x_0) = \rho_t(x_t)\rho_{0|t}(x_0 | x_t).$$

Conditioning on $x_0$, the drift vector field $-\nabla f(x_0)$ is a constant, so the Fokker-Planck formula for the conditional density $\rho_{t|0}(x_t | x_0)$ is

$$\frac{\partial \rho_{t|0}(x_t | x_0)}{\partial t} = \nabla \cdot (\rho_{t|0}(x_t | x_0)\nabla f(x_0)) + \Delta \rho_{t|0}(x_t | x_0).$$  \hspace{1cm} (30)

To derive the evolution of $\rho_t$, we take expectation over $x_0 \sim \rho_0$. Multiplying both sides of (30) by $\rho_0(x_0)$ and integrating over $x_0$, we obtain

$$\frac{\partial \rho_t(x)}{\partial t} = \int_{\mathbb{R}^n} \frac{\partial \rho_{t|0}(x | x_0)}{\partial t} \rho_0(x_0) \, dx_0$$

$$= \int_{\mathbb{R}^n} (\nabla \cdot (\rho_{t|0}(x | x_0)\nabla f(x_0)) + \Delta \rho_{t|0}(x | x_0)) \rho_0(x_0) \, dx_0$$

$$= \int_{\mathbb{R}^n} (\nabla \cdot (\rho_{t,0}(x, x_0)\nabla f(x_0)) + \Delta \rho_{t,0}(x, x_0)) \, dx_0$$

$$= \nabla \cdot (\rho_t(x) \int_{\mathbb{R}^n} \rho_{0|t}(x_0 | x)\nabla f(x_0) \, dx_0) + \Delta \rho_t(x)$$

$$= \nabla \cdot (\rho_t(x)\mathbb{E}_{\rho_{0|t}}[\nabla f(x_0) | x_t = x]) + \Delta \rho_t(x).$$  \hspace{1cm} (31)

Observe that the difference between the Fokker-Planck equations (31) for ULA and (8) for Langevin dynamics is in the first term, that the drift is now the conditional expectation $\mathbb{E}_{\rho_{0|t}}[\nabla f(x_0) | x_t = x]$, rather than the true gradient $\nabla f(x)$.

Recall the time derivative of relative entropy along any flow is given by

$$\frac{d}{dt} H_\nu(\rho_t) = \frac{d}{dt} \int_{\mathbb{R}^n} \rho_t \log \frac{\rho_t}{\nu} \, dx = \int_{\mathbb{R}^n} \frac{\partial \rho_t}{\partial t} \log \frac{\rho_t}{\nu} \, dx$$

since the second part of the chain rule is zero: $\int \rho_t \frac{\partial}{\partial t} \log \frac{\rho_t}{\nu} \, dx = \int \frac{\partial \rho_t}{\partial t} \, dx = \frac{d}{dt} \int \rho_t \, dx = 0.$
Therefore, the time derivative of relative entropy for ULA, using the Fokker-Planck equation (31) and integrating by parts, is given by:

\[
\frac{d}{dt} H_\nu(\rho_t) = \int_{\mathbb{R}^n} \left( \nabla \cdot \left( \rho_t(x) \mathbb{E}_{\rho_{0t}}[\nabla f(x_0) \mid x_t = x] \right) + \Delta \rho_t(x) \right) \log \frac{\rho_t(x)}{\nu(x)} \, dx
\]

\[
= \int_{\mathbb{R}^n} \left( \nabla \cdot \left( \rho_t(x) \left( \nabla \log \frac{\rho_t(x)}{\nu(x)} + \mathbb{E}_{\rho_{0t}}[\nabla f(x_0) \mid x_t = x] - \nabla f(x) \right) \right) \right) \log \frac{\rho_t(x)}{\nu(x)} \, dx
\]

\[
= - \int_{\mathbb{R}^n} \rho_t(x) \left\| \nabla \log \frac{\rho_t(x)}{\nu(x)} \right\|^2 \, dx + \int_{\mathbb{R}^n} \rho_t(x) \left( \nabla f(x) - \mathbb{E}_{\rho_{0t}}[\nabla f(x_0) \mid x_t = x], \nabla \log \frac{\rho_t(x)}{\nu(x)} \right) \, dx
\]

\[
= - J_\nu(\rho_t) + \int_{\mathbb{R}^n \times \mathbb{R}^n} \rho_{0t}(x, x_t) \left( \nabla f(x_t) - \nabla f(x_0), \nabla \log \frac{\rho_t(x_t)}{\nu(x_t)} \right) \, dx_0 \, dx
\]

\[
= - J_\nu(\rho_t) + \mathbb{E}_{\rho_{0t}} \left[ \left\langle \nabla f(x_t) - \nabla f(x_0), \nabla \log \frac{\rho_t(x_t)}{\nu(x_t)} \right\rangle \right] \tag{32}
\]

where in the last step we have renamed \( x \) as \( x_t \). The first term in (32) is the same as in the Langevin dynamics. The second term in (32) is the discretization error, which we can bound as follows. Using \( \langle a, b \rangle \leq \|a\|^2 + \frac{1}{4}\|b\|^2 \) and since \( \nabla f \) is \( L \)-Lipschitz,

\[
\mathbb{E}_{\rho_{0t}} \left[ \left\langle \nabla f(x_t) - \nabla f(x_0), \nabla \log \frac{\rho_t(x_t)}{\nu(x_t)} \right\rangle \right] \leq \mathbb{E}_{\rho_{0t}} \left[ \|\nabla f(x_t) - \nabla f(x_0)\|^2 \right] + \frac{1}{4} \mathbb{E}_{\rho_{0t}} \left[ \left\| \nabla \log \frac{\rho_t(x_t)}{\nu(x_t)} \right\|^2 \right]
\]

\[
= \mathbb{E}_{\rho_{0t}} \left[ \|\nabla f(x_t) - \nabla f(x_0)\|^2 \right] + \frac{1}{4} J_\nu(\rho_t)
\]

\[
\leq L^2 \mathbb{E}_{\rho_{0t}} \left[ \|x_t - x_0\|^2 \right] + \frac{1}{4} J_\nu(\rho_t) \tag{33}
\]

Recall from (29) the solution of ULA is \( x_t \overset{d}{=} x_0 - t\nabla f(x_0) + \sqrt{2t} z_0 \), where \( z_0 \sim \mathcal{N}(0, I) \) is independent of \( x_0 \). Then

\[
\mathbb{E}_{\rho_{0t}} \left[ \|x_t - x_0\|^2 \right] = \mathbb{E}_{\rho_{0t}} \left[ \| - t\nabla f(x_0) + \sqrt{2t} z_0 \|^2 \right]
\]

\[
= t^2 \mathbb{E}_{\rho_{0t}} \left[ \|\nabla f(x_0)\|^2 \right] + 2tn
\]

\[
\leq \frac{4t^2L^2}{\alpha} H_\nu(\rho_0) + 2t^2nL + 2tn
\]

where in the last inequality we have used Lemma 12. This bounds the discretization error by

\[
\mathbb{E}_{\rho_{0t}} \left[ \left\langle \nabla f(x_t) - \nabla f(x_0), \nabla \log \frac{\rho_t(x_t)}{\nu(x_t)} \right\rangle \right] \leq \frac{4t^2L^4}{\alpha} H_\nu(\rho_0) + 2t^2nL^3 + 2tnL^2 + \frac{1}{4} J_\nu(\rho_t).
\]

Therefore, from (32), the time derivative of KL divergence along ULA is bounded by

\[
\frac{d}{dt} H_\nu(\rho_t) \leq -\frac{3}{4} J_\nu(\rho_t) + \frac{4t^2L^4}{\alpha} H_\nu(\rho_0) + 2t^2nL^3 + 2tnL^2.
\]
Then by the LSI (4) assumption,
\[
\frac{d}{dt} H_\nu(\rho_t) \leq -\frac{3\alpha}{2} H_\nu(\rho_t) + \frac{4\ell^2 L^4}{\alpha} H_\nu(\rho_0) + 2t^2 n L^3 + 2tn L^2.
\]
We wish to integrate the inequality above for \(0 \leq t \leq \eta\). Using \(t \leq \eta\) and since \(\eta \leq \frac{1}{2\ell}\), we simplify the above to
\[
\frac{d}{dt} H_\nu(\rho_t) \leq -\frac{3\alpha}{2} H_\nu(\rho_t) + \frac{4\eta^2 L^4}{\alpha} H_\nu(\rho_0) + 2\eta^2 n L^3 + 2\eta n L^2
\]
\[
\leq -\frac{3\alpha}{2} H_\nu(\rho_t) + \frac{4\eta^2 L^4}{\alpha} H_\nu(\rho_0) + 3\eta n L^2.
\]
Multiplying both sides by \(e^{\frac{3\alpha}{2}t}\), we can write the above as
\[
\frac{d}{dt} \left( e^{\frac{3\alpha}{2}t} H_\nu(\rho_t) \right) \leq e^{\frac{3\alpha}{2}t} \left( \frac{4\eta^2 L^4}{\alpha} H_\nu(\rho_0) + 3\eta n L^2 \right).
\]
Integrating from \(t = 0\) to \(t = \eta\) gives
\[
e^{\frac{3\alpha}{2}\eta} H_\nu(\rho_\eta) - H_\nu(\rho_0) \leq \frac{2(e^{\frac{3\alpha}{2}\eta} - 1)}{3\alpha} \left( \frac{4\eta^2 L^4}{\alpha} H_\nu(\rho_0) + 3\eta n L^2 \right)
\]
\[
\leq 2\eta \left( \frac{4\eta^2 L^4}{\alpha} H_\nu(\rho_0) + 3\eta n L^2 \right)
\]
where in the last step we have used the inequality \(e^c \leq 1 + 2c\) for \(0 < c = \frac{3}{2}\alpha\eta \leq 1\), which holds because \(0 < \eta \leq \frac{1}{2\ell}\). Rearranging, the inequality above gives
\[
H_\nu(\rho_\eta) \leq e^{-\frac{3\alpha}{2}\eta} \left( 1 + \frac{8\eta^3 L^4}{\alpha} \right) H_\nu(\rho_0) + e^{-\frac{3\alpha}{2}\eta} 6\eta^2 n L^2.
\]
Since \(1 + \frac{8\eta^3 L^4}{\alpha} \leq 1 + \frac{\alpha\eta}{2} \leq e^{\frac{1}{2}\alpha\eta}\) for \(\eta \leq \frac{\alpha}{4\ell^2}\), and using \(e^{-\frac{3\alpha}{2}\eta} \leq 1\), we conclude that
\[
H_\nu(\rho_\eta) \leq e^{-\alpha\eta} H_\nu(\rho_0) + 6\eta^2 n L^2.
\]
This is the desired inequality, after renaming \(\rho_0 \equiv \rho_k\) and \(\rho_\eta \equiv \rho_{k+1}\). Note that the conditions \(\eta \leq \frac{1}{2\ell}\) and \(\eta \leq \frac{1}{3\alpha}\) above are also implied by the assumption \(\eta \leq \frac{\alpha}{4\ell^2}\) since \(\alpha \leq L\).

\[\ Boxed\]

### 8.2.2 Proof of Theorem 1

**Proof of Theorem 1.** Applying the recursion (12) from Lemma 3, we obtain
\[
H_\nu(\rho_k) \leq e^{-\alpha\eta k} H_\nu(\rho_0) + \frac{6\eta^2 n L^2}{1 - e^{-\alpha\eta}} \leq e^{-\alpha\eta k} H_\nu(\rho_0) + \frac{8\eta n L^2}{\alpha}
\]
where in the last step we have used the inequality \(1 - e^{-c} \geq \frac{3}{4} c\) for \(0 < c = \alpha\eta \leq \frac{1}{4}\), which holds since \(\eta \leq \frac{\alpha}{4\ell^2} \leq \frac{1}{4\ell}\).

