

Singularly perturbed differential equations

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Foreword

These notes are based on a series of lectures given at Freie Universität Berlin in spring 2008. They give a high-level overview of certain singular perturbation problems that appear in the modelling of real-world problems by differential equations. In doing so the notes focus on two prevalent classes of singularly perturbed differential equations: deterministic systems that have an invariant manifold, and coupled slow/fast systems, both stochastic and deterministic, which can be treated within the framework of averaging techniques. Parts of the notes are based on the textbook *Multiscale Methods: Averaging and Homogenization* by Greg Pavliotis and Andrew Stuart, a book which I highly recommend.

1 Introduction

Systems involving several time scales often assume the prototypical form

$$\begin{aligned}\dot{x}^\epsilon &= f(x^\epsilon, y^\epsilon, \epsilon) \\ \dot{y}^\epsilon &= \frac{1}{\epsilon}g(x^\epsilon, y^\epsilon, \epsilon), \quad x^\epsilon(0) = x_0, y^\epsilon(0) = y_0\end{aligned}\tag{1.1}$$

where $(x, y) \in \mathbf{R}^n \times \mathbf{R}^m$ and $0 < \epsilon \ll 1$ is a small parameter and we use the “overdot” to denote derivatives with respect to the free variable, i.e., $\dot{z}(t) = dz/dt$. If $f(\cdot, \cdot, \epsilon)$ and $g(\cdot, \cdot, \epsilon)$ are globally Lipschitz and uniformly bounded in ϵ , then $\dot{y}^\epsilon(t)$ will be of order $1/\epsilon$ faster than $\dot{x}^\epsilon(t)$. Accordingly, we call x the slow variables and y the fast variables of the system.

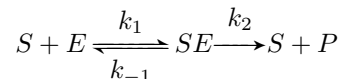
1.1 Motivation

Slow/fast systems naturally appear in the modelling of real-world processes. Typical examples involve:

Climate systems Many large-scale phenomena such as El Niño arise from the coupling between the tropical ocean and the atmosphere where the rapid weather changes in the atmosphere act as a stochastic force on the slowly evolving ocean.

Celestial mechanics The timescale of the earth’s orbital motion around the sun is much shorter than its period of rotation. Hence the tidal evolution of the earth-moon system depends on the slowly varying gravitational potential of the sun (see Figure 1).

Enzyme kinetics Enzyme-catalysed reactions with single-substrate mechanisms due to Michaelis and Menten are systematically written as



where it is assumed that the back reaction $S + P \rightarrow ES$ is negligible. If the concentration of the substrate S is high, the enzyme E is entirely saturated and only exists in its complex form ES . This entails that, after a short relaxation time depending upon the initial conditions, the concentrations of both the enzyme and the complex quickly converge to a steady-state.

Many-particle dynamics In systems that consist of different types of atoms which are coupled by interatomic forces, the lighter particles typically oscillate quickly around an average path that follows the slow motion of the heavy particles. As any numerical scheme has to resolve the fastest scale in the system, the singular perturbation in the system of equations (1.1) renders the numerical integration unstable as ϵ goes to zero. Therefore we may wish to replace it by the “simpler” equation

$$\dot{x} = \bar{f}(x), \quad x(0) = x_0,\tag{1.2}$$

which approximates the dynamics of the slow degrees of freedom when ϵ is small.

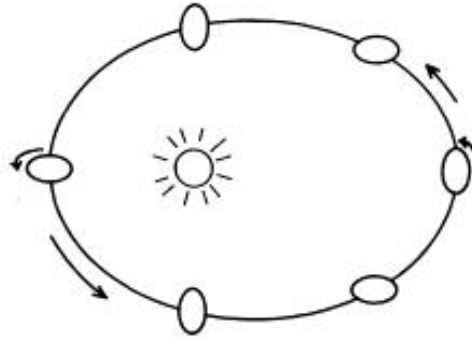


Fig. 1 Sun-earth-moon system

1.2 Elimination of fast variables

The specific form of the reduced system (1.2) depends

1. on the qualitative properties of the vector field $g(x, \cdot, \epsilon)$,
2. on the way the limit $x^\epsilon \rightarrow x$ is taken, and
3. on the type of approximation used.

