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The Variational Formulation of the Fokker–Planck Equation A Summary

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Research Report

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Abstract

The Fokker–Planck equation, or forward Kolmogorov equation, describes the evolution of the probability density for a stochastic process associated with an Ito stochastic differential equation. It pertains to a wide variety of time–dependent systems in which randomness plays a role. In this paper, we are concerned with Fokker–Planck equations for which the drift term is given by the gradient of a potential. For a broad class of potentials, we construct a time–discrete, iterative variational scheme whose solutions converge to the solution of the Fokker–Planck equation. The major novelty of this iterative scheme is that the time step is governed by the Wasserstein metric on probability measures. This formulation enables us to reveal an appealing, and previously unexplored, relationship between the Fokker–Planck equation and the associated free energy functional. Namely, we demonstrate that the dynamics may be regarded as a gradient flux, or a steepest descent, for the free energy with respect to the Wasserstein metric.

Keywords: Fokker–Planck equation, steepest descent, free energy, Wasserstein metric.

1 Introduction and overview

The Fokker–Planck equation plays a central role in statistical physics and in the study of fluctuations in physical and biological systems [7, 17, 18]. It is intimately connected with the theory of stochastic differential equations: A (normalized) solution to a given Fokker–Planck equation represents the probability density for the position (or velocity) of a particle whose motion is described by a corresponding Ito stochastic differential equation (or Langevin equation). We shall restrict our attention in this paper to the case where the drift coefficient is a gradient. The simplest relevant physical setting is that of a particle undergoing diffusion in a potential field [18].

It is known that, under certain conditions on the drift and diffusion coefficients, the stationary solution of a Fokker–Planck equation of the type that we consider here satisfies a variational principle. It minimizes a certain convex free energy functional over an appropriate admissible class of probability densities [12]. This free energy functional satisfies an H–theorem: It decreases in time for any solution of the Fokker-Planck equation [17]. In this work, we shall establish a deeper, and apparently previously unexplored, connection between the free energy functional and the Fokker–Planck dynamics. Specifically, we shall demonstrate that the solution of the Fokker–Planck equation follows, at each instant in time, the direction of steepest descent of the associated free energy functional.

The notion of a steepest descent, or a gradient flux, makes sense only in context with an appropriate metric. We shall show that the required metric in the case of the Fokker–Planck equation is the Wasserstein metric (defined in Section 3) on probability densities. As far as we know, the

Wasserstein metric cannot be written as an induced metric for a metric tensor (the space of probability measures is not a Riemannian manifold). Thus, in order to give meaning to the assertion that the Fokker–Planck equation may be regarded as a steepest descent, or gradient flux, of the free energy functional with respect to this metric, we switch to a discrete time formulation. We develop a discrete, iterative variational scheme whose solutions converge, in a sense to be made precise below, to the solution of the Fokker-Planck equation. The time-step in this iterative scheme is associated with the Wasserstein metric. For a different view on the use of implicit schemes for measures, see [6, 14].

For the purpose of comparison, let us consider the classical diffusion (or heat) equation

$$\frac{\partial \rho(t,x)}{\partial t} = \Delta \rho(t,x)\,, \quad t \in (0,\infty)\,, \quad x \in I\!R^n\,,$$

which is the Fokker–Planck equation associated with a standard n–dimensional Brownian motion. It is well–known (see, for example, [5, 19]) that this equation is the gradient flux of the Dirichlet integral $\frac{1}{2}\int_{I\!R^n} |\nabla \rho|^2\, dx$ with respect to the $L^2(I\!R^n)$ metric. The classical discretization is given by the scheme

$$\left.\begin{array}{l} \text{Determine } \rho^{(k)} \text{ that minimizes} \\ \frac{1}{2}\,\|\rho^{k-1} - \rho\|^2_{L^2(I\!R^n)} \;+\; \frac{h}{2}\int_{I\!R^n} |\nabla \rho|^2\, dx\,, \end{array}\right\}$$

over an appropriate class of densities ρ. Here, h is the time step size. On the other hand, we derive as a special case of our results below that the scheme

$$\left.\begin{array}{l} \text{Determine } \rho^{(k)} \text{ that minimizes} \\ \frac{1}{2}\, d(\rho^{k-1}, \rho)^2 \;+\; h\int_{I\!R^n} \rho \log \rho\, dx \\ \text{over all } \rho \in K\,, \end{array}\right\} \tag{1}$$