Given \(\delta > 0\), if we further assume \(\eta \leq \frac{\delta\alpha}{60\ell^2}\), then the above implies \(H_\nu(\rho_k) \leq e^{-\alpha\eta k} H_\nu(\rho_0) + \frac{\delta}{2}\).

This means for \(k \geq \frac{1}{\alpha\eta} \log \frac{2H_\nu(\rho_0)}{\delta}\), we have \(H_\nu(\rho_k) \leq \frac{\delta}{2} + \frac{\delta}{2} = \delta\), as desired. \(\ Boxed\)
8.3 Details for §4: Rényi divergence along Langevin dynamics

8.3.1 Properties of Rényi divergence

We recall that Rényi divergence is increasing in the order.

**Lemma 13.** For any probability distributions $\rho, \nu$, the map $q \mapsto R_{q,\nu}(\rho)$ is increasing for $q > 0$.

**Proof.** Let $0 < q \leq r$. We will show that $R_{q,\nu}(\rho) \leq R_{r,\nu}(\rho)$.

First suppose $q > 1$. We write $F_{q,\nu}(\rho)$ as an expectation over $\rho$ and use power mean inequality:

$$F_{q,\nu}(\rho) = \mathbb{E}_\nu \left[ \left( \frac{\nu}{\rho} \right)^q \right] = \mathbb{E}_\rho \left[ \left( \frac{\nu}{\rho} \right)^{q-1} \right] \leq \mathbb{E}_\rho \left[ \left( \frac{\nu}{\rho} \right)^{r-1} \right]^{\frac{q-1}{r-1}} = \mathbb{E}_\nu \left[ \left( \frac{\nu}{\rho} \right)^r \right]^{\frac{q-1}{r-1}} = F_{r,\nu}(\rho)^{\frac{q-1}{r-1}}.$$

Taking logarithm and dividing by $q - 1 > 0$ gives

$$R_{q,\nu}(\rho) = \frac{1}{q-1} \log F_{q,\nu}(\rho) \leq \frac{1}{r-1} \log F_{r,\nu}(\rho) = R_{r,\nu}(\rho).$$

The case $q = 1$ follows by taking limit $q \to 1$.

Now suppose $q \leq r < 1$, so $1 - q \geq 1 - r > 0$. We again write $F_{q,\nu}(\rho)$ as an expectation over $\rho$ and use power mean inequality:

$$F_{q,\nu}(\rho) = \mathbb{E}_\nu \left[ \left( \frac{\nu}{\rho} \right)^q \right] = \mathbb{E}_\rho \left[ \left( \frac{\nu}{\rho} \right)^{1-q} \right] \geq \mathbb{E}_\rho \left[ \left( \frac{\nu}{\rho} \right)^{1-r} \right]^{\frac{1-q}{1-r}} = \mathbb{E}_\nu \left[ \left( \frac{\nu}{\rho} \right)^r \right]^{\frac{1-q}{1-r}} = F_{r,\nu}(\rho)^{\frac{1-q}{1-r}}.$$

Taking logarithm and dividing by $q - 1 < 0$ (which flips the inequality) gives

$$R_{q,\nu}(\rho) = \frac{1}{q-1} \log F_{q,\nu}(\rho) \leq \frac{1}{r-1} \log F_{r,\nu}(\rho) = R_{r,\nu}(\rho).$$

The case $q < 1 \leq r$ follows since $R_{q,\nu}(\rho) \leq R_{1,\nu}(\rho) \leq R_{r,\nu}(\rho)$. \hfill \square

8.3.2 Proof of Lemma 4

**Proof of Lemma 4.** Since $f$ is $L$-smooth and $x^*$ is a stationary point of $f$, for all $x \in \mathbb{R}^n$ we have

$$f(x) \leq f(x^*) + \langle \nabla f(x^*), x - x^* \rangle + \frac{L}{2} \| x - x^* \|^2 = f(x^*) + \frac{L}{2} \| x - x^* \|^2.$$
Let $q > 1$. Then for $\rho = \mathcal{N}(x^*, \sigma^2 I)$ with $\frac{q \sigma^2}{2} > (q-1)L$,

$$F_{q,\nu}(\rho) = \int_{\mathbb{R}^n} \frac{\rho(x)^q}{\nu(x)^{q-1}} dx$$

$$= \frac{1}{(2\pi\sigma^2)^{\frac{na}{2}}} \int_{\mathbb{R}^n} e^{-\frac{q}{2\sigma^2} \|x-x^*\|^2 + (q-1)f(x)} dx$$

$$\leq \frac{1}{(2\pi\sigma^2)^{\frac{na}{2}}} \int_{\mathbb{R}^n} e^{-\frac{q}{2\sigma^2} \|x-x^*\|^2 + (q-1)f(x^*) + \frac{(q-1)L}{2} \|x-x^*\|^2} dx$$

$$= e^{(q-1)f(x^*)} \left(\frac{2\pi}{\sigma^2} - (q-1)L \right)^{\frac{q}{2}}$$

$$= e^{(q-1)f(x^*)} \left(\frac{2\pi}{\sigma^2} - (q-1)L \right) \frac{1}{(2\pi)^{\frac{na}{2}} \left(\frac{q \sigma^2}{2} - (q-1)L \right)^{\frac{n}{2}}}.$$ 

Therefore,

$$R_{q,\nu}(\rho) = \frac{1}{q-1} \log F_{q,\nu}(\rho) \leq f(x^*) - \frac{n}{2} \log 2\pi - \frac{n}{2(q-1)} \log \sigma^2 \left(\frac{q \sigma^2}{2} - (q-1)L \right).$$

In particular, if $\sigma^2 = \frac{1}{L}$, then $\frac{q \sigma^2}{2} - (q-1)L = L > 0$, and the bound above becomes

$$R_{q,\nu}(\rho) \leq f(x^*) + \frac{n}{2} \log \frac{L}{2\pi}.$$ 

The case $q = 1$ follows from Lemma 1, since $\frac{1}{4\pi e} < \frac{1}{2\pi}$.

**8.3.3 Proof of Lemma 5**

**Proof of Lemma 5.** We plug in $h^2 = \left(\frac{\rho}{\nu}\right)^q$ to the LSI definition (2) to obtain

$$\frac{q^2}{2\alpha} G_{q,\nu}(\rho) \geq qE_\nu \left[ \left(\frac{\rho}{\nu}\right)^q \log \frac{\rho}{\nu} \right] - F_{q,\nu}(\rho) \log F_{q,\nu}(\rho)$$

$$= \frac{q \partial}{\partial q} F_{q,\nu}(\rho) - F_{q,\nu}(\rho) \log F_{q,\nu}(\rho).$$
Therefore,
\[
\frac{q^2 G_{q,\nu}(\rho)}{2\alpha F_{q,\nu}(\rho)} \geq q \frac{\partial}{\partial q} \log F_{q,\nu}(\rho) - \log F_{q,\nu}(\rho)
\]
\[
= q \frac{\partial}{\partial q} \left( ((q - 1)R_{q,\nu}(\rho)) - (q - 1)R_{q,\nu}(\rho) \right)
\]
\[
= qR_{q,\nu}(\rho) + q(q - 1) \frac{\partial}{\partial q} R_{q,\nu}(\rho) - (q - 1)R_{q,\nu}(\rho)
\]
\[
= R_{q,\nu}(\rho) + q(q - 1) \frac{\partial}{\partial q} R_{q,\nu}(\rho)
\]
\[
\geq R_{q,\nu}(\rho)
\]
where in the last inequality we have used \( q \geq 1 \) and \( \frac{\partial}{\partial q} R_{q,\nu}(\rho) \geq 0 \) since \( q \mapsto R_{q,\nu}(\rho) \) is increasing by Lemma 13.

8.3.4 Proof of Lemma 6

**Proof of Lemma 6.** Let \( q > 0, q \neq 1 \). By the Fokker-Planck formula (8) and integration by parts,
\[
\frac{d}{dt} F_{q,\nu}(\rho_t) = \int_{\mathbb{R}^n} \frac{\rho_t}{\nu} \frac{\partial}{\partial t} \frac{\rho_t}{\nu} \log \frac{\rho_t}{\nu} \, dx
\]
\[
= q \int_{\mathbb{R}^n} \rho_t^{q-1} \frac{\partial}{\partial t} \rho_t \, dx
\]
\[
= q \int_{\mathbb{R}^n} \left( \frac{\rho_t}{\nu} \right)^{q-1} \nabla \cdot \left( \rho_t \nabla \log \frac{\rho_t}{\nu} \right) \, dx
\]
\[
= -q \int_{\mathbb{R}^n} \rho_t \left\langle \nabla \left( \frac{\rho_t}{\nu} \right)^{q-1}, \nabla \log \frac{\rho_t}{\nu} \right\rangle \, dx
\]
\[
= -q(q - 1) \int_{\mathbb{R}^n} \rho_t \left\langle \left( \frac{\rho_t}{\nu} \right)^{q-2} \nabla \frac{\rho_t}{\nu}, \left( \frac{\rho_t}{\nu} \right)^{-1} \nabla \frac{\rho_t}{\nu} \right\rangle \, dx
\]
\[
= -q(q - 1) E_{\nu} \left[ \left( \frac{\rho_t}{\nu} \right)^{q-2} \left\| \nabla \frac{\rho_t}{\nu} \right\|^2 \right]
\]
\[
= -q(q - 1) G_{q,\nu}(\rho_t).
\]
Therefore,
\[
\frac{d}{dt} R_{q,\nu}(\rho_t) = \frac{1}{q - 1} \frac{d}{dt} F_{q,\nu}(\rho_t) = -q \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)}.
\]
For \( q = 1 \), we have \( R_{1,\nu}(\rho_t) = H_{\nu}(\rho_t), G_{1,\nu}(\rho_t) = J_{\nu}(\rho_t), \) and \( F_{1,\nu}(\rho_t) = 1 \), and the claim (19) follows from Lemma 2.

\[27\]
8.3.5 Proof of Theorem 2

Proof of Theorem 2. By Lemma 5 and Lemma 6,

\[
\frac{d}{dt}R_{q,\nu}(\rho_t) = -q \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)} \leq -\frac{2\alpha}{q} R_{q,\nu}(\rho_t).
\]

Integrating gives

\[
R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha t}{q}} R_{q,\nu}(\rho_0)
\]
as desired. \hfill \Box

8.3.6 Hypercontractivity

Lemma 14. Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \). Let \( q_0 > 1 \), and suppose \( R_{q_0,\nu}(\rho_0) < \infty \). Define \( q_t = 1 + e^{2\alpha t}(q_0 - 1) \). Along the Langevin dynamics (7), for all \( t \geq 0 \),

\[
\left(1 - \frac{1}{q_t}\right) R_{q,\nu}(\rho_t) \leq \left(1 - \frac{1}{q_0}\right) R_{q_0,\nu}(\rho_0).
\]

(36)

In particular, for any \( q \geq q_0 \), we have \( R_{q,\nu}(\rho_t) \leq R_{q_0,\nu}(\rho_0) < \infty \) for all \( t \geq \frac{1}{2\alpha} \log \frac{q-1}{q_0-1} \).

