Forward Probability Equations

We shall now consider another approach to calculating probabilities for statistical dynamical systems, based on so-called forward probability equations.

Liouville equation for classical dynamical systems

Consider the classical ODE with random initial conditions

$$\frac{d}{dt}\tilde{X}(t) = f(\tilde{X},t)$$
$$\tilde{X}(t_0) = \tilde{x}_0$$

where $\tilde{x}_0$ is sampled from a probability distribution P_0 on $\mathbb{R}^d$ with density $\rho_0(x_0)$. This has solution denoted $\tilde{X}(t; x_0, t_0)$ or $\tilde{X}(t)$; if the initial value is implicit.

We shall now derive an equation of evolution for the probability density function. We start with the "fine-grained density"

$$\tilde{\rho}(x,t) = \delta^d(x - \tilde{X}(t)).$$

Then, by chain rule

$$\begin{aligned}
\partial_t \tilde{\rho}(x,t) &= \nabla_x \delta^d(x - \tilde{X}(t)) \cdot \left(-\frac{d}{dt}\tilde{X}(t)\right) \\
&= -f(\tilde{X}(t),t) \cdot \nabla_x \delta^d(x - \tilde{X}(t)) \\
&= -\nabla_x \cdot \left[f(\tilde{X}(t),t)\, \delta^d(x - \tilde{X}(t)) \right] \\
&= -\nabla_x \cdot \left[f(x,t)\, \delta^d(x - \tilde{X}(t)) \right] \\
&= -\nabla_x \cdot \left(f(x,t)\, \tilde{\rho}(x,t) \right).
\end{aligned}$$

The equation

$$\partial_t \tilde{\rho}(x,t) + \nabla_x \cdot \left(f(x,t)\, \tilde{\rho}(x,t) \right) = 0$$

is called the "fine-grained Liouville equation". It expresses conservation of probability in the state space. By averaging over the initial conditions $\tilde{x}_0$ we get the Liouville equation

$$\partial_t \rho(x,t) + \nabla_x \cdot \left(f(x,t)\, \rho(x,t) \right) = 0$$

for the density $\rho(x,t) = \langle \tilde{\rho}(x,t) \rangle$ in the state space.

An exact formal solution of this equation may be found by making a change of variables $x' = \tilde{x}(t; x_0, t_0)$ in the latter expression, with inverse $x_0 = \tilde{x}(t_0; x', t)$:

$$\begin{aligned}
\rho(x,t) &= \int \delta^d(x - \tilde{x}(t; x_0, t_0))\, \rho_0(x_0)\, d^d x_0 \\
&= \int \delta^d(x - x')\, \rho_0(\tilde{x}(t_0; x', t)) \frac{d^d x'}{\left| \frac{\partial \tilde{x}}{\partial x_0}(t; x_0, t_0) \right|} \\
&= \frac{\rho_0(\tilde{x}(t_0; x, t))}{\left| \frac{\partial \tilde{x}}{\partial x_0}(t; x_0, t_0) \right| \Big|_{x_0 = \tilde{x}(t_0; x, t)}} \\
&= \rho_0(\tilde{x}(t_0; x, t)) \left| \frac{\partial \tilde{x}}{\partial x}(t_0; x, t) \right|
\end{aligned}$$

The Liouville equation is often rewritten as

$$\partial_t \rho(x,t) = \hat{\mathcal{L}}(t)\, \rho(x,t)$$

where

$$\hat{\mathcal{L}}(t)\, \rho \equiv - \nabla_x \cdot \left(f(x,t)\, \rho \right)$$

is the so-called Liouville operator.

A smooth invariant measure of the dynamical system

$$\dot{x} = f(x)$$

with an autonomous (time-independent) vector field $f(x)$ is characterized as an eigenvector with eigenvalue 0 of the Liouville operator:

$$\hat{\mathcal{L}}(\rho_*) = 0 \quad \text{or} \quad \nabla_x \cdot \left(f(x)\,\rho_*(x)\right) = 0$$

