P358 Project Fokker-Planck

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1 Background

Before the emergence of quantum mechanics and chaos theory, physics up until the nineteenth century mostly consisted of the modelling of natural phenomena by deterministic solutions of differential equations. During that time period it was commonly believed that if one knew all of the initial conditions of a system, one would be able to predict the future with certainty. Quantum mechanics and chaos theory prompted a statistical interpretation of physics due to the probabilistic measurement process in quantum mechanics, the unpredictable behaviors of simple differential equations in chaos theory and Brownian motion.

In 1827, a botanist named Robert Brown investigated the motion of small pollen grains suspended in water. The pollen grains seemed to have an extremely random and irregular state of motion and was called *Brownian motion*. In 1905, Einstein published an article titled *Concerning the motion, as required by the molecular-kinetic theory of heat, of particles suspended in liquids at rest*. Simultaneously an identical explanation was developed by Smoluchowski in 1906. Smoluchowski was responsible for the later systematic development of the theory which is why the Fokker-Planck equation is sometimes called the Smoluchowski equation, especially when applied to particle position distributions. Additionally, the equation is referred to as the Kolmogorov equations in probability theory. In 1931, Andrei Kolmogorov sought to derive a theory of continuous Markov processes by extending discrete Markov processes.

The Fokker-Planck equation is a partial differential equation that describes the time evolution of the probability density function under the influence of arbitrary potentials and stochastic forces. This allows for the equation to be used in various fields outside of physics. For example, in mathematical finance the Fokker-Planck equation is used to inversely find the local volatility of an option. The local volatility is the equivalent of the diffusion coefficient D, see below. The Fokker-Planck equation can also be applied to evolutionary dynamics, or the study of the mathematical principles according to which biological organisms as well as cultural ideas evolve.

2 Motivation

Before we begin to motivate the Fokker-Planck equation let us write it in one dimension:

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\frac{\partial}{\partial x}(-F(x)W(x,t)) + D\frac{\partial^2 W}{\partial x^2}. \tag{1}$$

Here, W is a time dependent probability distribution, k is the Boltzmann constant, T is the temperature, $F(x)$ is the force acting on the particle distribution, and D is the diffusion coefficient. For our purposes D is viewed as constant, but D can also depend on both position and time. The first term relates the change in the probability distribution, W, to an external force, F. The second term incorporates the diffusion due to surrounding particles.

The canonical example of this equation is Brownian motion. Brownian motion is the random motion of a particle suspended within a fluid. The motion is due to the impulses caused by collision with fast moving particles within the medium. It is not feasible to model the motion exactly due to the large number

of collisions. Instead, the motion can be modeled using stochastic variables. Classical Brownian motion is modeled according to:

$$\frac{\partial W(x,t)}{\partial t} = D\frac{\partial^2 W}{\partial x^2}. \tag{2}$$

This is just Equation 1 without external forces, and with a constant diffusion coefficient D. The constant diffusion is due to the homogeneity of the surrounding medium. Einstein's derivation of the above equation will be discussed in the Theory section and was important in the development of the Fokker-Planck equation and other stochastic methods. However, this simple example shows the power of the Fokker-Planck equation to allow us to create models for processes that involve a large number of particles.

Now lets try to build an equation to model the movement of a set of dust particles with non-negligible mass suspended in air with motion restricted to a vertical line. We can no longer say that there are no external forces on our particles. Let our force be:

$$F(x) = -mg + qE(x) \tag{3}$$

where m is the mass of the dust particle, g is the acceleration due to gravity, q is the charge on a single dust particle, and $E(x)$ is an electric field dependent on the vertical position of our particle. Let the diffusion of our particles in air be some constant, D_0. We can now model the movement of the distribution of dust particles using the Fokker-Planck equation as:

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\frac{\partial}{\partial x}((mg - qE(x))W(x,t)) + D\frac{\partial^2 W}{\partial x^2}. \tag{4}$$

We know that in the limit of a large neutral particle that the solution to this must be $W(x,t) = \delta(x - x(t))$, where $x(t)$ is the one-dimensional equation of motion for a single particle.

Overall, our motivation to study the Fokker-Planck equation comes from the desire to model distributions of particles that are subject to both external forces and diffusion. The most well known example of this is Brownian motion.