Proof. We will show \( \frac{d}{dt} \left\{ \left(1 - \frac{1}{q_t}\right) R_{q,\nu}(\rho_t) \right\} \leq 0 \), which implies the desired relation (36). Since \( q_t = 1 + e^{2\alpha t}(q_0 - 1) \), we have \( \dot{q}_t = \frac{d}{dt} q_t = 2\alpha(q_t - 1) \). Note that

\[
\frac{d}{dt} R_{q,\nu}(\rho_t) = \frac{d}{dt} \left( \frac{\log F_{q,\nu}(\rho_t)}{q_t - 1} \right)
\]

\[= \frac{\dot{q}_t \log F_{q,\nu}(\rho_t)}{(q_t - 1)^2} + \dot{q}_t \mathbb{E}_\nu \left[ \left( \frac{\rho_t}{\nu} \right)^q \log \frac{\rho_t}{\nu} \right] - q_t(q_t - 1) G_{q,\nu}(\rho_t)
\]

\[= -2\alpha R_{q,\nu}(\rho_t) + 2\alpha \mathbb{E}_\nu \left[ \left( \frac{\rho_t}{\nu} \right)^q \log \frac{\rho_t}{\nu} \right] F_{q,\nu}(\rho_t) - q_t \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)}.
\]

In the second equality above we have used our earlier calculation (35) which holds for fixed \( q \). Then by LSI in the form (34), we have

\[
\frac{d}{dt} R_{q,\nu}(\rho_t) \leq -2\alpha R_{q,\nu}(\rho_t) + 2\alpha \left(\frac{q_t}{2\alpha} \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)} + \frac{1}{q_t} \log F_{q,\nu}(\rho_t) \right) - q_t \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)}
\]

\[= -2\alpha R_{q,\nu}(\rho_t) + 2\alpha \left(1 - \frac{1}{q_t}\right) R_{q,\nu}(\rho_t)
\]

\[= -\frac{2\alpha}{q_t} R_{q,\nu}(\rho_t).
\]
Therefore,
\[
\frac{d}{dt} \left\{ \left(1 - \frac{1}{q_t}\right) R_{q_t,\nu}(\rho_t) \right\} = \frac{q_t}{q_t^2} R_{q_t,\nu}(\rho_t) + \left(1 - \frac{1}{q_t}\right) \frac{d}{dt} R_{q_t,\nu}(\rho_t) \\
\leq \frac{2\alpha(q_t - 1)}{q_t^2} R_{q_t,\nu}(\rho_t) - \left(1 - \frac{1}{q_t}\right) \frac{2\alpha}{q_t} R_{q_t,\nu}(\rho_t) \\
= 0,
\]
as desired.

Now given \( q \geq q_0 \), let \( t_0 = \frac{1}{2\alpha} \log \frac{q-1}{q_0-1} \) so \( q_t = q \). Then \( R_{q,\nu}(\rho_{t_0}) \leq \frac{q}{(q-1)\rho_0} R_{q_0,\nu}(\rho_0) \leq R_{q_0,\nu}(\rho_0) < \infty \). For \( t > t_0 \), by applying Theorem 2 starting from \( \rho_{t_0} \), we obtain \( R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha}{q}(t-t_0)} R_{q_0,\nu}(\rho_{t_0}) \leq R_{q,\nu}(\rho_{t_0}) \leq R_{q_0,\nu}(\rho_0) < \infty \).

By combining Theorem 2 and Lemma 14, we obtain the following characterization of the behavior of Renyi divergence along the Langevin dynamics under LSI.

**Corollary 2.** Suppose \( \nu \) satisfies LSI with constant \( \alpha > 0 \). Suppose \( \rho_0 \) satisfies \( R_{q_0,\nu}(\rho_0) < \infty \) for some \( q_0 > 1 \). Along the Langevin dynamics (7), for all \( q \geq q_0 \) and \( t \geq t_0 := \frac{1}{2\alpha} \log \frac{q-1}{q_0-1} \),
\[
R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha}{q}(t-t_0)} R_{q_0,\nu}(\rho_0).
\]

**Proof.** By Lemma 14, at \( t = t_0 \) we have \( R_{q,\nu}(\rho_{t_0}) \leq R_{q_0,\nu}(\rho_0) \). For \( t > t_0 \), by applying Theorem 2 starting from \( \rho_{t_0} \), we have \( R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha}{q}(t-t_0)} R_{q,\nu}(\rho_{t_0}) \leq e^{-\frac{2\alpha}{q}(t-t_0)} R_{q_0,\nu}(\rho_0) \).

### 8.4 Proofs for §5: Rényi divergence along ULA

#### 8.4.1 Proof of Lemma 7

**Proof of Lemma 7.** By Cauchy-Schwarz inequality,
\[
F_{q,\nu}(\rho) = \int \frac{\rho^q}{\nu^q} \, dx \\
= \int \nu \left( \frac{\rho}{\nu} \right)^q \left( \frac{\nu}{\nu} \right)^{q-1} \, dx \\
\leq \left( \int \nu \left( \frac{\rho}{\nu} \right)^{2q} \, dx \right)^{\frac{1}{2}} \left( \int \nu \left( \frac{\nu}{\nu} \right)^{2(q-1)} \, dx \right)^{\frac{1}{2}} \\
= F_{2q,\nu}(\rho)^{\frac{1}{2}} F_{2q-1,\nu}(\nu)^{\frac{1}{2}}.
\]
Taking logarithm gives
\[
(q - 1)R_{q,\nu}(\rho) \leq \frac{(2q - 1)}{2} R_{2q,\nu}(\rho) + \frac{(2q - 2)}{2} R_{2q-1,\nu}(\nu).
\]
Dividing both sides by \( q - 1 > 0 \) gives the desired inequality (21).
8.4.2 Proof of Lemma 8

We will use the following auxiliary results. Recall that given a map $T : \mathbb{R}^n \to \mathbb{R}^n$ and a probability distribution $\rho$, the pushforward $T_\# \rho$ is the distribution of $T(x)$ when $x \sim \rho$.

**Lemma 15.** Let $T : \mathbb{R}^n \to \mathbb{R}^n$ be a differentiable bijective map. For any probability distributions $\rho, \nu$, and for all $q > 0$,

$$R_{q,T_\# \nu}(T_\# \rho) = R_{q,\nu}(\rho).$$

**Proof.** Let $\tilde{\rho} = T_\# \rho$ and $\tilde{\nu} = T_\# \nu$. By the change of variable formula,

$$\rho(x) = \det(\nabla T(x)) \tilde{\rho}(T(x)),
\nu(x) = \det(\nabla T(x)) \tilde{\nu}(T(x)).$$

Since $T$ is differentiable and bijective, $\det(\nabla T(x)) \neq 0$. Therefore,

$$\frac{\tilde{\rho}(T(x))}{\tilde{\nu}(T(x))} = \frac{\rho(x)}{\nu(x)}.$$

Now let $X \sim \nu$, so $T(X) \sim \tilde{\nu}$. Then for all $q > 0$.

$$F_{q,\tilde{\nu}}(\tilde{\rho}) = \mathbb{E}_{\tilde{\nu}} \left[ \left( \frac{\tilde{\rho}}{\tilde{\nu}} \right)^q \right] = \mathbb{E}_{X \sim \nu} \left[ \left( \frac{\tilde{\rho}(T(X))}{\tilde{\nu}(T(X))} \right)^q \right] = \mathbb{E}_{X \sim \nu} \left[ \left( \frac{\rho(X)}{\nu(X)} \right)^q \right] = F_{q,\nu}(\rho).$$

Suppose $q \neq 1$. Taking logarithm on both sides and dividing by $q-1 \neq 0$ yields $R_{q,\tilde{\nu}}(\tilde{\rho}) = R_{q,\nu}(\rho)$, as desired. The case $q = 1$ follows from taking limit $q \to 1$, or by an analogous direct argument:

$$H_{\tilde{\nu}}(\tilde{\rho}) = \mathbb{E}_{\tilde{\nu}} \left[ \frac{\tilde{\rho}}{\tilde{\nu}} \log \frac{\tilde{\rho}}{\tilde{\nu}} \right] = \mathbb{E}_{X \sim \nu} \left[ \frac{\tilde{\rho}(T(X))}{\tilde{\nu}(T(X))} \log \frac{\tilde{\rho}(T(X))}{\tilde{\nu}(T(X))} \right] = \mathbb{E}_{X \sim \nu} \left[ \frac{\rho(X)}{\nu(X)} \log \frac{\rho(X)}{\nu(X)} \right] = H_{\nu}(\rho).$$

We have the following standard result on how the LSI constant changes under a Lipschitz mapping. We recall that $T : \mathbb{R}^n \to \mathbb{R}^n$ is $L$-Lipschitz if $\|T(x) - T(y)\| \leq L\|x - y\|$ for all $x, y \in \mathbb{R}^n$. For completeness, we provide the proof of Lemma 16 in Appendix A.3.1.

**Lemma 16.** Suppose a probability distribution $\nu$ satisfies LSI with constant $\alpha > 0$. Let $T : \mathbb{R}^n \to \mathbb{R}^n$ be a differentiable $L$-Lipschitz map. Then $\tilde{\nu} = T_\# \nu$ satisfies LSI with constant $\alpha/L^2$.

We also recall the following result on how the LSI constant changes along Gaussian convolution. We provide the proof of Lemma 17 in Appendix A.3.2.

**Lemma 17.** Suppose a probability distribution $\nu$ satisfies LSI with constant $\alpha > 0$. For $t > 0$, the probability distribution $\tilde{\nu}_t = \nu * \mathcal{N}(0, 2tI)$ satisfies LSI with constant $(\frac{1}{\alpha} + 2t)^{-1}$.  

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We now derive a formula for the decrease of Rényi divergence along simultaneous heat flow. We note the resulting formula (38) is similar to the formula (19) for the decrease of Rényi divergence along the Langevin dynamics. A generalization of the following formula is also useful for analyzing a proximal sampling algorithm under isoperimetry [17].

**Lemma 18.** For any probability distributions \( \rho_0, \nu_0 \), and for any \( t \geq 0 \), let \( \rho_t = \rho_0 * N(0, 2tI) \) and \( \nu_t = \nu_0 * N(0, 2tI) \). Then for all \( q > 0 \),

\[
\frac{d}{dt} R_{q,\nu_t}(\rho_t) = -q \frac{G_{q,\nu_t}(\rho_t)}{F_{q,\nu_t}(\rho_t)}.
\]  

(38)

**Proof.** By definition, \( \rho_t \) and \( \nu_t \) evolve following the simultaneous heat flow:

\[
\frac{\partial \rho_t}{\partial t} = \Delta \rho_t, \quad \frac{\partial \nu_t}{\partial t} = \Delta \nu_t.
\]

(39)

We will use the following identity for any smooth function \( h: \mathbb{R}^n \to \mathbb{R} \),

\[
\Delta(h^q) = \nabla \cdot (qh^{q-1}\nabla h) = q(q-1)h^{q-2}\|\nabla h\|^2 + qh^{q-1}\Delta h.
\]

We will also use the integration by parts formula (57). Then along the simultaneous heat flow (39),

\[
\frac{d}{dt} F_{q,\nu_t}(\rho_t) = \frac{d}{dt} \int \frac{\rho_t^q}{\nu_t^q} dx
\]

\[
= \int q \left( \frac{\rho_t}{\nu_t} \right)^{q-1} \frac{\partial \rho_t}{\partial t} dx - \int (q-1) \left( \frac{\rho_t}{\nu_t} \right)^q \frac{\partial \nu_t}{\partial t} dx
\]

\[
= \int \Delta \left( \left( \frac{\rho_t}{\nu_t} \right)^{q-1} \right) \rho_t dx - (q-1) \int \Delta \left( \left( \frac{\rho_t}{\nu_t} \right)^q \right) \nu_t dx
\]

\[
= q \int \Delta \left( \left( \frac{\rho_t}{\nu_t} \right)^{q-1} \right) \rho_t dx - (q-1) \int \Delta \left( \left( \frac{\rho_t}{\nu_t} \right)^q \right) \nu_t dx
\]

\[
= q \int \Delta \left( \left( \frac{\rho_t}{\nu_t} \right)^{q-1} \right) \rho_t dx - (q-1) \int \Delta \left( \left( \frac{\rho_t}{\nu_t} \right)^q \right) \nu_t dx
\]

\[
= -q(q-1) G_{q,\nu_t}(\rho_t).
\]