Regarding the latter, the limiting equation clearly depends, for example, on the norm that measures the deviations $\|x^\epsilon - x\|$, or on the time interval in which the approximation shall hold. Issues of weak and strong convergence as well as approximations on compact or exponentially long time intervals will be discussed later on. Regarding the first two topics, we will briefly mention two basic perturbation techniques that are employed in analysing slow/fast systems such as (1.1).

Invariant manifolds A suggestive way of writing (1.1) is as follows:

$$\begin{aligned} \dot{x}^\epsilon &= f(x^\epsilon, y^\epsilon, \epsilon) \\ \epsilon \dot{y}^\epsilon &= g(x^\epsilon, y^\epsilon, \epsilon), \quad x^\epsilon(0) = x_0, y^\epsilon(0) = y_0. \end{aligned}$$

Clearly, for arbitrary initial conditions (x_0, y_0) the right hand side of the second equation will be of order 1, so letting ϵ approach zero does not make sense at the moment. However, we may choose (x_0, y_0) such that the fast equation becomes stationary, i.e. $g(x_0, y_0, 0) = 0$. Moreover, if ϵ is sufficiently small, it seems reasonable to replace (1.1) with the differential algebraic equation

$$\begin{aligned} \dot{x} &= f(x, y, 0) \\ 0 &= g(x, y, 0), \quad x(0) = x_0, y(0) = y_0. \end{aligned} \tag{1.3}$$

By construction, the dynamics remain on the invariant manifold

$$S = \{(x, y) \in \mathbf{R}^n \times \mathbf{R}^m \mid g(x, y, 0) = 0\} \subset \mathbf{R}^n \times \mathbf{R}^m.$$

In simple cases we can solve the algebraic equation $g(x, y, 0) = 0$ for the dependent variable x , provided that the Jacobian $(\partial g / \partial y)$ is regular on S . This yields an equation $x = h(y)$ that we can plug into the first equation, by which we find

$$\dot{x} = f(x, h(x), 0), \quad x(0) = x_0.$$

In other words, if the slow/fast system (1.1) admits an invariant manifold, we may approximate the slow equation by the reduced system (1.2) where $\bar{f}(x) = f(x, h(x), 0)$. The condition on the initial values may be relaxed if the fast subsystem is strictly hyperbolic, i.e., the invariant manifold is “attractive” such that all trajectories that are launched in the vicinity of the invariant manifold are quickly absorbed by it. Assertions regarding the behaviour of solutions for finite ϵ and convergence as $\epsilon \rightarrow 0$ are made by the *geometric singular perturbation theory* that is due to Tikhonov [18], Gradštein [6] and Fenichel [5].

Averaging and homogenisation in time Yet another way to derive a reduced system of the form (1.2) consists in averaging over the fast variables. To this end we rescale the free variable according to $t \mapsto t/\epsilon$ and introduce the *microscopic time*

$$\tau = t/\epsilon \quad \Rightarrow \quad \frac{d}{dt} = \frac{1}{\epsilon} \frac{d}{d\tau}.$$

By chain rule, (1.1) turns out to be equivalent to the system

$$\begin{aligned} \dot{z}^\epsilon &= \epsilon f(z^\epsilon, \xi^\epsilon, \epsilon) \\ \dot{\xi}^\epsilon &= g(z^\epsilon, \xi^\epsilon, \epsilon), \quad z^\epsilon(0) = x_0, \xi^\epsilon(0) = y_0 \end{aligned}$$

where $(z(\tau), \xi(\tau)) = (x(\epsilon\tau), y(\epsilon\tau))$. We keep the “overdot” notation to denote the derivative with respect to the free variable. Let us consider the solution on the time interval $[0, T]$; by continuity of the solution we conclude that the slow limit solution for $\epsilon \rightarrow 0$ is constant on the interval $[0, T]$, i.e.,