3 Theory

We will motivate the Fokker-Planck equation by echoing the derivation by Albert Einstein. We will start with a physical example, specifically the motion of small particles on the surface of water. An important assumption made in Einstein's approach is that the observed motion of the particles is caused by the interaction between the water molecules and the particles resting on the surface. The collisions between the observed particles and the water molecules are assumed to be very frequent and alters the trajectory of the particle based on some probability distribution ϕ. Moreover, the trajectory of one particle is independent of the trajectories of other particles. Also, the trajectories of the same particle over different time intervals are independent of each other.

For simplicity we will consider the particles in one dimension. Assume the system has a total of N particles in the system and a small time step τ. The position of the of the particles will change by a small step size of Δ according to our model. Note that the step size Δ can have different values for each particle and can be either positive or negative. We will assume the number of particles that experience these spatial shifts over the time interval τ is governed by the probability distribution ϕ. Note that over the time interval τ the spatial shift goes from Δ to $\Delta + d\Delta$. Thus, $N\phi(\Delta)d\Delta$ is the number of particles that experience the spatial shift. We assume that ϕ is normalized $\int_{-\infty}^{\infty}\phi(\Delta)d\Delta = 1$. We also assume that there is an equal likelihood of a particles taking a positive Δ displacement and a negative Δ displacement, implying that ϕ is even, $\phi(-\Delta) = \phi(\Delta)$.

We will define the function $W(x,t)$ to be the number of particles per unit volume. We can determine how the number of particles per unit volume change over the time interval τ according to our physical assumptions. For simplicity, we will consider the change in volume in a single spatial dimension x,

$$W(x, t+\tau) = \int_{-\infty}^{\infty} \phi(\Delta) W(x+\Delta, t) d\Delta. \tag{5}$$

We can expand the left hand side of the above equation about the variable τ since it is a small value we have;

$$W(x, t+\tau) = W(x,t) + \tau \frac{\partial W}{\partial t} + \mathcal{O}(\tau^2). \tag{6}$$

We can also taylor expand the right hand side of the equation about the variable of Δ since it is also assumed to be a small value;

$$W(x+\Delta, t) = W(x,t) + \Delta \frac{\partial W}{\partial x} + \frac{\Delta^2}{2} \frac{\partial^2 W}{\partial x^2} + \mathcal{O}(\Delta^3). \tag{7}$$

Using the results from equations 5, 6, and 7, we arrive at the following result;

$$\begin{aligned} W(x,t) + \tau \frac{\partial W}{\partial t} =& \int_{-\infty}^{\infty} W(x,t) + \Delta \frac{\partial W}{\partial x} + \frac{\Delta^2}{2} \frac{\partial^2 W}{\partial x^2} \phi(\Delta) d\Delta \\ =& W \int_{-\infty}^{\infty} \phi(\Delta) d\Delta + \frac{\partial W}{\partial x} \int_{-\infty}^{\infty} \Delta \phi(\Delta) d\Delta + \frac{\partial^2 W}{\partial x^2} \int_{-\infty}^{\infty} \frac{\Delta^2}{2} \phi(\Delta) d\Delta. \end{aligned} \tag{8}$$

Note that we move the partial derivatives outside of the integral since they are not dependent on the small displacement Δ. Recall that we have constrained the distribution ϕ, such that it is an even function and is normalized. Based on these constraints, it follows that the second term of equation 8 will be zero, since it is an odd integrand over symmetric bounds. The result from this cancellation is the following expression;

$$\frac{\partial W}{\partial t} = \frac{\partial^2 W}{\partial x^2} \frac{1}{\tau} \int_{-\infty}^{\infty} \frac{\Delta^2}{2} \phi(\Delta) d\Delta = D \frac{\partial^2 W}{\partial x^2}. \tag{9}$$