(40)

Note that the identity (40) above is analogous to the identity (35) along the Langevin dynamics. Therefore, for \( q \neq 1 \),

\[
\frac{d}{dt} R_{q,\nu_t}(\rho_t) = \frac{1}{q - 1} \frac{d}{dt} F_{q,\nu_t}(\rho_t) = -q \frac{G_{q,\nu_t}(\rho_t)}{F_{q,\nu_t}(\rho_t)},
\]
as desired. The case \( q = 1 \) follows from taking limit \( q \to 1 \), or by an analogous direct calculation. We will use the following identity for \( h : \mathbb{R}^n \to \mathbb{R}_{>0} \),

\[
\Delta \log h = \nabla \cdot \left( \frac{\nabla h}{h} \right) = \frac{\Delta h}{h} - \| \nabla \log h \|^2.
\]

Then along the simultaneous heat flow (39),

\[
\frac{d}{dt} H_{\nu_t}(\rho_t) = \int \rho_t \log \frac{\rho_t}{\nu_t} \, dx
= \int \frac{\partial \rho_t}{\partial t} \log \frac{\rho_t}{\nu_t} \, dx + \int \rho_t \frac{\nu_t}{\rho_t} \frac{\partial}{\partial t} \left( \frac{\rho_t}{\nu_t} \right) \, dx
= \int \Delta \rho_t \log \frac{\rho_t}{\nu_t} \, dx + \int \nu_t \left( \frac{1}{\nu_t} \frac{\partial \rho_t}{\partial t} \, dx - \frac{\rho_t}{\nu_t^2} \frac{\partial \nu_t}{\partial t} \right) \, dx
= \int \rho_t \Delta \log \frac{\rho_t}{\nu_t} \, dx - \int \frac{\rho_t}{\nu_t} \Delta \nu_t \, dx
= \int \rho_t \left( \frac{\nu_t}{\rho_t} \Delta \left( \frac{\rho_t}{\nu_t} \right) - \left\| \nabla \log \frac{\rho_t}{\nu_t} \right\|^2 \right) \, dx - \int \frac{\rho_t}{\nu_t} \Delta \nu_t \, dx
= -J_{\nu_t}(\rho_t),
\]

as desired. Note that this is also analogous to the identity (9) along the Langevin dynamics. \( \square \)

We are now ready to prove Lemma 8.

**Proof of Lemma 8.** We will prove that along each step of ULA (11) from \( x_k \sim \rho_k \) to \( x_{k+1} \sim \rho_{k+1} \), the Rényi divergence with respect to \( \nu_\eta \) decreases by a constant factor:

\[
R_{q,\nu_\eta}(\rho_{k+1}) \leq e^{-\beta \eta^q} R_{q,\nu_\eta}(\rho_k). \tag{41}
\]

Iterating the bound above yields the desired claim (22).

We decompose each step of ULA (11) into a sequence of two steps:

\[
\tilde{\rho}_k = (I - \eta \nabla f) \# \rho_k, \tag{42a}
\rho_{k+1} = \tilde{\rho}_k \ast \mathcal{N}(0, 2\eta I). \tag{42b}
\]

In the first step (42a), we apply a smooth deterministic map \( T(x) = x - \eta \nabla f(x) \). Since \( \nabla f \) is \( L \)-Lipschitz and \( \eta < \frac{1}{L} \), \( T \) is a bijection. Then by Lemma 15,

\[
R_{q,\nu_\eta}(\rho_k) = R_{q,\tilde{\nu}_\eta}(\tilde{\rho}_k) \tag{43}
\]

where \( \tilde{\nu}_\eta = (I - \eta \nabla f) \# \nu_\eta \). Recall by Assumption 1 that \( \nu_\eta \) satisfies LSI with constant \( \beta \). Since the map \( T(x) = x - \eta \nabla f(x) \) is \( (1 + \eta L) \)-Lipschitz, by Lemma 16 we know that \( \tilde{\nu}_\eta \) satisfies LSI with constant \( \frac{\beta}{(1 + \eta L)^2} \).
In the second step (42b), we convolve with a Gaussian distribution, which is the result of evolving along the heat flow at time $\eta$. For $0 \leq t \leq \eta$, let $\tilde{\rho}_{k,t} = \tilde{\rho}_k \ast \mathcal{N}(0, 2tI)$ and $\tilde{\nu}_{\eta,t} = \tilde{\nu}_\eta \ast \mathcal{N}(0, 2tI)$, so $\tilde{\rho}_{k,\eta} = \tilde{\rho}_{k+1}$ and $\tilde{\nu}_{\eta,\eta} = \nu_\eta$. By Lemma 18,

$$\frac{d}{dt} R_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t}) = -q \frac{G_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t})}{F_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t})}.$$ 

Since $\tilde{\nu}_\eta$ satisfies LSI with constant $\frac{\beta}{(1+\eta L)^2}$, by Lemma 17 we know that $\tilde{\nu}_{\eta,t}$ satisfies LSI with constant $\frac{(1+\eta L)^2 + 2t}{2} \geq \frac{(1+\eta L)^2 + 2\eta}{2}$ for $0 \leq t \leq \eta$. In particular, since $\eta \leq \min\{\frac{1}{3L}, \frac{1}{5L}\}$, the LSI constant is $\frac{(1+\eta L)^2 + 2\eta}{2} \geq \frac{(16+2\eta)}{9} = \frac{\beta}{2}$. Then by Lemma 5,

$$\frac{d}{dt} R_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t}) = -q \frac{G_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t})}{F_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t})} \leq -\frac{\beta}{q} R_{q,\tilde{\nu}_{\eta,t}}(\tilde{\rho}_{k,t}).$$

Integrating over $0 \leq t \leq \eta$ gives

$$R_{q,\tilde{\nu}_\eta}(\rho_{k+1}) = R_{q,\tilde{\nu}_\eta}(\tilde{\rho}_{k,\eta}) \leq e^{-\frac{\beta\eta}{q}} R_{q,\tilde{\nu}_\eta}(\tilde{\rho}_k).\quad (44)$$

Combining (43) and (44) gives the desired inequality (41).

8.4.3 Proof of Theorem 5

Proof of Theorem 5. This follows directly from Lemma 7 and Lemma 8.

8.5 Details for §6: Poincaré Inequality

8.5.1 Proof of Lemma 9

Proof of Lemma 9. We plug in $g^2 = \left(\frac{\beta}{\eta}\right)^q$ to Poincaré inequality (24) and use the monotonicity condition from Lemma 13 to obtain

$$\frac{q^2}{4\alpha} G_{q,\nu}(\rho) \geq F_{q,\nu}(\rho) - F_{q,2,\nu}(\rho)^2$$

$$= e^{(q-1)R_{q,\nu}(\rho)} - e^{(q-2)R_{q,2,\nu}(\rho)}$$

$$\geq e^{(q-1)R_{q,\nu}(\rho)} - e^{(q-2)R_{q,\eta}(\rho)}$$

$$= F_{q,\nu}(\rho) \left(1 - e^{-R_{q,\nu}(\rho)}\right).$$

Dividing both sides by $F_{q,\nu}(\rho)$ and rearranging yields the desired inequality.

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8.5.2 Proof of Theorem 3

Proof of Theorem 3. By Lemma 6 and Lemma 9,
\[ \frac{d}{dt} R_{q,\nu}(\rho_t) = -q \frac{G_{q,\nu}(\rho_t)}{F_{q,\nu}(\rho_t)} \leq - \frac{4\alpha}{q} \left( 1 - e^{-R_{q,\nu}(\rho_t)} \right). \]

We now consider two possibilities:

1. If \( R_{q,\nu}(\rho_0) \geq 1 \), then as long as \( R_{q,\nu}(\rho_t) \geq 1 \), we have \( 1 - e^{-R_{q,\nu}(\rho_t)} \geq 1 - e^{-1} > \frac{1}{2} \), so
\[ \frac{d}{dt} R_{q,\nu}(\rho_t) \leq - \frac{2\alpha}{q} \] which implies \( R_{q,\nu}(\rho_t) \leq R_{q,\nu}(\rho_0) - \frac{2\alpha t}{q} \).

2. If \( R_{q,\nu}(\rho_0) \leq 1 \), then \( R_{q,\nu}(\rho_t) \leq 1 \), and thus \( \frac{1 - e^{-R_{q,\nu}(\rho_t)}}{R_{q,\nu}(\rho_t)} \geq \frac{1}{1 + R_{q,\nu}(\rho_t)} \geq \frac{1}{2} \). Thus, in this case
\[ \frac{d}{dt} R_{q,\nu}(\rho_t) \leq - \frac{2\alpha}{q} R_{q,\nu}(\rho_t), \] and integrating gives \( R_{q,\nu}(\rho_t) \leq e^{-\frac{2\alpha t}{q} R_{q,\nu}(\rho_0)} \), as desired.

\[ \square \]

8.5.3 Proof of Lemma 10

We will use the following auxiliary results, which are analogous to Lemma 16 and Lemma 17. We provide the proof of Lemma 19 in Appendix A.3.3, and the proof of Lemma 20 in Appendix A.3.4.

Lemma 19. Suppose a probability distribution \( \nu \) satisfies Poincaré inequality with constant \( \alpha > 0 \). Let \( T: \mathbb{R}^n \to \mathbb{R}^n \) be a differentiable \( L \)-Lipschitz map. Then \( \tilde{\nu} = T_{\#}\nu \) satisfies Poincaré inequality with constant \( \alpha / L^2 \).

Lemma 20. Suppose a probability distribution \( \nu \) satisfies Poincaré inequality with constant \( \alpha > 0 \). For \( t > 0 \), the probability distribution \( \tilde{\nu}_t = \nu \ast \mathcal{N}(0, 2tI) \) satisfies Poincaré inequality with constant \( \left( \frac{1}{\alpha} + 2t \right)^{-1} \).

We are now ready to prove Lemma 10.

Proof of Lemma 10. Following the proof of Lemma 8, we decompose each step of ULA (11) into two steps:

\[ \tilde{\rho}_k = (I - \eta \nabla f)_{\#}\rho_k, \]
\[ \rho_{k+1} = \tilde{\rho}_k \ast \mathcal{N}(0, 2\eta I). \]

The first step (45a) is a deterministic bijective map, so it preserves Rényi divergence by Lemma 15: \( R_{q,\nu_\eta}(\rho_k) = R_{q,\tilde{\nu}_\eta}(\tilde{\rho}_k) \), where \( \tilde{\nu}_\eta = (I - \eta \nabla f)_{\#}\nu_\eta \). Recall by Assumption 2 that \( \nu_\eta \) satisfies Poincaré inequality with constant \( \beta \). Since the map \( T(x) = x - \eta \nabla f(x) \) is \( (1 + \eta L) \)-Lipschitz, by Lemma 19 we know that \( \tilde{\nu}_\eta \) satisfies Poincaré inequality with constant \( \frac{\beta}{(1 + \eta L)^2} \).