The latter concrete statement is called the (generalized) Liouville theorem. The special case originally considered is when the dynamics is "conservative" or satisfies

$$\nabla_x \cdot f(x) = 0.$$

This property is called "conservative" since then $\rho_* = \text{const.}$ is a time-independent density, so that the d-dimensional volume d^dx in phase-space is conserved. Note in this case that we can also write

$$\hat{\mathcal{L}}(\rho) = -f(x) \cdot \nabla_x \rho.$$

Hamiltonian dynamical systems are an example of conservative dynamics. In this case

$$x = \begin{bmatrix} r \\ p \end{bmatrix}, \qquad f(x) = \begin{bmatrix} \nabla_p H(r,p) \\ -\nabla_r H(r,p) \end{bmatrix}, \qquad r, p \in \mathbb{R}^d$$

so that

$$\nabla_x \cdot f = (\nabla_r, \nabla_p) \cdot (\nabla_p H, -\nabla_r H) = 0.$$

In this case,

$$\mathcal{L}\rho = -f \cdot \nabla_x \rho = -(\nabla_p H, -\nabla_r H) \cdot (\nabla_r \rho, \nabla_p \rho) = \nabla_r H \cdot \nabla_p \rho - \nabla_p H \cdot \nabla_r \rho$$

$$= \{H, \rho\} \leftarrow \text{poisson bracket.}$$

<u>Example</u> N-particle molecular dynamics with interaction potential $U(r_n - r_m)$ between pairs of particles. Then

$$H = \sum_{n=1}^{N} \frac{p_n^2}{2m} + \sum_{n<m} U(r_n - r_m)$$

and the Liouville equation becomes

$$\partial_t \rho + \sum_{n=1}^{N} \left(\frac{p_n}{m} \cdot \nabla_{r_n} \rho + F_n(r) \cdot \nabla_{p_n} \rho \right) = 0$$

where $\rho = \rho(r,p)$ with $r = (r_1, \dots r_N)$, $p = (p_1, \dots, p_N)$ and

$$F_n(r) = - \sum_{m \neq n} \nabla U(r_n - r_m); \quad \text{force on } n\text{th particle.}$$

These results can be used to study the time-dependence of averages of arbitrary random variables ("observables") of the system

$$\tilde{A}(t) = A(\tilde{x}(t)).$$

On one hand,

$$\langle \tilde{A}(t) \rangle = \int d^d x_0 \; A(\tilde{X}(t; x_0, t_0)) \, \rho_0(x_0)$$

On the other hand

$$\langle \tilde{A}(t) \rangle = \int d^d x \; A(x) \, \rho(x,t).$$

From latter,

$$\frac{d}{dt} \langle \tilde{A}(t) \rangle = \int d^d x \; A(x) (\mathcal{L}(t) \rho)(x,t) = \int d^d x \; (\mathcal{L}^*(t) A)(x) \, \rho(x,t)$$

$$= \langle \mathcal{L}^*(t) \, \tilde{A}(t) \rangle$$

where $\mathcal{L}^*(t)$ is formal L^2-adjoint of $\mathcal{L}$ defined by

$$(\mathcal{L}^*(t) A)(x) = f(x,t) \cdot \nabla A(x)$$

This can also be seen directly from chain rule

$$\frac{d}{dt}\tilde{A}(t) = \frac{d}{dt} A(\tilde{x}(t;x_0,t_0)) = f(\tilde{x}(t),t)\cdot\nabla_x A(\tilde{x}(t)) = (\hat{\mathcal{L}}^*(t)A)$$

Note that if $\tilde{A}(t)$ has also some explicit time-dependence, $\tilde{A}(t) = A(\tilde{x}(t),t)$, then instead $\frac{d}{dt}\tilde{A}(t) = (\partial_t + \hat{\mathcal{L}}^*(t))\tilde{A}(t)$.

A dynamical system is conservative if and only if the Liouville operator is skew-adjoint:

$$\nabla_x\cdot f(x,t) = 0 \iff \hat{\mathcal{L}}^*(t) = -\hat{\mathcal{L}}(t).$$

This can be seen by noting that

$$\begin{aligned}(\hat{\mathcal{L}}(t)+\hat{\mathcal{L}}^*(t))\phi &= f(t)\cdot\nabla_x\phi - \nabla_x\cdot(f(t)\phi)\\ &= -(\nabla_x\cdot f)\,\phi\end{aligned}$$

for all smooth, bounded functions $\phi(x)$ on state space.