We have arrived at the Diffusion equation, where $D = \frac{1}{\tau} \int_{-\infty}^{\infty} \frac{\Delta^2}{2} \phi(\Delta) d\Delta$. This is the Fokker-Planck equation (see section 1) in the simplest ensemble, i.e. with no drift present in the particles. We will physically motivate the so-called drift term of the Fokker-Planck equation. Consider a constant time-independent potential well U acting on the ensemble of particles. Clearly we can assume that there will also be a force F present on each of the particles due to this potential well. Now the small displacements Δ for each particle will be driven by both this potential well and the probabilistic interactions. We can describe the drift on the particles via the force at each position $F(x)W(x,t)$. The change in the distribution of particles at each time interval τ will be a balancing match between the statistical diffusion process and the presence of the potential well. Note the drift term used is divided by kT since this is a measure of the average kinetic energy of the particles, where k is the Boltzmann constant and T is the temperature of the system. In short, this argument is saying that the potential well of the system will have more influence on the trajectory of the particle if the system is at a low temperature and less influence when the thermal bath is at a high temperature. Note that the temperature of the system is assumed to be constant in this case. Again recall that $W(x,t)$ is the number of particles per unit volume and at a small time step we want to see how this distribution is changing due to the drift in only the x-dimension over a small change in time. This physical argument gives us the following drift correction to the equation;

$$\text{Drift} = -\frac{1}{kT} \frac{\partial}{\partial x} \Big(F(x) W(x,t) \Big). \tag{10}$$

Note that this term is negative since these interactions from the potential well will 'resist' or 'counteract' the statistical diffusion term. Adding this term to the Diffusion equation we arrive at the one dimensional Fokker-Planck equation;

$$\frac{\partial W(x,t)}{\partial t} = -\frac{1}{kT} \frac{\partial}{\partial x} \Big(F(x) W(x,t) \Big) + D \frac{\partial^2 W}{\partial x^2}. \tag{11}$$

4 Methods

4.1 Explicit method for Fokker-Planck

We will initially consider an explicit numerical method for (1) with the force given by

$$F(x) = -\frac{\partial U}{\partial x}, \tag{12}$$

and potential given by

$$U(x) = a_0 kT(a_4 x^4 + a_3 x^3 + a_2 x^2 a_1 x), \tag{13}$$

with known constants a_n, and with boundary conditions

$$W(x = 0, t = 0) = W(x = 1, t = 0) = 0. \tag{14}$$

We will use finite-differencing with symmetric first spacial derivatives and forward time derivatives to discretize Equation 1. We apply the chain rule to Equation 1 and obtain

$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{kT}\left[-\frac{\partial F(x)}{\partial x}W(x,t) - \frac{\partial W(x,t)}{\partial x}F(x)\right] + D\frac{\partial^2 W}{\partial x^2}. \tag{15}$$

Using a central finite difference approximation, Equation 15 is simplified to be

$$\frac{W_{i,j+1} - W_{i,j}}{\Delta t} = \frac{1}{kT}\left[-\frac{F_{i+1,j} - F_{i-1,j}}{2\Delta x}W_{i,j} - \frac{W_{i+1,j} - W_{i-1,j}}{2\Delta x}F_{i,j}\right] + D\frac{W_{i+1,j} - 2W_{i,j} + W_{i-1,j}}{(\Delta x)^2}, \tag{16}$$

where there are time steps Δt and position steps Δx, with $W_{i,j}$ for $W(x_i, t_j)$ and with $F_{i,j}$ for $F(x_i, t_j)$ (given the potential supplied in Equation 13, we can calculate the partial derivative directly rather than use the finite differencing shown and decrease the truncation error).

From Equation 18, we obtain an explicit recurrence relation for the probability density function of a particle in a potential well,

$$W_{i,j+1} = W_{i,j} + \frac{\Delta t}{kT}\left[-\frac{F_{i+1,j} - F_{i-1,j}}{2\Delta x}W_{i,j} - \frac{W_{i+1,j} - W_{i-1,j}}{2\Delta x}F_{i,j}\right] + \Delta t D\frac{W_{i+1,j} - 2W_{i,j} + W_{i-1,j}}{(\Delta x)^2}. \tag{17}$$

Using the boundary conditions (14), and starting with a Gaussian distribution as an initial condition

$$W(x, t = 0) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu)^2}{2\sigma^2}},$$

(or some other initial distribution) we obtain a system of linear equations from (17) that we step through and solve directly. It should be noted that our truncation error is on the order $O(h^2)$ for the central difference approximation for the local position steps, but $O(h)$ for the forward difference approximation in the time steps.

In order to enforce the boundary conditions (14) we add ghost points on either side of our set of support points. For node centered support points we set $W^n_{-1} = 0$ and $W^n_{J+1} = 0$. For cell centered support points we set $W^n_{-1/2} = -W^n_{1/2}$ and $W^n_{J+1/2} = -W^n_{J-1/2}$.

