Sampling via Nonlinear Diffusion Equations

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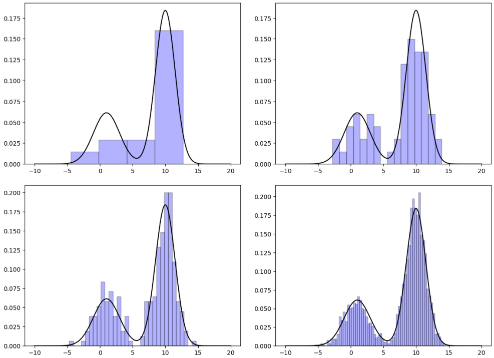
Motivation

Setup: Let $\tilde{\rho}$ be a probability measure on Euclidean space $\mathbb{R}^d$.

Goal: We seek $\{x_i\}_{i=1}^n \subset \mathbb{R}^d$ such that the empirical measure $\frac{1}{n}\sum_{i=1}^n \delta_{x_i}$ converges to $\tilde{\rho}$ as $n \to \infty$.

- Our definition of “convergence" depends on the context of the problem. For example, we may define convergence in terms of the 2-Wasserstein metric.



Classical Approach: Langevin Dynamics

Assumption: The target measure $\tilde{\rho}$ is strongly log-concave, i.e. $\tilde{\rho}(x) = e^{-V(x)}$ for a λ-convex function $V : \mathbb{R}^d \to \mathbb{R}$, $\lambda > 0$.

For any initialization $\{x_{i,0}\}_{i=1}^n$, evolving particles by the stochastic differential equation

$$\begin{cases} dx_i(t) = \nabla \log(\tilde{\rho}(x_i))dt + dW_i \\ x_i(0) = x_{i,0}. \end{cases}$$

ensures that $\lim_{t\to\infty} \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i(t)} = \tilde{\rho}$.

Remark (Continuum Perspective)

At time t, the particles approximate $\rho(t,x)$, the solution to the **Fokker-Planck equation**:

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \nabla \log(\tilde{\rho})) = \Delta \rho \quad t \geq 0 \\ \rho(0,x) = \rho_0(x). \end{cases}$$

$\rho(t,x)$ converges to $\tilde{\rho}$ as $t \to \infty$.

The Nonlinear Diffusion Equation

A drawback of Langevin dynamics is that the target measure $\tilde{\rho}$ must be strongly log-concave, i.e. $\tilde{\rho} = e^{-V(x)}dx$ for a λ-convex function V.

A new approach allows us to consider target measures of the form

$$\tilde{\rho}(x) = ((f')^{-1}(Z - V(x)))_+,$$

where

- Z is a normalizing constant.
- $V : \mathbb{R}^d \to \mathbb{R}$ and $f : [0, \infty) \to \mathbb{R}$ are smooth.
- V is λ-convex for some $\lambda > 0$.
- f is convex and $s \mapsto s^d f(s^{-d})$ is convex and nonincreasing on $(0, \infty)$.

Key idea: If $\rho(t, x)$ is a solution to the **Generalized Fokker-Planck equation**:

$$\begin{cases} \partial_t \rho - \nabla \cdot (\rho \nabla V) = \nabla \cdot (\rho \nabla f'(\rho)) & t \geq 0 \\ \rho(0, x) = \rho_0(x), \end{cases}$$

then $\rho(t, x)$ still converges to $\tilde{\rho}$ as $t \to \infty$.

My Project

Develop a particle method to approximate $\rho(t, x)$, the solution to the Generalized Fokker-Planck equation.

Example: Consider the function

$$f(s) = \begin{cases} s\ln(s) - s & m = 1 \\ \frac{s^m}{m-1} & m \neq 1 \end{cases}$$

and the external potential $V(x) = \frac{x^2}{2(m+1)}$.

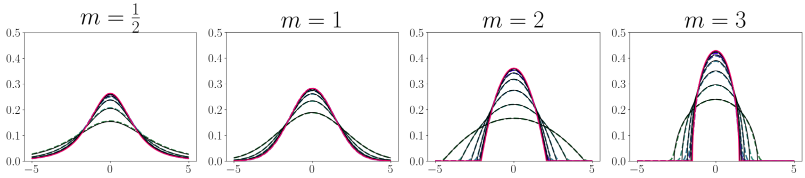


Figure: Numerical solutions are plotted with dashed lines, exact solutions are plotted with solid lines. Solutions are plotted in increments of one unit of time, up until $t_{max} = 6$.

References

- Craig, Katy, Karthik Elamvazhuthi, Matt Haberland, and Olga Turanova. “A blob method for inhomogeneous diffusion with applications to multi-agent control and sampling.” Mathematics of Computation (2023).
- Craig, Katy, Matt Jacobs, and Olga Turanova. “A blob method for general nonlinear diffusion.” In preparation.
- Jin, Shi, Lei Li, and Jian-Guo Liu. “Random batch methods (RBM) for interacting particle systems.” Journal of Computational Physics (2020).

Approximation of the Generalized Fokker-Planck Equation

Consider the function

$$f_\varepsilon(s) = \begin{cases} \frac{\delta(\varepsilon)}{2}|s|^2 + {}^{\delta(\varepsilon)}f(s) - {}^{\delta(\varepsilon)}f(0) & s \geq 0 \\ +\infty & s < 0, \end{cases}$$

where ${}^{\varepsilon}f$ is the Moreau-Yosida regularization of f and $\delta(\varepsilon) \to 0$ as $\varepsilon \to 0$.

Let φ_ε be a mollifier.

We approximate the Generalized Fokker-Planck equation via

$$\begin{cases} \partial_t \rho_\varepsilon = \nabla \cdot (\rho_\varepsilon \nabla (p_\varepsilon + V)) \\ p_\varepsilon = f'_\varepsilon(\varphi_\varepsilon * \rho_\varepsilon) \\ \rho_\varepsilon(0, x) = \rho^0_\varepsilon(x). \end{cases} \qquad (\text{PDE}_\varepsilon)$$

From PDE to ODE

Suppose that $\rho^0_\varepsilon(x) = \sum_{i=1}^{n} m_i \delta_{x_i^0}(x)$. Then, there exists a unique solution of PDE$_\varepsilon$ of the form $\rho_\varepsilon(t,x) = \sum_{i=1}^{n} m_i \delta_{x_i(t)}(x)$, where

$$\begin{cases} \dot{x}_j(t) = -\nabla p_\varepsilon(x_j(t)) - \nabla V(x_j(t)) \\ x_j(0) = x_j^0. \end{cases}$$

Elementary calculations show that the trajectory of the jth particle at time t is given by

$$\begin{cases} \dot{x}_j(t) = -f''_\varepsilon \left(\sum_{i=1}^{n} m_i \varphi_\varepsilon(x_j(t) - x_i(t)) \right) \sum_{i=1}^{n} m_i \nabla \varphi_\varepsilon(x_j(t) - x_i(t)) - \nabla V(x_j(t)) \\ x_j(0) = x_j^0. \end{cases}$$