Appendix F

Implementing evolution

F.1 Koopmania

The way in which time evolution acts on observables may be rephrased in the language of functional analysis, by introducing the *Koopman operator*, whose action on a state space function $a(x)$ is to replace it by its downstream value time t later, $a(x) \to a(x(t))$ evaluated at the trajectory point $x(t)$:

$$\mathcal{K}^t a(x) \;=\; a(f^t(x))\,. \tag{F.1}$$

Observable $a(x)$ has no explicit time dependence; all the time dependence comes from its evaluation at $x(t)$ rather than at $x = x(0)$.

Suppose we are starting with an initial density of representative points $\rho(x)$: then the average value of $a(x)$ evolves as

$$\langle a\rangle(t) \;=\; \frac{1}{|\rho_\mathcal{M}|}\int_\mathcal{M} dx\, a(f^t(x))\rho(x) \;=\; \frac{1}{|\rho_\mathcal{M}|}\int_\mathcal{M} dx\, \left[\mathcal{K}^t a(x)\right]\rho(x)\,.$$

An alternative point of view (analogous to the shift from the Heisenberg to the Schrödinger picture in quantum mechanics) is to push dynamical effects into the density. In contrast to the Koopman operator which advances the trajectory by time t, the Perron-Frobenius operator (16.10) depends on the trajectory point time t in the past, so the Perron-Frobenius operator is the adjoint of the Koopman operator

$$\int_\mathcal{M} dx\, \left[\mathcal{K}^t a(x)\right]\rho(x) = \int_\mathcal{M} dx\, a(x)\left[\mathcal{L}^t \rho(x)\right]\,. \tag{F.2}$$

Checking this is an easy change of variables exercise. For finite dimensional deterministic invertible flows the Koopman operator (F.1) is simply the inverse of

the Perron-Frobenius operator (16.6), so in what follows we shall not distinguish the two. However, for infinite dimensional flows contracting forward in time and for stochastic flows such inverses do not exist, and there you need to be more careful.

The family of Koopman's operators $\{\mathcal{K}^t\}_{t\in\mathbb{R}_+}$ forms a semigroup parameterized by time

(a) $\mathcal{K}^0 = \mathbf{1}$

(b) $\mathcal{K}^t\mathcal{K}^{t'} = \mathcal{K}^{t+t'} \qquad t, t' \geq 0 \qquad$ (semigroup property) ,

with the *generator* of the semigroup, the generator of infinitesimal time translations defined by

$$\mathcal{A} \;=\; \lim_{t\to 0^+} \frac{1}{t}\left(\mathcal{K}^t - \mathbf{1}\right)\,.$$

(If the flow is finite-dimensional and invertible, $\mathcal{A}$ is a generator of a group). The explicit form of $\mathcal{A}$ follows from expanding dynamical evolution up to first order, as in (2.5):

$$\mathcal{A}\, a(x) \;=\; \lim_{t\to 0^+} \frac{1}{t}\left(a(f^t(x)) - a(x)\right) \;=\; v_i(x)\partial_i a(x)\,. \tag{F.3}$$

Of course, that is nothing but the definition of the time derivative, so the equation of motion for $a(x)$ is

$$\left(\frac{d}{dt} - \mathcal{A}\right)a(x) \;=\; 0\,. \tag{F.4}$$

appendix F.2

The finite time Koopman operator (F.1) can be formally expressed by exponentiating the time evolution generator $\mathcal{A}$ as

$$\mathcal{K}^t = e^{t\mathcal{A}}\,. \tag{F.5}$$

exercise F.1

The generator $\mathcal{A}$ looks very much like the generator of translations. Indeed, for a constant velocity field dynamical evolution is nothing but a translation by time × velocity:

exercise 16.10

$$e^{tv\frac{\partial}{\partial x}}a(x) = a(x + tv)\,. \tag{F.6}$$

As we will not need to implement a computational formula for general $e^{t\mathcal{A}}$ in what follows, we relegate making sense of such operators to appendix F.2. Here

appendix F.2

we limit ourselves to a brief remark about the notion of “spectrum” of a linear operator.

The Koopman operator $\mathcal{K}$ acts multiplicatively in time, so it is reasonable to suppose that there exist constants $M > 0$, $\beta \geq 0$ such that $\|\mathcal{K}^t\| \leq M e^{t\beta}$ for all $t \geq 0$. What does that mean? The operator norm is define in the same spirit in which we defined the matrix norms in sect. J.2: We are assuming that no value of $\mathcal{K}^t \rho(x)$ grows faster than exponentially for any choice of function $\rho(x)$, so that the fastest possible growth can be bounded by $e^{t\beta}$, a reasonable expectation in the light of the simplest example studied so far, the exact escape rate (17.20). If that is so, multiplying $\mathcal{K}^t$ by $e^{-t\beta}$ we construct a new operator $e^{-t\beta}\mathcal{K}^t = e^{t(\mathcal{A}-\beta)}$ which decays exponentially for large t, $\|e^{t(\mathcal{A}-\beta)}\| \leq M$. We say that $e^{-t\beta}\mathcal{K}^t$ is an element of a *bounded* semigroup with generator $\mathcal{A} - \beta\mathbf{1}$. Given this bound, it follows by the Laplace transform

$$\int_0^\infty dt\, e^{-st}\mathcal{K}^t = \frac{1}{s-\mathcal{A}}\,, \qquad \mathrm{Re}\, s > \beta\,, \tag{F.7}$$

that the *resolvent* operator $(s-\mathcal{A})^{-1}$ is bounded (“resolvent” = able to cause separation into constituents)

section J.2

$$\left\| \frac{1}{s-\mathcal{A}} \right\| \leq \int_0^\infty dt\, e^{-st} M e^{t\beta} = \frac{M}{s-\beta}\,.$$