where K is the set of all probability densities on $I\!R^n$ having finite second moments, is also a discretization of the diffusion equation when d is the Wasserstein metric. In particular, this allows us to regard the diffusion equation as a steepest descent of the functional $\int_{I\!R^n} \rho \log \rho\, dx$ with respect to the Wasserstein metric. This reveals a novel link between the diffusion equation and the Gibbs–Boltzmann entropy ($-\int_{I\!R^n} \rho \log \rho\, dx$) of the density ρ. Furthermore, this formulation allows us to attach a precise interpretation to the conventional notion that diffusion arises from the tendency of the system to maximize entropy.

The connection between the Wasserstein metric and dynamical problems involving dissipation or diffusion (such as strongly overdamped fluid flow or nonlinear diffusion equations) seems to have first been recognized by Otto in [15]. The results in [15] together with our recent research on variational principles of entropy and free energy type for measures [12, 11], provide the

impetus for the present investigation. The work in [12] was motivated by the desire to model and characterize metastability and hysteresis in physical systems. We plan to explore in subsequent research the relevance of the developments in the present paper to the study of such phenomena.

2 The Fokker–Planck equation, stationary solutions, and the free energy functional

We are concerned with Fokker-Planck equations having the form

$$\frac{\partial \rho}{\partial t} = \;\mathrm{div}\,(\nabla \Psi(x)\rho) + \beta^{-1}\Delta \rho\,, \quad \rho(x,0) = \rho^0(x), \tag{2}$$

where the potential $\Psi(x) : I\!R^n \to [0,\infty)$ is a smooth function, $\beta > 0$ is a given constant, and $\rho^0(x)$ is a probability density on $I\!R^n$. The solution $\rho(t,x)$ of (2) must, therefore, be a probability density on $I\!R^n$ for almost every fixed time t. That is, $\rho(t,x) \geq 0$ for almost every $(t,x) \in (0,\infty) \times I\!R^n$, and $\int_{I\!R^n} \rho(t,x)\, dx = 1$ for almost every $t \in (0,\infty)$.

It is well known that the Fokker-Planck equation (2) is inherently related to the Ito stochastic differential equation [4, 7, 17, 18]

$$dX(t) = -\nabla \Psi(X(t))dt + \sqrt{2\beta^{-1}}\, dW(t)\,, \quad X(0) = X^0\,. \tag{3}$$

Here, $W(t)$ is a standard n–dimensional Wiener process, and X^0 is an n–dimensional random vector with probability density ρ^0. Equation (3) is a model for the motion of a particle undergoing diffusion in the potential field Ψ. $X(t) \in I\!R^n$ then represents the position of the particle, and the positive parameter β is proportional to the inverse temperature. The solution $\rho(t,x)$ of the Fokker-Planck equation (2) furnishes the probability density at time t for finding the particle at position x.

If the potential Ψ satisfies appropriate growth conditions, then there is a unique stationary solution $\rho_s(x)$ of the Fokker–Planck equation, and it takes the form of the Gibbs distribution [7, 17]

$$\rho_s(x) = Z^{-1} \exp(-\beta \Psi(x)), \tag{4}$$

where the partition function Z is given by the expression

$$Z = \int_{I\!R^n} \exp(-\beta \Psi(x))\, dx.$$

Note that, in order for equation (4) to make sense, Ψ must grow rapidly enough to ensure that Z is finite. The probability measure $\rho_s(x)\, dx$, when it exists, is the unique invariant measure for the Markov process $X(t)$ defined by the stochastic differential equation (3).

It is readily verified (see, for example, [12]) that the Gibbs distribution ρ_s satisfies a variational principle – it minimizes over all probability densities on $\mathbb{R}^n$ the free energy functional

$$F(\rho) = E(\rho) + \beta^{-1} S(\rho), \tag{5}$$

where

$$E(\rho) := \int_{\mathbb{R}^n} \Psi \rho \, dx \tag{6}$$

plays the role of an energy functional, and

$$S(\rho) := \int_{\mathbb{R}^n} \rho \log \rho \, dx \tag{7}$$

is the negative of Gibbs-Boltzmann entropy functional.