The second step (45b) is convolution with a Gaussian distribution, which is the result of evolving along the heat flow at time \( \eta \). For \( 0 \leq t \leq \eta \), let \( \tilde{\rho}_{k,t} = \tilde{\rho}_k \ast \mathcal{N}(0, 2tI) \) and \( \tilde{\nu}_{\eta,t} = \tilde{\nu}_\eta \ast \mathcal{N}(0, 2tI) \), so
\(\tilde{\rho}_{k,n} = \tilde{\rho}_{k+1}\) and \(\tilde{\nu}_{n,n} = \nu_n\). Since \(\tilde{\nu}_n\) satisfies Poincaré inequality with constant \((1+\eta L)^2 + 2\eta\)^{-1}, by Lemma 20 we know that \(\tilde{\nu}_{n,t}\) satisfies Poincaré inequality with constant \((1+\eta L)^2 + 2\eta\)^{-1} for \(0 \leq t \leq \eta\). In particular, since \(\eta \leq \min\{\frac{1}{3L}, \frac{1}{93}\}\), the Poincaré constant is \((1+\eta L)^2 + 2\eta\)^{-1} \(\geq (\frac{16}{93} + \frac{2}{93})^{-1} = \frac{\beta}{2}\). Then by Lemma 18 and Lemma 9,

\[
\frac{d}{dt} R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t}) = -q G_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t}) \leq -\frac{2\beta}{q} \left(1 - e^{-R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t})}\right).
\]

We now consider two possibilities, as in Theorem 3:

1. If \(R_{q,\nu_n}(\rho_k) = R_{q,\tilde{\nu}_{n,0}}(\tilde{\rho}_{k,0}) \geq 1\), then as long as \(R_{q,\nu_n}(\rho_{k+1}) = R_{q,\tilde{\nu}_{n,0}}(\tilde{\rho}_{k,n}) \geq 1\), we have \(1 - e^{-R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t})} \geq 1 - e^{-1} > \frac{1}{2}\), so \(\frac{d}{dt} R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t}) \leq -\frac{2\beta}{q}\), which implies \(R_{q,\nu_n}(\rho_{k+1}) \leq R_{q,\nu_n}(\rho_k) - \frac{2\eta k}{q}\). Iterating this step, we have that \(R_{q,\nu_n}(\rho_k) \leq R_{q,\nu_n}(\rho_0) - \frac{2\eta k}{q}\) if \(R_{q,\nu_n}(\rho_0) \geq 1\) and as long as \(R_{q,\nu_n}(\rho_k) \geq 1\).

2. If \(R_{q,\nu_n}(\rho_k) = R_{q,\tilde{\nu}_{n,0}}(\tilde{\rho}_{k,0}) \leq 1\), then \(R_{q,\tilde{\nu}_{n,0}}(\tilde{\rho}_{k,0}) \leq 1\), and thus \(\frac{1}{1 - e^{-R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t})}} \geq 1 + R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t}) \geq \frac{1}{2}\). Thus, in this case \(\frac{d}{dt} R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t}) \leq -\frac{2\beta}{q} R_{q,\tilde{\nu}_{n,t}}(\tilde{\rho}_{k,t})\). Integrating over \(0 \leq t \leq \eta\) gives \(R_{q,\nu_n}(\rho_{k+1}) = R_{q,\tilde{\nu}_{n,0}}(\tilde{\rho}_{k,n}) \leq e^{-\frac{2\eta}{q} R_{q,\tilde{\nu}_{n,0}}(\tilde{\rho}_{k,0})} = e^{-\frac{2\eta}{q} R_{q,\nu_n}(\rho_k)}\). Iterating this step gives \(R_{q,\nu_n}(\rho_k) \leq e^{-\frac{2\eta k}{q} R_{q,\nu_n}(\rho_0)}\) if \(R_{q,\nu_n}(\rho_0) \leq 1\), as desired.

\[\square\]

### 8.5.4 Proof of Theorem 6

**Proof of Theorem 6.** By Lemma 10 (which applies since \(2q > 2\)), after \(k_0\) iterations we have \(R_{2q,\nu_n}(\rho_{k_0}) \leq 1\). Applying the second case of Lemma 10 starting from \(k_0\) gives \(R_{2q,\nu_n}(\rho_k) \leq e^{-\frac{\beta q (k-k_0)}{2q}} R_{2q,\nu_n}(\rho_{k_0}) \leq e^{-\frac{\beta q (k-k_0)}{2q}}\). Then by Lemma 7,

\[
R_{q,\nu}(\rho_k) \leq \left(\frac{q - \frac{1}{2}}{q - 1}\right) R_{2q,\nu_n}(\rho_k) + R_{2q-1,\nu}(\nu_k) \leq \left(\frac{q - \frac{1}{2}}{q - 1}\right) e^{-\frac{\beta q (k-k_0)}{2q}} + R_{2q-1,\nu}(\nu_k)
\]

as desired.

\[\square\]

### 8.6 Proofs for §7: Properties of biased limit

#### 8.6.1 Bounding relative Fisher information

Let \(H(\rho) = -\mathbb{E}_\rho[\log \rho]\) be Shannon entropy, \(J(\rho) = \mathbb{E}_\rho[\|\nabla \log \rho\|^2]\) be the Fisher information, and \(K(\rho) = \mathbb{E}_\rho[\|\nabla^2 \log \rho\|^2_{\text{HS}}]\) be the second-order Fisher information. We can write relative entropy as

\[
H_\nu(\rho) = \mathbb{E}_\rho[\log \frac{\rho}{\nu}] = -H(\rho) + \mathbb{E}_\rho[f]
\]

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and we can write relative Fisher information as
\[
J_\nu(\nu) = \mathbb{E}_{\nu_\eta} \left[ \left\| \nabla \log \frac{\nu}{\nu_\eta} \right\|^2 \right] = J(\nu_\eta) + 2\mathbb{E}_{\nu_\eta} \left[ \langle \nabla \log \nu_\eta, \nabla f \rangle \right] + \mathbb{E}_{\nu_\eta} [\|\nabla f\|^2] \\
= J(\nu) + \mathbb{E}_{\nu_\eta} [\|\nabla f\|^2 - 2\Delta f]
\]

(46)

where the last step follows from integration by parts.

We first prove the following, which only requires second-order smoothness.

**Lemma 21.** Assume \( f \) is \( L \)-smooth \((-LI \leq \nabla^2 f \leq LI)\) and \( \eta \leq \frac{1}{2L} \). Then
\[
J_\nu(\nu_\eta) \leq \mathbb{E}_{\nu_\eta} [\|\nabla f\|^2 - \Delta f] + \eta nL^2.
\]

**Proof.** We examine how entropy changes from \( \nu_\eta \) to \( \mu_\eta \) and back, which will give us an estimate on the Fisher information. By the change-of variable formula for \( \nu_\eta = (I - \eta \nabla f)_\# \nu_\eta \), we have
\[
\log \nu_\eta(x) = \log \det(I - \eta \nabla f(x)) + \log \mu_\eta(x - \eta \nabla f(x)).
\]

(47)

By taking expectation over \( x \sim \nu \) (equivalently, \( x - \eta \nabla f(x) \sim \mu \)), we get
\[
H(\nu_\eta) = H(\mu_\eta) - \mathbb{E}_{\nu_\eta} [\log \det(I - \eta \nabla^2 f)].
\]

(48)

On the other hand, recall that along the heat flow \( \rho_t = \rho_0 * \mathcal{N}(0, 2tI) \), we have the relations
\[
\frac{d}{dt} H(\rho_t) = J(\rho_t), \\
\frac{d}{dt} J(\rho_t) = -K(\rho_t) \leq 0.
\]

See for example [72]. Thus, \( \nu_\eta = \mu_\eta * \mathcal{N}(0, 2\eta I) \) satisfies
\[
H(\nu_\eta) = H(\mu_\eta) + \int_0^\eta J(\rho_t) \, dt \geq H(\mu_\eta) + \eta J(\nu_\eta)
\]

(49)

where \( \rho_t = \rho_0 * \mathcal{N}(0, 2tI) \) is the heat flow from \( \rho_0 = \mu_\eta \) to \( \rho_\eta = \nu_\eta \), and the last inequality holds since \( t \mapsto J(\rho_t) \) is decreasing. Combining (48) and (49), we get
\[
\eta J(\nu_\eta) \leq H(\nu_\eta) - H(\mu_\eta) = -\mathbb{E}_{\nu_\eta} [\log \det(I - \eta \nabla^2 f)].
\]

(50)

Let \( \lambda_1, \ldots, \lambda_d \) be the eigenvalues of \( \nabla^2 f \). Since \( f \) is \( L \)-smooth, \( |\lambda_i| \leq L \). Using the inequality \( \log(1 - \eta \lambda_i) \geq -\eta \lambda_i - \eta^2 \lambda_i^2 \), which holds since \( \eta |\lambda_i| \leq \frac{1}{2} \) since \( \eta \leq \frac{1}{2L} \), we have
\[
-\mathbb{E}_{\nu_\eta} [\log \det(I - \eta \nabla^2 f)] = \sum_{i=1}^n \mathbb{E}_{\nu_\eta} [-\log(1 - \eta \lambda_i)] \\
\leq \sum_{i=1}^n \mathbb{E}_{\nu_\eta} [\eta \lambda_i + \eta^2 \lambda_i^2] \\
= \eta \mathbb{E}_{\nu_\eta} [\Delta f] + \eta^2 \mathbb{E}_{\nu_\eta} [\|\nabla^2 f\|^2_{\text{HS}}] \\
\leq \eta \mathbb{E}_{\nu_\eta} [\Delta f] + \eta^2 nL^2.
\]

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Plugging this to (50) gives
\[ J(\nu_\eta) \leq -\frac{1}{\eta} \mathbb{E}_{\nu_\eta}[\log \det(I - \eta \nabla^2 f)] \leq \mathbb{E}_{\nu_\eta}[\Delta f] + \eta nL^2. \]  

(51)

Therefore, we can bound the relative Fisher information (46):
\[ J_\nu(\nu_\eta) = J(\nu_\eta) + \mathbb{E}_{\nu_\eta}[\|\nabla f\|^2 - 2\Delta f] \leq \mathbb{E}_{\nu_\eta}[\|\nabla f\|^2 - \Delta f] + \eta nL^2. \]

8.6.2 Bounding the expected value

Recall that for \( \nu = e^{-f} \), we have \( \mathbb{E}_\nu[\|\nabla f\|^2 - \Delta f] = 0 \). Under third-order smoothness, we will prove \( \mathbb{E}_{\nu_\eta}[\|\nabla f\|^2 - \Delta f] = O(\eta) \).

Lemma 22. Assume \( f \) is \((L, M)\)-smooth. Then for \( \eta \leq \frac{1}{2L} \),
\[ \mathbb{E}_{\nu_\eta}[\|\nabla f\|^2 - \Delta f] \leq \eta n \left( L^2 + M \sqrt{J(\mu_\eta)} \right). \]  

(52)

Proof. We examine how the expected value of \( f \) changes from \( \nu_\eta \) to \( \mu_\eta \) and back, which will give us an estimate on the desired quantity.