4.1.1 Explicit Stability Conditions

4.2 Implicit method for Fokker-Planck

We next consider an implicit scheme in order to guarantee stability. For more than one dimension, we might consider an Alternating-Direction Implicit (ADI) method, however for a Fokker-Planck equation in

one dimension we simply apply finite differences fully implicitly,

$$\begin{aligned}\frac{W_{i,j+1}-W_{i,j-1}}{2\Delta t} =& \frac{1}{kT}\left[-\frac{F_{i+1,j}-F_{i-1,j}}{2\Delta x}W_{i,j+1} - \frac{W_{i+1,j+1}-W_{i-1,j+1}}{2\Delta x}F_{i,j}\right] \\ &+ D\frac{W_{i+1,j+1}-2W_{i,j+1}+W_{i-1,j+1}}{(\Delta x)^2}.\end{aligned} \tag{18}$$

Although the implicit is more expensive to compute, it guarantees stability. We plan to implement the method both by using the differencing shown for $F_{i,j}$ and by computing the derivatives directly (which the Chang & Cooper scheme stays away from in order to guarantee particle preservation)[1].

5 Projected Test Cases

In our exploration of the Fokker-Planck equation we will analyze potentials of which we can intuitively find our expected output. First, let us analyze a particle within a constant potential filed and within a medium with constant diffusion, $D = 1/2$. Additionally, let our initial condition be a δ centered at $x = 0$. It is easiest to work from our expectation at infinite time back to our initial condition. At infinite time we would no longer be able to say much about the position of our particle because the only motion in it would have been caused by diffusion. Therefore, we would expect a uniform distribution distribution across all space. To analyze times in between zero and infinity lets notice that this system is governed by Equation 2. The known solution to this is:

$$W(x,t) = \frac{1}{\sqrt{2\pi t}}e^{-x^2/2t}. \tag{19}$$

The above equation is a normal distribution that has a time dependent standard deviation.

Next, let us look at a system which can be solved using much simpler means. The system is a large particle in one dimensional free fall from a height h. Here we pick D to be some small constant and our potential is simply $U = mgx$, where x is the height above zero, g is the acceleration due to gravity and m is the mass of the particle. The initial condition is known to be $\delta(x - h)$. We know from kinematics that the particle will move according to: $x = (1/2)gt^2$. Therefore, we would expect our peak to evolve with time according to that equation.

Now let us look at a particle in a potential well centered about $x = \pi/2$ with width π with constant diffusion. From quantum mechanics we know the probability distribution of the location of the particle is:

$$W(x) = \frac{\sqrt{2}}{\pi}sin^2(nx). \tag{20}$$

We are not certain whether the distribution from Fokker-Planck at large time will approach the above probability distribution. The logic for why it would approach the above distribution is as follows: The solution above is not time dependent so the initial condition is irrelevant. Additionally, as time increases the initial condition of our solution will begin to matter less due to the diffusion term. Therefore, both solutions are essentially independent of the initial condition and solve the same set of boundary conditions so, they should be the same. In other words, the solution to the Poisson equation is the solution to the diffusion equation for time approaching infinity and time independent potential. Another possible solution that we are able to reason for the described conditions is a uniform distribution across the potential well. The uniform distribution would come from the diffusion obscuring our peak over time until the peak is equally likely to be everywhere within the well.

Another interesting potential would be to consider the Lennard-Jones interaction. This potential well describes the interaction between two different atoms or molecules, say atoms i and j. The parameters ϵ_{ij} and σ_{ij} are used to describe the strength of the interaction between the particles and the size of the particles, respectively. This interaction is described analytically below;

$$U_{\mathrm{LJ}} = 4\epsilon_{ij}\left\{\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right\}. \tag{21}$$

We could then pick the parameters ϵ_{ij} and σ_{ij} such that we could possibly simulate the interaction between simply gases, i.e. noble gases, or Methane gas since these molecules and be modeled as 'super-atoms'. Note that it is not clear what exactly the resulting probability distributions after a long will be since this potential well also depends on the variables ϵ_{ij} and σ_{ij}, which we have not determined yet.