If one is interested in the spectrum of $\mathcal{K}$, as we will be, the resolvent operator is a natural object to study. The main lesson of this brief aside is that for the continuous time flows the Laplace transform is the tool that brings down the generator in (16.29) into the resolvent form (16.31) and enables us to study its spectrum.

F.2 Implementing evolution

(R. Artuso and P. Cvitanović)

We now come back to the semigroup of operators $\mathcal{K}^t$. We have introduced the generator of the semigroup (16.27) as

$$\mathcal{A} = \left.\frac{d}{dt}\mathcal{K}^t\right|_{t=0}\,.$$

If we now take the derivative at arbitrary times we get

$$\begin{aligned}\left(\frac{d}{dt}\mathcal{K}^t\psi\right)(x) &= \lim_{\eta\to 0}\frac{\psi(f^{t+\eta}(x)) - \psi(f^t(x))}{\eta}\\ &= v_i(f^t(x))\left.\frac{\partial}{\partial\tilde{x}_i}\psi(\tilde{x})\right|_{\tilde{x}=f^t(x)}\\ &= \left(\mathcal{K}^t\mathcal{A}\psi\right)(x)\end{aligned}$$

which can be formally integrated like an ordinary differential equation yielding

exercise F.1

$$\mathcal{K}^t = e^{t\mathcal{A}}\,. \tag{F.8}$$

This guarantees that the Laplace transform manipulations in sect. 16.5 are correct. Though the formal expression of the semigroup (F.8) is quite simple one has to take care in implementing its action. If we express the exponential through the power series

$$\mathcal{K}^t = \sum_{k=0}^{\infty}\frac{t^k}{k!}\mathcal{A}^k\,, \tag{F.9}$$

we encounter the problem that the infinitesimal generator (16.27) contains non-commuting pieces, i.e., there are i, j combinations for which the commutator does not satisfy

$$\left[\frac{\partial}{\partial x_i}, v_j(x)\right] = 0\,.$$

To derive a more useful representation, we follow the strategy used for finite-dimensional matrix operators in sects. 4.2 and 4.3 and use the semigroup property to write

$$\mathcal{K}^t = \prod_{m=1}^{t/\delta\tau}\mathcal{K}^{\delta\tau}$$

as the starting point for a discretized approximation to the continuous time dynamics, with time step $\delta\tau$. Omitting terms from the second order onwards in the expansion of $\mathcal{K}^{\delta\tau}$ yields an error of order $O(\delta\tau^2)$. This might be acceptable if the time step $\delta\tau$ is sufficiently small. In practice we write the Euler product

$$\mathcal{K}^t = \prod_{m=1}^{t/\delta\tau}\left(1 + \delta\tau\mathcal{A}_{(m)}\right) + O(\delta\tau^2) \tag{F.10}$$

where

$$\left(\mathcal{A}_{(m)}\psi\right)(x) = v_i(f^{m\delta\tau}(x))\left.\frac{\partial\psi}{\partial\tilde{x}_i}\right|_{\tilde{x}=f^{m\delta\tau}(x)}$$

As far as the x dependence is concerned, $e^{\delta\tau\mathcal{A}_i}$ acts as

$$e^{\delta\tau\mathcal{A}_i}\begin{Bmatrix} x_1 \\ \cdot \\ x_i \\ x_d \end{Bmatrix} \to \begin{Bmatrix} x_1 \\ \cdot \\ x_i + \delta\tau v_i(x) \\ x_d \end{Bmatrix} . \qquad \text{(F.11)}$$

exercise 2.6

We see that the product form (F.10) of the operator is nothing else but a prescription for finite time step integration of the equations of motion - in this case the simplest Euler type integrator which advances the trajectory by $\delta\tau$×velocity at each time step.