<u>Example</u>: We now give a non-trivial example of the Liouville equation for a non-conservative dynamics, the <u>incompressible Navier-Stokes equation.</u>

$$\partial_t u + (u\cdot\nabla)u = -\nabla p + \nu\Delta u + f(t)$$

where $f(t)$ is a body force, possibly time dependent.
This is an infinite dimensional dynamical system, whose states space consists of divergence-free velocity fields with finite energy or $u\in L^2_\sigma(\mathbb{R}^d)$.

It can be considered as an example of an ODE in function space, with the analogy

ODE		NS
x	$\Longleftrightarrow$	u
x_i	$\Longleftrightarrow$	$u_\alpha(x)$
i	$\Longleftrightarrow$	(x, α)

We can write the Navier-Stokes equation as

$$\frac{d}{dt} u(t) = F_\nu [u(t), t]$$

where

$$F_\nu [u, t; x] = -(u \cdot \nabla) u - \nabla p + \nu \Delta u + f(t).$$

This can also be written in terms of Fourier modes in a periodic domain $V = [-\frac{L}{2}, \frac{L}{2}]^d$,

$$a(k,t) = \int_V d^d x \; e^{-i k \cdot x} \; u(x,t)$$

that satisfy $a^*(k,t) = a(-k,t)$ and $k \cdot a(k,t) = 0$ as

$$\frac{d}{dt} a(k,t) = \sum_{p+q=k} -i \, (a(p,t) \cdot q) \left[a(q,t) - (k \cdot a(q,t)) \frac{k}{k^2} \right]$$

$$- \nu k^2 a(k,t) + \hat{f}(k,t).$$

Note that since

$$u(x) = \frac{1}{2L^d} \sum_k \left[a(k)\, e^{ik\cdot x} + a^*(k)\, e^{-ik\cdot x} \right]$$

one has

$$\frac{\partial}{\partial a_j(k)} u_i(x) = \frac{1}{2L^d} \delta_{ij}\, e^{ik\cdot x} \;, \qquad \frac{\partial}{\partial a_j^*(k)} u_i(x) = \frac{1}{2L^d} \delta_{ij}\, e^{-ik\cdot x}$$

so that

$$\frac{\delta}{\delta u_i(x)} = \frac{1}{2} \sum_k \left(e^{ik\cdot x} \frac{\partial}{\partial a_i(k)} + e^{-ik\cdot x} \frac{\partial}{\partial a_i^*(k)} \right)$$

If all three Fourier modes are restricted to wavenumbers less than K, then the dynamics is called Fourier-truncated Navier-Stokes:

$$F_\nu^{(K)}[u,t;x] = \frac{1}{L^d} \sum_{|k|<K} e^{ik x} \Bigg(\sum_{\substack{p+q=k \\ |p|<K,\, |q|<K}} i\,(a(p)\cdot q) \left[a(q) - (k\cdot a(q)) \frac{k}{k^2} \right] - \nu k^2 a(k) + \hat{f}(k,t) \Bigg)$$

It was shown by T.D. Lee (1952) that truncated Euler $(\nu=0,\, f=0)$ satisfies a Liouville theorem:

$$\sum_i \int d^d x \; \frac{\delta}{\delta u_i(x)} F_{0,i}^{(K)}[u;x] = 0$$

This result allows methods of equilibrium statistical mechanics to be applied to the truncated Euler system.

However, for the general case with $\nu \neq 0$ and $f \neq 0$, there is no Liouville theorem and one must solve the full Liouville equation

$$\partial_t \rho[u,t] = \hat{\mathcal{L}}(t)\, \rho[u,t]$$

to find the probability density in function space, with

$$\hat{\mathcal{L}}(t)\rho[u] = -\sum_i \int d^d x \, \frac{\delta}{\delta u_i(x)} \left\{ F_i[u,t;x]\, \rho[u] \right\}.$$

This equation is sometimes called the Hopf equation, because it is closely related to the similar functional evolution eqn derived by E. Hopf for the characteristic functional of the velocity in 1952.

Note, in particular, the invariant measure $\rho_*[u]$ which determines all the (single-time) statistics of turbulent flow, satisfies

$$\hat{\mathcal{L}}\rho_*[u] = 0$$

in the case where the body force is time independent.

Unfortunately there is no known analytical solution to this equation in function space! It is furthermore very hard to solve this equation numerically (much more so than NS itself)