Even when the Gibbs measure is not defined, the free energy (5) of a density $\rho(t,x)$ satisfying the Fokker–Planck equation (2) may be defined, provided that $F(\rho^0)$ is finite. This free energy functional then serves as a Lyapunov function for the Fokker-Planck equation: If $\rho(t,x)$ satisfies (2), then $F(\rho(t,x))$ can only decrease with time [17]. Thus, the free energy functional is an H–function for the dynamics. The developments that follow will enable us to regard the Fokker-Planck dynamics as a gradient flux, or a steepest descent, of the free energy with respect to a particular metric on an appropriate class of probability measures. The requisite metric is the Wasserstein metric on the set of probability measures having finite second moments.

3 The Wasserstein metric

The Wasserstein distance, $d(\mu_1, \mu_2)$, between two (Borel) probability measures μ_1 and μ_2 on $\mathbb{R}^n$ is defined by the formula

$$d(\mu_1, \mu_2)^2 = \inf_{p \in \mathcal{P}(\mu_1, \mu_2)} \int_{\mathbb{R}^n \times \mathbb{R}^n} |x - y|^2 \, p(dxdy), \tag{8}$$

where $\mathcal{P}(\mu_1, \mu_2)$ is the set of all probability measures on $\mathbb{R}^n \times \mathbb{R}^n$ with first marginal μ_1 and second marginal μ_2, and the symbol $|\cdot|$ denotes the usual Euclidean norm on $\mathbb{R}^n$. More precisely, a probability measure p is in $\mathcal{P}(\mu_1, \mu_2)$ if and only if for each Borel subset $A \subset \mathbb{R}^n$ there holds

$$p(A \times \mathbb{R}^n) = \mu_1(A) \ , \ \ p(\mathbb{R}^n \times A) = \mu_2(A).$$

It is well known that d defines a metric on the set of probability measures μ on R^n having finite second moments: $\int_{R^n} |x|^2 \mu(dx) < \infty$ [10, 16]. We note that the Wasserstein metric may be equivalently defined by [16]

$$d(\mu_1, \mu_2)^2 = \inf \mathbf{E}|X - Y|^2 \, , \tag{9}$$

where $\mathbf{E}(U)$ denotes the expectation of the random variable U, and the infimum is taken over all random variables X and Y such that X has distribution μ_1 and Y has distribution μ_2. Since

$$\mathbf{E}|X - Y|^2 = \mathbf{E}|X|^2 + \mathbf{E}|Y|^2 - 2\mathbf{E}(X \cdot Y) \, ,$$

and since $\mathbf{E}(|X|^2)$ and $\mathbf{E}(|Y|^2)$ are fixed, we see that the infimum in (9) is attained when the correlation of the random variables X and Y is maximal. The Wasserstein metric defines a weak topology on probability measures.

The variational problem (8) is an example of a Monge–Kantorovich mass transference problem with the particular cost function $c(x,y) = |x-y|^2$ [16]. In that context, an infimizer $p^* \in \mathcal{P}(\mu_1, \mu_2)$ is referred to as an optimal transference plan. When μ_1 and μ_2 have finite second moments, the existence of such a p^* for (8) is readily verified. For a probabilistic proof that the infimum in (8) is attained under such conditions, see [10]. Brenier [2] has established the existence of a *one–to–one* optimal transference plan in the case that the measures μ_1 and μ_2 have bounded support and are absolutely continuous with respect to Lebesgue measure. Caffarelli [3] and Gangbo and McCann [8, 9] have recently extended Brenier's results to more general cost functions c and to cases in which the measures do not have bounded support.

If the measures μ_1 and μ_2 are absolutely continuous with respect to the Lebesgue measure, with densities ρ_1 and ρ_2, respectively, we will write $\mathcal{P}(\rho_1, \rho_2)$ for the set of probability measures having first marginal μ_1 and second marginal μ_2. Correspondingly, we will denote by $d(\rho_1, \rho_2)$ the Wasserstein distance between μ_1 and μ_2. This is the situation that we will be concerned with in the sequel.