F.2.1 A symplectic integrator

The procedure we described above is only a starting point for more sophisticated approximations. As an example on how to get a sharper bound on the error term consider the Hamiltonian flow $\mathcal{A} = \mathcal{B} + C$, $\mathcal{B} = p_i \frac{\partial}{\partial q_i}$, $C = -\partial_i V(q) \frac{\partial}{\partial p_i}$. Clearly the potential and the kinetic parts do not commute. We make sense of the formal solution (F.10) by splitting it into infinitesimal steps and keeping terms up to $\delta\tau^2$ in

exercise F.2

$$\mathcal{K}^{\delta\tau} = \hat{\mathcal{K}}^{\delta\tau} + \frac{1}{24}(\delta\tau)^3[\mathcal{B} + 2C, [\mathcal{B}, C]] + \cdots , \qquad \text{(F.12)}$$

where

$$\hat{\mathcal{K}}^{\delta\tau} = e^{\frac{1}{2}\delta\tau\mathcal{B}} e^{\delta\tau C} e^{\frac{1}{2}\delta\tau\mathcal{B}} . \qquad \text{(F.13)}$$

The approximate infinitesimal Liouville operator $\hat{\mathcal{K}}^{\delta\tau}$ is of the form that now generates evolution as a sequence of mappings induced by (16.30), a free flight by $\frac{1}{2}\delta\tau\mathcal{B}$, scattering by $\delta\tau\partial V(q')$, followed again by $\frac{1}{2}\delta\tau\mathcal{B}$ free flight:

$$\begin{aligned} e^{\frac{1}{2}\delta\tau\mathcal{B}} \begin{Bmatrix} q \\ p \end{Bmatrix} &\to \begin{Bmatrix} q' \\ p' \end{Bmatrix} = \begin{Bmatrix} q - \frac{\delta\tau}{2} p \\ p \end{Bmatrix} \\ e^{\delta\tau C} \begin{Bmatrix} q' \\ p' \end{Bmatrix} &\to \begin{Bmatrix} q'' \\ p'' \end{Bmatrix} = \begin{Bmatrix} q' \\ p' + \delta\tau\partial V(q') \end{Bmatrix} \\ e^{\frac{1}{2}\delta\tau\mathcal{B}} \begin{Bmatrix} q'' \\ p'' \end{Bmatrix} &\to \begin{Bmatrix} q''' \\ p''' \end{Bmatrix} = \begin{Bmatrix} q' - \frac{\delta\tau}{2} p'' \\ p'' \end{Bmatrix} \end{aligned} \qquad \text{(F.14)}$$

Collecting the terms we obtain an integration rule for this type of symplectic flow which is better than the straight Euler integration (F.11) as it is accurate up to order $\delta\tau^2$:

$$\begin{aligned} q_{n+1} &= q_n - \delta\tau\, p_n - \frac{(\delta\tau)^2}{2}\partial V\left(q_n - \delta\tau p_n/2\right) \\ p_{n+1} &= p_n + \delta\tau\partial V\left(q_n - \delta\tau p_n/2\right) \end{aligned} \qquad \text{(F.15)}$$

The Jacobian matrix of one integration step is given by

$$M = \begin{pmatrix} 1 & -\delta\tau/2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ \delta\tau\partial V(q') & 1 \end{pmatrix} \begin{pmatrix} 1 & -\delta\tau/2 \\ 0 & 1 \end{pmatrix} . \qquad \text{(F.16)}$$

Note that the billiard flow (8.11) is an example of such symplectic integrator. In that case the free flight is interrupted by instantaneous wall reflections, and can be integrated out.

Commentary

Remark F.1 Koopman operators. The "Heisenberg picture" in dynamical systems theory has been introduced by Koopman and Von Neumann [F.1, F.2], see also ref. [16.12]. Inspired by the contemporary advances in quantum mechanics, Koopman [F.1] observed in 1931 that $\mathcal{K}^t$ is unitary on $L^2(\mu)$ Hilbert spaces. The Koopman operator is the classical analogue of the quantum evolution operator $\exp\left(i\hat{H}t/\hbar\right)$ – the kernel of $\mathcal{L}^t(y,x)$ introduced in (16.16) (see also sect. 17.2) is the analogue of the Green's function discussed here in chapter 31. The relation between the spectrum of the Koopman operator and classical ergodicity was formalized by von Neumann [F.2]. We shall not use Hilbert spaces here and the operators that we shall study *will not* be unitary. For a discussion of the relation between the Perron-Frobenius operators and the Koopman operators for finite dimensional deterministic invertible flows, infinite dimensional contracting flows, and stochastic flows, see Lasota-Mackey [16.12] and Gaspard [1.8].

Remark F.2 Symplectic integration. The reviews [F.12] and [F.13] offer a good starting point for exploring the symplectic integrators literature. For a higher order integrators of type (F.13), check ref. [F.18].

Exercises

F.1. **Exponential form of semigroup elements.** Check that the Koopman operator and the evolution generator commute, $\mathcal{K}^t\mathcal{A} = \mathcal{A}\mathcal{K}^t$, by considering the action of both operators on an arbitrary state space function $a(x)$.

F.2. **Non-commutativity.** Check that the commutators in (F.12) are not vanishing by showing that

$$[\mathcal{B}, C] = -p\left(V'' \frac{\partial}{\partial p} - V' \frac{\partial}{\partial q}\right).$$

F.3. **Symplectic leapfrog integrator.** Implement (F.15) for 2-dimensional Hamiltonian flows; compare it with Runge-Kutta integrator by integrating trajectories in some (chaotic) Hamiltonian flow.

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