A possible test case for all of the above potentials is that we could vary the temperature of the thermal path T. We would expect at higher temperatures for the diffusive process to drive the change of probability distribution. While, at lower temperatures we would that the drift term due to the potential well will drive the system. In other word we would expect very cold systems to rest inside the potential well and as the temperature increases the strength of this interaction decreases.

The above examples are not an exhaustive list of those we will analyze in our final project. We will build additional examples that show case properties of the Fokker-Planck equation or examples that can be verified analytically or logically.

6 Test Cases and Results

6.1 Explicit Method

We used the explicit method of described in section 4.1 to solve the Fokker-Planck equation for a potential well defined by the following fourth order polynomial.

$$U(x) = a_0 kT \left(a_4 x^4 + a_3 x^3 + a_2 x^2 + a_1 x\right) \tag{22}$$

We used the following numerical values for the constants; $a_0 = 300, a_1 = -0.38, a_2 = 1.37, a_3 = -2$, and $a_4 = 1$, which corresponds to the above graph.

If we have no diffusion, it follows that the equilibrium positions of this potential are at the minimums, i.e. where the force is zero ($-\frac{\partial U}{\partial x} = 0$). The global minimum of the potential is at ≈ 0.78. There is, however, a local minimum at the position ≈ 0.26, note that this will correspond to the system being meta-stable. Prior to using our explicit integration solver we know that the solution as $t \to \infty$ is the following expression,

$$W(t \to \infty) = Ae^{U(x)/D}, \tag{23}$$

where $U(x)$ is our potential as a function of only space, D is a constant diffusion, and A is a normalization constant.

References

[1] J.S Chang and G Cooper. A practical difference scheme for fokker-planck equations. *Journal of Computational Physics*, 6(1):1 – 16, 1970.

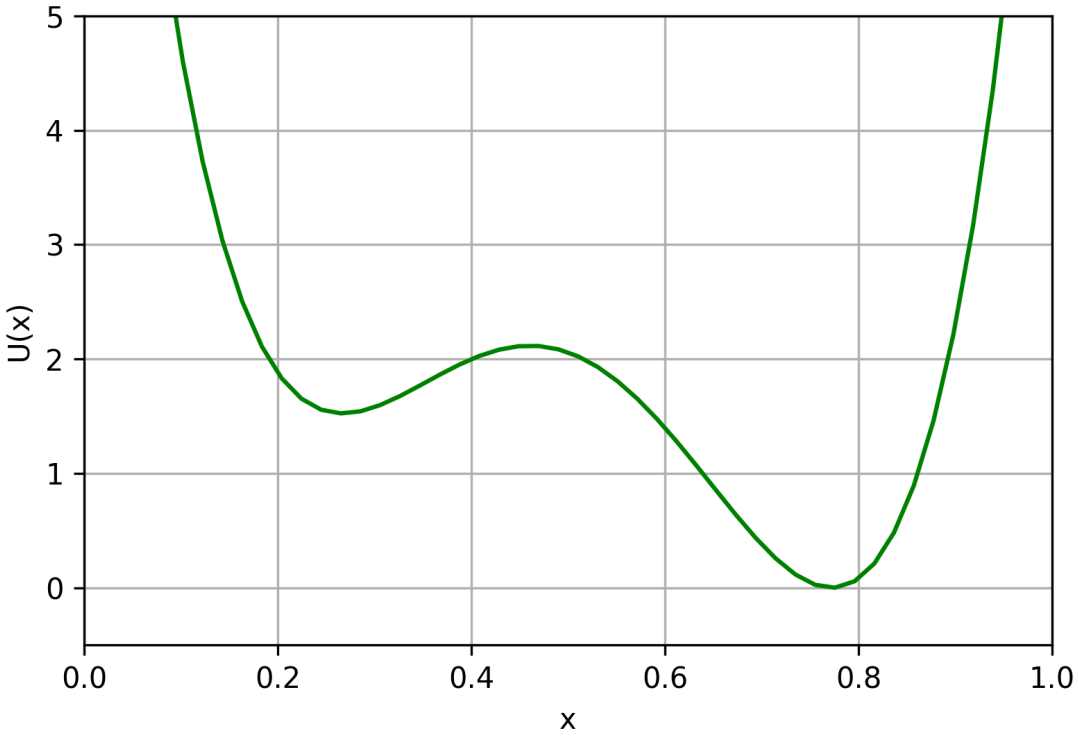

Figure 1: Potential Well