4 The discrete scheme

We shall now construct a time–discrete scheme that is designed to converge in an appropriate sense (to be made precise below) to a solution of the Fokker-Planck equation. The scheme that we shall describe was motivated by a similar scheme developed by Otto in an investigation of pattern formation in magnetic fluids [15]. We shall make the following assumptions concerning the potential Ψ introduced in Section (2):

$$\Psi \in C^\infty(\mathbb{R}^n);$$

$$\Psi(x) \ \geq \ 0 \ \text{ for all } x \in \mathbb{R}^n \, ; \tag{10}$$

$$|\nabla \Psi(x)| \ \leq \ C\,(\Psi(x) + 1) \ \text{ for all } x \in \mathbb{R}^n \, , \tag{11}$$

for some constant $C < \infty$. Notice that our assumptions on Ψ allow for cases in which $\int_{R^n} \exp(-\beta\Psi) \, dx$ is not defined, so that the stationary density ρ_s given by (4) does not exist. These assumptions allow us to treat a wide

class of Fokker–Planck equations. In particular, the classical diffusion equation $\frac{\partial \rho}{\partial t} = \beta^{-1}\Delta\rho$, for which $\Psi \equiv$ const., falls into this category. We also introduce the set K of admissible probability densities:

$$K := \left\{ \rho : \mathbb{R}^n \to [0,\infty) \text{ measurable} \,\middle|\, \int_{R^n} \rho(x)\,dx = 1\,, M(\rho) < \infty \right\},$$

where

$$M(\rho) = \int_{R^n} |x|^2\,\rho(x)\,dx\,.$$

With these conventions in hand, we now formulate the iterative discrete scheme:

$$\left.\begin{array}{l} \text{Determine } \rho^{(k)} \text{ that minimizes} \\ \frac{1}{2}\,d(\rho^{(k-1)},\rho)^2 \;+\; h\,F(\rho) \\ \text{over all } \rho \in K\,. \end{array}\right\} \tag{12}$$

Here we use the notation $\rho^{(0)} = \rho^0$. The scheme (12) is the obvious generalization of the scheme (1) set forth in the Introduction for the diffusion equation. We have established existence and uniqueness of solutions to this iterative scheme. We refer the reader to [13] for the proof of the ensuing Proposition.

PROPOSITION (EXISTENCE AND UNIQUENESS OF SOLUTIONS TO THE SCHEME) *Given $\rho^0 \in K$, there exists a unique solution of the scheme (12).*

We now state our main result. We can demonstrate that an appropriate interpolation of the solution to the scheme (12) converges to the unique solution of the Fokker-Planck equation. Specifically, the convergence result that we have established is:

THEOREM (CONVERGENCE TO THE SOLUTION OF THE FOKKER–PLANCK EQUATION). *Let $\rho^0 \in K$ satisfy $F(\rho^0) < \infty$, and for given $h > 0$, let $\{\rho_h^{(k)}\}_{k\in N}$ be the solution of (12). Define the interpolation $\rho_h : (0,\infty)\times\mathbb{R}^n \to [0,\infty)$ by*

$$\rho_h(t) \;=\; \rho_h^{(k)} \quad \textit{for } t \in [k\,h,(k+1)\,h) \textit{ and } k \in \mathbb{N}\cup\{0\}$$

Then as $h \downarrow 0$,

$$\rho_h(t) \;\rightharpoonup\; \rho(t) \quad \textit{weakly in } L^1(\mathbb{R}^n) \quad \textit{for all } t \in (0,\infty)\,, \tag{13}$$

where $\rho \in C^\infty((0,\infty)\times\mathbb{R}^n)$ is the unique solution of

$$\frac{\partial \rho}{\partial t} = \operatorname{div}(\rho\nabla\Psi) + \beta^{-1}\Delta\rho\,, \tag{14}$$

with initial condition

$$\rho(t) \;\rightharpoonup\; \rho^0 \quad \textit{strongly in } L^1(\mathbb{R}^n) \quad \textit{for} \quad t \downarrow 0 \tag{15}$$

and

$$M(\rho),\, E(\rho) \;\in\; L^\infty((0,T)) \quad \textit{for all } T < \infty\,. \tag{16}$$

REMARKS.

1. A finer analysis reveals that

$$\rho_h \;\to\; \rho \quad \textit{strongly in } L^1((0,T)\times\mathbb{R}^n) \quad \textit{for all } T < \infty\,.$$

2. With minor modifications to the scheme (12), we can establish an analogous convergence theorem for Fokker–Planck equations with time dependent diffusion coefficient (i.e., for $\beta = \beta(t)$).

We refer the reader once again to the article [13] for a detailed proof of this Theorem.

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