Let \( x \sim \nu_\eta \) and \( y = x - \eta \nabla f(x) \sim \mu_\eta \), so \( x' = y + \sqrt{2\eta} Z \sim \nu_\eta \) where \( Z \sim \mathcal{N}(0, I) \) is independent. Since \( f \) is \( L \)-smooth, we have the bound:
\[ f(y) \leq f(x) - \eta \left( 1 - \frac{\eta L}{2} \right) \|\nabla f(x)\|^2. \]

Taking expectation over \( x \sim \nu_\eta \) (equivalently, \( y \sim \mu_\eta \)) yields
\[ \mathbb{E}_{\mu_\eta}[f] \leq \mathbb{E}_{\nu_\eta}[f] - \eta \left( 1 - \frac{\eta L}{2} \right) \mathbb{E}_{\nu_\eta}[\|\nabla f\|^2]. \]

On the other hand, let \( \rho_t = \rho_0 * \mathcal{N}(0, 2tI) \) be the heat flow from \( \rho_0 = \mu_\eta \) to \( \rho_\eta = \nu_\eta \), and recall that along the heat flow, \( \frac{d}{dt} \mathbb{E}_{\rho_t}[f] = \mathbb{E}_{\rho_t}[\Delta f] \). Then
\[ \mathbb{E}_{\nu_\eta}[f] = \mathbb{E}_{\mu_\eta}[f] + \int_0^\eta \mathbb{E}_{\rho_t}[\Delta f] dt. \]

Combining the two relations above,
\[ \eta \left( 1 - \frac{\eta L}{2} \right) \mathbb{E}_{\nu_\eta}[\|\nabla f(x)\|^2] \leq \mathbb{E}_{\nu_\eta}[f] - \mathbb{E}_{\mu_\eta}[f] = \int_0^\eta \mathbb{E}_{\rho_t}[\Delta f] dt. \]
Therefore,
\[
\eta \left(1 - \frac{\eta L}{2}\right) \mathbb{E}_{\nu \eta} [||\nabla f||^2 - \Delta f] \leq \int_{0}^{\eta} \mathbb{E}_{\rho_t} [\Delta f] \, dt - \eta \left(1 - \frac{\eta L}{2}\right) \mathbb{E}_{\nu \eta} [\Delta f] \\
= \int_{0}^{\eta} \left(\mathbb{E}_{\rho_t} [\Delta f] - \mathbb{E}_{\rho \eta} [\Delta f]\right) \, dt + \frac{\eta^2 L}{2} \mathbb{E}_{\nu \eta} [\Delta f] \\
\leq \int_{0}^{\eta} \left(\mathbb{E}_{\rho_t} [\Delta f] - \mathbb{E}_{\rho \eta} [\Delta f]\right) \, dt + \frac{\eta^2 nL^2}{2}.
\]

Since \( \rho_t \) evolves following the heat flow, by Lemma 23 we have for any \( 0 \leq t \leq \eta \):
\[
W_2(\rho_t, \rho \eta)^2 \leq (\eta - t)^2 J(\rho_t) \leq (\eta - t)^2 J(\rho_0) = (\eta - t)^2 J(\mu \eta)
\]
where the second inequality above follows from the fact that Fisher information is decreasing along heat flow.

Since we assume \( \nabla^2 f \) is \( M \)-Lipschitz, the Laplacian \( \Delta f = \text{Tr}(\nabla^2 f) \) is \( (nM) \)-Lipschitz. Then by the dual formulation of \( W_1 \) distance,
\[
\mathbb{E}_{\rho_t} [\Delta f] - \mathbb{E}_{\rho \eta} [\Delta f] \leq nM W_1(\rho_t, \rho \eta) \leq nM W_2(\rho_t, \rho \eta) \leq (\eta - t) nM \sqrt{J(\mu \eta)}.
\]
Integrating over \( 0 \leq t \leq \eta \) gives
\[
\int_{0}^{\eta} \left(\mathbb{E}_{\rho_t} [\Delta f] - \mathbb{E}_{\rho \eta} [\Delta f]\right) \, dt \leq \frac{\eta^2}{2} nM \sqrt{J(\mu \eta)}.
\]

Plugging this to (53) gives
\[
\eta \left(1 - \frac{\eta L}{2}\right) \mathbb{E}_{\nu \eta} [||\nabla f||^2 - \Delta f] \leq \frac{\eta^2}{2} nM \sqrt{J(\mu \eta)} + \frac{\eta^2 nL^2}{2}.
\]
Since \( 1 - \frac{\eta L}{2} \geq \frac{3}{4} > \frac{1}{2} \) for \( \eta \leq \frac{1}{2L} \), this also implies
\[
\frac{\eta}{2} \mathbb{E}_{\nu \eta} [||\nabla f||^2 - \Delta f] \leq \frac{\eta^2}{2} nM \sqrt{J(\mu \eta)} + \frac{\eta^2 nL^2}{2}.
\]

Dividing by \( \frac{\eta}{2} \) gives the claim. \( \Box \)

**Remark 6.** We see from (53) that if \( \Delta \Delta f \geq 0 \), then \( \mathbb{E}_{\rho_t} [\Delta f] - \mathbb{E}_{\rho \eta} [\Delta f] \leq 0 \). Thus, we also get the bound \( J_{\nu}(\nu \eta) \leq \eta nL^2 \) assuming \( f \) is \( L \)-smooth and \( \Delta \Delta f \geq 0 \).

In the proof above, we use the following lemma on the distance along the heat flow. Note that a simple coupling argument gives \( W_2(\rho_0, \rho \eta)^2 \leq O(\eta) \), rather than \( O(\eta^2) \) below (when \( J(\rho_0) < \infty \)).

\[\text{Recall } W_1(\rho, \nu) = \sup \{ \mathbb{E}_{\rho}[g] - \mathbb{E}_{\nu}[g] : g \text{ is } 1\text{-Lipschitz} \}.\]
Lemma 23. For any probability distribution $\rho_0$ and for any $\eta > 0$, let $\rho_\eta = \rho_0 \ast \mathcal{N}(0, 2\eta I)$. Then

$$W_2(\rho_\eta, \rho_0)^2 \leq \eta^2 J(\rho_0). \quad (53)$$

Proof. By definition, $\rho_\eta$ evolves following the heat flow $\frac{\partial \rho_t}{\partial t} = \Delta \rho_t$ from time $t = 0$ to time $t = \eta$. Fix $\eta > 0$, and let us rescale time to be from 0 to 1: Let $\tilde{\rho}_\tau = \rho_{\eta \tau}$, so $\tilde{\rho}_0 = \rho_0$ and $\tilde{\rho}_1 = \rho_\eta$. Then $\tilde{\rho}_\tau$ evolves following a rescaled heat flow:

$$\frac{\partial \tilde{\rho}_\tau}{\partial \tau} = \eta \Delta \tilde{\rho}_\tau = \eta \Delta \tilde{\rho}_\tau = \eta \nabla \cdot (\tilde{\rho}_\tau \nabla \log \tilde{\rho}_\tau) \quad (54)$$

Since $(\tilde{\rho}_\tau)_{0 \leq \tau \leq 1}$ connects $\tilde{\rho}_0 = \rho_0$ to $\tilde{\rho}_1 = \rho_\eta$, its length must exceed the $W_2$ distance:

$$W_2(\rho_\eta, \rho_0)^2 \leq \int_0^1 \EE_{\tilde{\rho}_\tau}[\|\eta \nabla \log \tilde{\rho}_\tau\|^2] d\tau = \eta^2 \int_0^1 J(\tilde{\rho}_\tau) d\tau \leq \eta^2 J(\rho_0).$$

In the last step we have used Fisher information is decreasing along the heat flow: $J(\tilde{\rho}_\tau) \leq J(\rho_0)$. \qed

8.6.3 Bounding the Fisher information

Lemma 24. 1. If $f$ is $L$-smooth and $\eta \leq \frac{1}{2L}$, then

$$J(\nu_\eta) \leq \frac{3}{2} n L.$$  

2. If $f$ is $(L, M)$-smooth and $\eta \leq \frac{1}{2L}$, then

$$J(\mu_\eta) \leq 12n(L + 3nM^2).$$

Proof. First, since $f$ is $L$-smooth and $\eta \leq \frac{1}{2L}$, from (51) we can bound

$$J(\nu_\eta) \leq \EE_{\nu_\eta}[\Delta f] + \eta \EE_{\nu_\eta}[\|\nabla^2 f\|_{\text{HS}}^2] \leq nL + \eta nL^2 \leq \frac{3}{2} n L. \quad (55)$$

Second, by taking gradient in the formula (47) for $\mu_\eta = (I - \eta \nabla f)_\# \nu_\eta$, we get

$$\nabla \log \nu_\eta(x) = -\eta \nabla^3 f(x) A(x)^{-1} + A(x) \nabla \log \mu_\eta(x - \eta \nabla f(x))$$

or equivalently,

$$\nabla \log \mu_\eta(x - \eta \nabla f(x)) = A(x)^{-1} \nabla \log \nu_\eta(x) + \eta A(x)^{-1} \nabla^3 f(x) A(x)^{-1} \quad (56)$$

where

$$A(x) = I - \eta \nabla^2 f(x).$$

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satisfies \( \frac{1}{2} I \preceq A(x) \preceq \frac{3}{2} I \) since \(-LI \preceq \nabla^2 f(x) \preceq LI\) and \(\eta \leq \frac{1}{2L}\). In particular,
\[
\frac{2}{3} I \preceq A(x)^{-1} \preceq 2I.
\]
Therefore, the first term in (56) we can bound as
\[
\| A(x)^{-1} \nabla \log \nu_\eta(x) \|_2 \leq 2 \| \nabla \log \nu_\eta(x) \|_2.
\]
For the second term, using the assumption \(\| \nabla^3 f(x) \|_{\text{op}} \leq M\) and Lemma 25, we have
\[
\| A(x)^{-1} \nabla^3 f(x) A(x)^{-1} \|_2 \leq 2 \| \nabla^3 f(x) A(x)^{-1} \|_2 \leq 4nM.
\]
Therefore, from (56), we get
\[
\| \nabla \log \mu_\eta(x - \eta \nabla f(x)) \|_2 \leq \| \nabla \log \nu_\eta(x) \|_2 + 4nM.
\]
This implies
\[
\| \nabla \log \mu_\eta(x - \eta \nabla f(x)) \|_2^2 \leq 8 \| \nabla \log \nu_\eta(x) \|_2^2 + 32n^2 M^2.
\]
Taking expectation over \(x \sim \nu_\eta\) (equivalently, \(x - \eta \nabla f(x) \sim \mu_\eta\)), we conclude that
\[
J(\mu_\eta) \leq 8J(\nu_\eta) + 32n^2 M^2 \leq 12nL + 32n^2 M^2 \leq 12n(L + 3nM^2).
\]

In the above, we use the following bound from smoothness.

**Lemma 25.** Let \(T \in \mathbb{R}^{d \times d \times d}\) be a 3-tensor with \(\|T\|_{\text{op}} \leq M\). For any symmetric matrix \(B \in \mathbb{R}^{d \times d}\) with \(\|B\|_{\text{op}} \leq \beta\), the vector \(TB \in \mathbb{R}^n\) satisfies \(\|TB\|_2 \leq n\beta M\).

**Proof.** Since \(\|T\|_{\text{op}} \leq M\), for any \(u, v, w \in \mathbb{R}^d\) with \(\|u\| = \|v\| = \|w\| = 1\), \(|T[u, v, w]| \leq M\). In particular, for any \(u \in \mathbb{R}^d\) with \(\|u\| = 1\), \(p = T[u, u] \in \mathbb{R}^d\) satisfies \(\|p\|_2 \leq M\). We eigendecompose \(B = \sum_{i=1}^d \lambda_i u_i u_i^\top\) with eigenvectors \(u_1, \ldots, u_n \in \mathbb{R}^n\) and eigenvalues \(\lambda_1, \ldots, \lambda_n \in \mathbb{R}\) with \(\|u_i\|_2 = 1\), \(|\lambda_i| \leq \beta\). Then
\[
\|TB\|_2 = \left\| T \sum_{i=1}^n \lambda_i u_i u_i^\top \right\|_2 \leq \sum_{i=1}^n |\lambda_i| \cdot \|T[u_i, u_i]\|_2 \leq \sum_{i=1}^n \beta M = n\beta M.
\]
8.6.4 Proof of upper bound in Theorem 7

Proof of upper bound in Theorem 7. By combining Lemmas 21, 22, and 24:

\[ J_\nu(\nu_\eta) \leq \mathbb{E}_{\nu_\eta}[\|\nabla f \|^2 - \Delta f] + \eta nL^2 \]
\[ \leq \eta n\left(2L^2 + M\sqrt{J(\mu_\eta)}\right) \]
\[ \leq \eta n\left(2L^2 + M\sqrt{12n(L + 3nM^2)}\right) \]
\[ \leq \eta n\left(2L^2 + M(4\sqrt{nL} + 6nM)\right) \]
\[ \leq 2\eta n\left(L^2 + 2\sqrt{nLM} + 3nM^2\right) . \]

\[ \square \]

8.6.5 Proof of lower bound in Theorem 7

For the lower bound, we first prove the following properties. Observe that for \( \nu \propto e^{-f} \), \( \mathbb{E}_\nu[\nabla f] = 0 \) and \( \mathbb{E}_\nu[\langle x, \nabla f(x) \rangle] = n \). These properties still hold when we take the expectation under the biased limit.

Lemma 26. For any \( f \) and \( \eta > 0 \), the biased limit \( \nu_\eta \) satisfies:

1. \( \mathbb{E}_{\nu_\eta}[\nabla f] = 0 \).
2. \( \mathbb{E}_{\nu_\eta}[\langle x, \nabla f(x) \rangle] = d + \frac{\eta}{2}\mathbb{E}_{\nu_\eta}[\|\nabla f\|^2] \).

Proof. Let \( x \sim \nu_\eta \), \( y = x - \eta\nabla f(x) \sim \mu_\eta \), and \( x' = y + \sqrt{2}\eta z \sim \nu_\eta \) where \( z \sim \mathcal{N}(0, I) \) is independent. Then

\[ x' = x - \eta\nabla f(x) + \sqrt{2}\eta z. \]

By taking expectation over \( x \sim \nu_\eta \) (so \( x' \sim \nu_\eta \)), we get:

\[ \mathbb{E}_{\nu_\eta}[x'] = \mathbb{E}_{\nu_\eta}[x] - \mathbb{E}_{\nu_\eta}[\nabla f(x)] \]

which implies \( \mathbb{E}_{\nu_\eta}[\nabla f] = 0 \).

Next, by taking covariance, we get:

\[ \text{Cov}_{\nu_\eta}(x') = \text{Cov}_{\nu_\eta}(x - \eta\nabla f(x)) + 2\eta I \]
\[ = \text{Cov}_{\nu_\eta}(x - \eta\text{Cov}_{\nu_\eta}(x, \nabla f(x))) - \eta\text{Cov}_{\nu_\eta}(\nabla f(x), x) + \eta^2\text{Cov}_{\nu_\eta}(\nabla f(x)) + 2\eta I \]

so

\[ \text{Cov}_{\nu_\eta}(x, \nabla f(x)) + \text{Cov}_{\nu_\eta}(\nabla f(x), x) = \eta\text{Cov}_{\nu_\eta}(\nabla f(x)) + 2I. \]
Since $\mathbb{E}_{\nu_\eta} [\nabla f] = 0$, this means
\[
\mathbb{E}_{\nu_\eta} [x \nabla f(x)^\top] + \mathbb{E}_{\nu_\eta} [\nabla f(x) x^\top] = \eta \mathbb{E}_{\nu_\eta} [\nabla f(x) \nabla f(x)^\top] + 2I.
\]

Taking trace and dividing by 2 gives
\[
\mathbb{E}_{\nu_\eta} [\langle x, \nabla f(x) \rangle] = n + \frac{\eta}{2} \mathbb{E}_{\nu_\eta} [\|\nabla f(x)\|^2].
\]

We are now ready to prove the lower bound.

**Proof of lower bound in Theorem 7.** From Lemma 26 part 2, using the identity $d = \mathbb{E}_{\nu_\eta} [\langle x, -\nabla \log \nu_{\eta} \rangle]$ and Cauchy-Schwarz inequality, we can derive the bound:
\[
\frac{\eta}{2} \mathbb{E}_{\nu_\eta} [\|\nabla f(x)\|^2] = \mathbb{E}_{\nu_\eta} [\langle x, \nabla f(x) \rangle] - d
= \mathbb{E}_{\nu_\eta} \left[ \langle x, \nabla \log \frac{\nu_\eta}{\nu} \rangle \right]
= \mathbb{E}_{\nu_\eta} \left[ \langle x - \mathbb{E}_{\nu_\eta} [x], \nabla \log \frac{\nu_\eta}{\nu} \rangle \right]
\leq \sqrt{\text{Var}_{\nu_\eta}(x)} \cdot \sqrt{J_{\nu}(\nu_\eta)}.
\]

Rearranging gives us the desired result. In the second step above we can subtract $\mathbb{E}_{\nu_\eta} [x]$ because for any $c \in \mathbb{R}^n$, by Lemma 26 part 1,
\[
\mathbb{E}_{\nu_\eta} \left[ \langle c, \nabla \log \frac{\nu_\eta}{\nu} \rangle \right] = \langle c, \mathbb{E}_{\nu_\eta} [\nabla \log \nu_\eta] + \mathbb{E}_{\nu_\eta} [\nabla f] \rangle = 0.
\]

### 8.6.6 Proof of Theorem 8

The following proof is due to Sinho Chewi.

**Proof of Theorem 8.** Suppose we run ULA from $x_0 \sim \rho_0$ to obtain $x_k \sim \rho_k$, so $\rho_k \to \nu_\eta$ as $k \to \infty$. Let $\alpha_k$ denote the LSI constant of $\rho_k$, i.e. the largest constant $\tilde{\alpha} > 0$ such that (4) holds. Since $0 \leq \eta \leq \frac{1}{L}$ and $f$ is $\alpha$-strongly convex, the map $x \mapsto x - \eta \nabla f(x)$ is $(1 - \eta \alpha)$-Lipschitz. Since $x_k \sim \rho_k$ is $\alpha_k$-LSI, by Lemma 16, the distribution of $x_k - \eta \nabla f(x_k)$ satisfies LSI with constant $\alpha_k/(1 - \eta \alpha)^2$. Then by Lemma 17, $x_{k+1} = x_k - \eta \nabla f(x_k) + \sqrt{2\eta} z_k \sim \rho_{k+1}$ satisfies $\alpha_{k+1}$-LSI with
\[
\frac{1}{\alpha_{k+1}} \leq \frac{(1 - \eta \alpha)^2}{\alpha_k} + 2\eta.
\]
Suppose we start $\alpha_0 \geq \frac{\alpha}{2}$. We claim that $\alpha_k \geq \frac{\alpha}{2}$ for all $k \geq 0$. Indeed, if $\frac{1}{\alpha_k} \leq \frac{2}{\alpha}$, then since $\eta \leq \frac{1}{L} \leq \frac{1}{\alpha}$, we have

$$\frac{1}{\alpha_{k+1}} \leq \frac{(1 - \eta \alpha)^2}{\alpha/2} + 2\eta = \frac{2}{\alpha} - 2\eta(1 - \eta \alpha) \leq \frac{2}{\alpha}.$$ 

Thus by induction, $\alpha_k \geq \frac{\alpha}{2}$ for all $k \geq 0$. Taking the limit $k \to \infty$, this shows that $\nu_\eta = \lim_{k \to \infty} \rho_k$ also satisfies LSI with constant $\beta \geq \frac{\alpha}{2}$.

9 Discussion

In this paper we proved convergence guarantees on KL divergence and Rényi divergence along ULA under isoperimetric assumptions and bounded Hessian, without assuming convexity or bounds on higher derivatives. In particular, under LSI and bounded Hessian, we prove a complexity guarantee of $O(\kappa^2 n) \delta$ to achieve $H_\nu(\rho_k) \leq \delta$, where $\kappa := L/\alpha$ is the condition number. We note the dependence on $\kappa$ may not be tight. In particular, the asymptotic bias in KL divergence from our result scales linearly with step size, while from the Gaussian example we see it should scale quadratically with step size. We can achieve a smaller bias using a different algorithm, e.g. the underdamped Langevin algorithm [56] or the proximal Langevin algorithm [77]. However, it remains open whether we can provide a better analysis of ULA under LSI and smoothness that yields the optimal bias.

Our convergence results for ULA in Rényi divergence hold assuming the biased limit satisfies isoperimetry (Assumptions 1 and 2), which we can verify assuming strong log-concavity and smoothness of the target distribution. It would be interesting to verify when Assumptions 1 and 2 hold more generally, whether they can be relaxed, or if they follow from assuming isoperimetry and smoothness for the target density.

Another intriguing question is whether there is an affine-invariant version of the Langevin dynamics. This might lead to a sampling algorithm with logarithmic dependence on smoothness parameters, rather than the current polynomial dependence. There are some approaches that achieve affine invariance in continuous time, for example via interacting Langevin dynamics [36] or the Newton Langevin dynamics [22]; however, the discretization analysis remains a challenge.

Since the publication of the conference version of this paper [71], some of our techniques and results have been generalized. The one-step interpolation technique that we use in Lemma 3 proves to be useful for analyzing ULA or its variants under various assumptions. It has been extended to analyze ULA for sampling on manifolds, for example, on a complete Riemannian manifold [75]; or on a product of spheres with applications to solving semidefinite programming [50]. It has also been used to analyze ULA for sampling from distributions with sub-Gaussian tail growth and Hölder-continuous gradient [33]; for sampling from heavy-tailed distributions [40]; for sampling in Rényi divergence under a family of isoperimetric inequalities interpolating between LSI and Poincaré [21]; and for sampling from non-log-concave distributions with convergence in Fisher information [7]. The interpolation technique has also been useful for analyzing other sampling algorithms, e.g. the
Proximal Langevin Algorithm (which uses the proximal method for $f$ rather than gradient descent), which yields a smaller (and tight) asymptotic bias [77]. It has also been used to analyze the Mirror Langevin Algorithm (which uses Hessian metric and discretizes in the dual space) for sampling under mirror isoperimetric inequalities [45]. Further, the calculation along simultaneous heat flow (Lemma 18) is also useful for analyzing the convergence of a new proximal sampler algorithm under isoperimetry [17].

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A Appendix

A.1 Review on notation and basic properties

Throughout, we represent a probability distribution \( \rho \) on \( \mathbb{R}^n \) via its probability density function with respect to the Lebesgue measure, so \( \rho: \mathbb{R}^n \to \mathbb{R} \) with \( \int_{\mathbb{R}^n} \rho(x) dx = 1 \). We typically assume \( \rho \) has full support and smooth density, so \( \rho(x) > 0 \) and \( x \mapsto \rho(x) \) is differentiable. Given a function \( f: \mathbb{R}^n \to \mathbb{R} \), we denote the expected value of \( f \) under \( \rho \) by

\[
\mathbb{E}_\rho[f] = \int_{\mathbb{R}^n} f(x) \rho(x) \, dx.
\]

We use the Euclidean inner product \( (x, y) = \sum_{i=1}^n x_i y_i \) for \( x = (x_i)_{1 \leq i \leq n}, y = (y_i)_{1 \leq i \leq n} \in \mathbb{R}^n \). For symmetric matrices \( A, B \in \mathbb{R}^{n \times n} \), let \( A \preceq B \) denote that \( B - A \) is positive semidefinite. For \( \mu \in \mathbb{R}^n, \Sigma > 0 \), let \( \mathcal{N}(\mu, \Sigma) \) denote the Gaussian distribution on \( \mathbb{R}^n \) with mean \( \mu \) and covariance matrix \( \Sigma \).

Given a smooth function \( f: \mathbb{R}^n \to \mathbb{R} \), its gradient \( \nabla f: \mathbb{R}^n \to \mathbb{R}^n \) is the vector of partial derivatives:

\[
\nabla f(x) = \left( \frac{\partial f(x)}{\partial x_1}, \ldots, \frac{\partial f(x)}{\partial x_n} \right).
\]

The Hessian \( \nabla^2 f: \mathbb{R}^n \to \mathbb{R}^{n \times n} \) is the matrix of second partial derivatives:

\[
\nabla^2 f(x) = \begin{pmatrix}
\frac{\partial^2 f(x)}{\partial x_i \partial x_j}
\end{pmatrix}_{1 \leq i,j \leq n}.
\]

The Laplacian \( \Delta f: \mathbb{R}^n \to \mathbb{R} \) is the trace of its Hessian:

\[
\Delta f(x) = \text{Tr}(\nabla^2 f(x)) = \sum_{i=1}^n \frac{\partial^2 f(x)}{\partial x_i^2}.
\]
Given a smooth vector field \( v = (v_1, \ldots, v_n) : \mathbb{R}^n \to \mathbb{R}^n \), its divergence \( \nabla \cdot v : \mathbb{R}^n \to \mathbb{R} \) is

\[
(\nabla \cdot v)(x) = \sum_{i=1}^{n} \frac{\partial v_i(x)}{\partial x_i}.
\]

In particular, the divergence of gradient is the Laplacian:

\[
(\nabla \cdot \nabla f)(x) = \sum_{i=1}^{n} \frac{\partial^2 f(x)}{\partial x_i^2} = \Delta f(x).
\]

For any function \( f : \mathbb{R}^n \to \mathbb{R} \) and vector field \( v : \mathbb{R}^n \to \mathbb{R}^n \) with sufficiently fast decay at infinity, we have the following integration by parts formula:

\[
\int_{\mathbb{R}^n} \langle v(x), \nabla f(x) \rangle \, dx = -\int_{\mathbb{R}^n} f(x)(\nabla \cdot v)(x) \, dx.
\]

Furthermore, for any two functions \( f, g : \mathbb{R}^n \to \mathbb{R} \),

\[
\int_{\mathbb{R}^n} f(x) \Delta g(x) \, dx = -\int_{\mathbb{R}^n} \langle \nabla f(x), \nabla g(x) \rangle \, dx = \int_{\mathbb{R}^n} g(x) \Delta f(x) \, dx.
\]

When the argument is clear, we omit the argument \((x)\) in the formulae for brevity. For example, the last integral above becomes

\[
\int f \Delta g \, dx = -\int \langle \nabla f, \nabla g \rangle \, dx = \int g \Delta f \, dx. \quad (57)
\]

### A.2 Derivation of the Fokker-Planck equation

Consider a stochastic differential equation

\[
dx_t = v(X_t) \, dt + \sqrt{2} \, dW_t \quad (58)
\]

where \( v : \mathbb{R}^n \to \mathbb{R}^n \) is a smooth vector field and \((W_t)_{t \geq 0}\) is the Brownian motion on \( \mathbb{R}^n \) with \( W_0 = 0 \).

We will show that if \( X_t \) evolves following (58), then its probability density function \( \rho_t(x) \) evolves following the Fokker-Planck equation:

\[
\frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\rho_t v) + \Delta \rho_t. \quad (59)
\]

We can derive this heuristically as follows; we refer to standard textbooks for rigorous derivation [57].

For any smooth test function \( \phi : \mathbb{R}^n \to \mathbb{R} \), let us compute the time derivative of the expectation

\[
A(t) = \mathbb{E}_{\rho_t}[\phi] = \mathbb{E}[\phi(X_t)].
\]
On the one hand, we can compute this as
\[
\dot{A}(t) = \frac{d}{dt} A(t) = \frac{d}{dt} \int_{\mathbb{R}^n} \rho_t(x) \phi(x) \, dx = \int_{\mathbb{R}^n} \frac{\partial \rho_t(x)}{\partial t} \phi(x) \, dx. \tag{60}
\]

On the other hand, by (58), for small $\eta > 0$ we have
\[
X_{t+\eta} = X_t + \int_t^{t+\eta} v(X_s) \, ds + \sqrt{2}(W_{t+\eta} - W_t)
\]
\[
= X_t + \eta v(X_t) + \sqrt{2}(W_{t+\eta} - W_t) + O(\eta^2)
\]
\[
\sim N(0, I)
\]
where $Z \sim N(0, I)$ is independent of $X_t$, since $W_{t+\eta} - W_t \sim N(0, \eta I)$. Then by Taylor expansion,
\[
\dot{\phi}(X_{t+\eta}) = \dot{\phi} \left( X_t + \eta v(X_t) + \sqrt{2}\eta Z + O(\eta^2) \right)
\]
\[
= \phi(X_t) + \eta \langle \nabla \phi(X_t), v(X_t) \rangle + \sqrt{2}\eta \langle \nabla \phi(X_t), Z \rangle + \frac{1}{2} 2\eta \langle Z, \nabla^2 \phi(X_t) Z \rangle + O(\eta^2).
\]

Now we take expectation on both sides. Since $Z \sim N(0, I)$ is independent of $X_t$,
\[
A(t + \eta) = \mathbb{E}[\phi(X_{t+\eta})]
\]
\[
= \mathbb{E} \left[ \phi(X_t) + \eta \langle \nabla \phi(X_t), v(X_t) \rangle + \sqrt{2}\eta \langle \nabla \phi(X_t), Z \rangle + \frac{1}{2} 2\eta \langle Z, \nabla^2 \phi(X_t) Z \rangle \right] + O(\eta^2)
\]
\[
= A(t) + \eta \left( \mathbb{E}[\langle \nabla \phi(X_t), v(X_t) \rangle] + \mathbb{E}[\Delta \phi(X_t)] \right) + O(\eta^2).
\]

Therefore, by integration by parts, this second approach gives
\[
\dot{A}(t) = \lim_{\eta \to 0} \frac{A(t + \eta) - A(t)}{\eta}
\]
\[
= \mathbb{E}[\langle \nabla \phi(X_t), v(X_t) \rangle] + \mathbb{E}[\Delta \phi(X_t)]
\]
\[
= \int_{\mathbb{R}^n} \langle \nabla \phi(x), \rho_t(x) v(x) \rangle \, dx + \int_{\mathbb{R}^n} \rho_t(x) \Delta \phi(x) \, dx
\]
\[
= -\int_{\mathbb{R}^n} \phi(x) \nabla \cdot (\rho_t v(x)) \, dx + \int_{\mathbb{R}^n} \phi(x) \Delta \rho_t(x) \, dx
\]
\[
= \int_{\mathbb{R}^n} \phi(x) \left( -\nabla \cdot (\rho_t v(x)) + \Delta \rho_t(x) \right) \, dx. \quad \tag{61}
\]

Comparing (60) and (61), and since $\phi$ is arbitrary, we conclude that
\[
\frac{\partial \rho_t(x)}{\partial t} = -\nabla \cdot (\rho_t v(x)) + \Delta \rho_t(x)
\]
as claimed in (59).

When $v = -\nabla f$, the stochastic differential equation (58) becomes the Langevin dynamics (7) from Section 2.3, and the Fokker-Planck equation (59) becomes (8).

In the proof of Lemma 3, we also apply the Fokker-Planck equation (59) when $v = -\nabla f(x_0)$ is a constant vector field to derive the evolution equation (30) for one step of ULA.
A.3 Remaining proofs

A.3.1 Proof of Lemma 16

Proof of Lemma 16. Let \( g : \mathbb{R}^n \to \mathbb{R} \) be a smooth function, and let \( \tilde{g} : \mathbb{R}^n \to \mathbb{R} \) be the function \( \tilde{g}(x) = g(T(x)) \). Let \( X \sim \nu \), so \( T(X) \sim \tilde{\nu} \). Note that

\[
E_{\tilde{\nu}}[g^2] = E_{X \sim \nu}[g(T(X))^2] = E_{\nu}[\tilde{g}^2], \\
E_{\tilde{\nu}}[g^2 \log g^2] = E_{X \sim \nu}[g(T(X))^2 \log g(T(X))^2] = E_{\nu}[\tilde{g}^2 \log \tilde{g}^2].
\]

Furthermore, we have \( \nabla \tilde{g}(x) = \nabla T(x) \nabla g(T(x)) \). Since \( T \) is \( L \)-Lipschitz, \( \|\nabla T(x)\| \leq L \). Then

\[
\|\nabla \tilde{g}(x)\| \leq \|\nabla T(x)\| \|\nabla g(T(x))\| \leq L \|\nabla g(T(x))\|.
\]

This implies

\[
E_{\tilde{\nu}}[\|\nabla g\|^2] = E_{X \sim \nu}[\|\nabla g(T(X))\|^2] \geq \frac{E_{\nu}[\|\nabla \tilde{g}\|^2]}{L^2}.
\]

Therefore,

\[
\frac{E_{\tilde{\nu}}[\|\nabla g\|^2]}{E_{\tilde{\nu}}[g^2 \log g^2] - E_{\nu}[\tilde{g}^2] \log E_{\nu}[\tilde{g}^2]} \geq \frac{1}{L^2} \frac{E_{\nu}[\|\nabla \tilde{g}\|^2]}{E_{\nu}[\tilde{g}^2] \log E_{\nu}[\tilde{g}^2]} \geq \frac{\alpha}{2L^2}
\]

where the last inequality follows from the assumption that \( \nu \) satisfies LSI with constant \( \alpha \). This shows that \( \tilde{\nu} \) satisfies LSI with constant \( \alpha/L^2 \), as desired. \( \square \)

A.3.2 Proof of Lemma 17

Proof of Lemma 17. We recall the following convolution property of LSI [15]: If \( \nu, \tilde{\nu} \) satisfy LSI with constants \( \alpha, \tilde{\alpha} > 0 \), respectively, then \( \nu \ast \tilde{\nu} \) satisfies LSI with constant \( \left( \frac{1}{\alpha} + \frac{1}{\tilde{\alpha}} \right)^{-1} \). Since \( \mathcal{N}(0, 2tI) \) satisfies LSI with constant \( \frac{1}{27t} \), the claim follows. \( \square \)

A.3.3 Proof of Lemma 19

Proof of Lemma 19. Let \( g : \mathbb{R}^n \to \mathbb{R} \) be a smooth function, and let \( \tilde{g} : \mathbb{R}^n \to \mathbb{R} \) be the function \( \tilde{g}(x) = g(T(x)) \). Let \( X \sim \nu \), so \( T(X) \sim \tilde{\nu} \). Note that

\[
\text{Var}_{\tilde{\nu}}(g) = \text{Var}_{X \sim \nu}(g(T(X))) = \text{Var}_\nu(\tilde{g}).
\]

Furthermore, we have \( \nabla \tilde{g}(x) = \nabla T(x) \nabla g(T(x)) \). Since \( T \) is \( L \)-Lipschitz, \( \|\nabla T(x)\| \leq L \). Then

\[
\|\nabla \tilde{g}(x)\| \leq \|\nabla T(x)\| \|\nabla g(T(x))\| \leq L \|\nabla g(T(x))\|.
\]
This implies

\[ E_{\tilde{\nu}}[\|\nabla g\|^2] = E_{X \sim \nu}[\|\nabla g(T(X))\|^2] \geq \frac{E_{\nu}[\|\nabla g\|^2]}{L^2}. \]

Therefore,

\[ \frac{E_{\nu}[\|\nabla g\|^2]}{\text{Var}_{\nu}(g)} \geq \frac{1}{L^2} \frac{E_{\nu}[\|\nabla g\|^2]}{\text{Var}_{\nu}(\tilde{g})} \geq \frac{\alpha}{L^2} \]

where the last inequality follows from the assumption that \( \nu \) satisfies Poincaré inequality with constant \( \alpha \). This shows that \( \tilde{\nu} \) satisfies Poincaré inequality with constant \( \alpha/L^2 \), as desired.

\[ \square \]

A.3.4 Proof of Lemma 20

Proof of Lemma 20. We recall the following convolution property of Poincaré inequality [23]: If \( \nu, \tilde{\nu} \) satisfy Poincaré inequality with constants \( \alpha, \tilde{\alpha} > 0 \), respectively, then \( \nu * \tilde{\nu} \) satisfies Poincaré inequality with constant \( (\frac{1}{\alpha} + \frac{1}{\tilde{\alpha}})^{-1} \). Since \( \mathcal{N}(0, 2tI) \) satisfies Poincaré inequality with constant \( \frac{1}{2t} \), the claim follows.

\[ \square \]