$$\lim_{\epsilon \rightarrow 0} z^\epsilon(\tau) = x_0 \quad \forall \tau \in [0, T]$$

whereas $\xi(t) = \varphi_{x_0}^t(y_0)$ is the solution of the *associated equation*

$$\dot{\xi} = g(x_0, \xi, 0), \quad \xi(0) = y_0, \tag{1.4}$$

on $[0, T]$. This changes if we speed up time and consider the behaviour of the solution on an infinite time interval $[0, T/\epsilon]$: Switching back to the original variables $t = \epsilon\tau$ and $x^\epsilon(t) = z^\epsilon(t/\epsilon)$ (while keeping in mind that $\tau \in [0, T/\epsilon]$ is equivalent to $t \in [0, T]$), we arrive at the classical averaging formulation

$$\dot{x}^\epsilon = f(x^\epsilon, \varphi_x^{t/\epsilon}(y_0), \epsilon), \quad x^\epsilon(0) = x_0. \tag{1.5}$$

Note that the fast variable y^ϵ has been replaced by the solution of the associated problem (1.4) which depends parametrically on the current value $x^\epsilon(t) = x$ of the slow variable.

The representation (1.5) explains the idea of the fast dynamics acting as random perturbations to the slow dynamics, since $y^\epsilon \approx \varphi_x^{t/\epsilon}(y_0)$ has now become a “fast forcing function”. Seeking a *closure* of the last equation amounts to taking the limit $\epsilon \rightarrow 0$. The limiting equation reads

$$\dot{x} = \bar{f}(x), \quad x(0) = x_0,$$

with

$$\bar{f}(x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(x, \varphi_x^t(y_0), 0) dt,$$

provided that the integral exists.¹ Note that \bar{f} may still depend on the initial value y_0 . If, however, the associated system admits an ergodic probability measure μ_x , i.e.,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T h(\varphi_x^t(y_0)) dt = \int h(y) d\mu_x(y)$$

for almost all initial values y_0 and any integrable function $h \in L^1(\mathbf{R}^m)$, then \bar{f} is independent of y_0 and can be computed by simply taking the ensemble average

$$\bar{f}(x) = \int f(x, y, 0) d\mu_x(y).$$

The latter is often more convenient than computing time averages. Statements so as to guarantee that the original slow/fast system can be replaced by the forced equation (1.5) and averaged over the fast perturbations are known by the name of *averaging principles* and go back to the works of Bogolyubov / Mitropol'skii [2] and Khas'minskii [8] from the sixties.

A remark is in order. Averaging principles make assertions about approximation properties of averaged differential equations on compact time intervals. Yet it may happen that the right hand side of (1.5) averages to zero under the fast dynamics, in case of which the dynamics become trivial on the interval $[0, T]$ and the relevant dynamics happen on a time interval of order $1/\epsilon$ or even $\exp(-1/\epsilon)$. Convergence results in this respect are due to Khas'minskii and are often quoted as *homogenisation results* or *diffusive limits*.

¹ If the fast forcing function is periodic with period $T < \infty$, the integral will be computed over a single period.

1.3 Perturbation techniques

The analyses of singularly perturbed differential equations such as (1.1) often boil down to linear operator equations of the type (see, e.g., [12] for a treatment of stochastic systems)

$$\partial\phi^\epsilon(u, t) = \mathcal{L}^\epsilon\phi^\epsilon(u, t), \quad \phi^\epsilon(u, 0) = \psi(u). \quad (1.6)$$

Here \mathcal{L}^ϵ is a differential operator that is defined on some Banach space subject to suitable boundary conditions and $u \in \mathbf{R}^{n+m}$ is a shorthand for (x, y) . If we confine our attention to the aforementioned class of problems (averaging or geometric singular perturbation) the operator typically takes the form

$$\mathcal{L}^\epsilon = \mathcal{L}_0 + \frac{1}{\epsilon}\mathcal{L}_1$$

where \mathcal{L}_0 and \mathcal{L}_1 “generate” the slow and fast dynamics, respectively. (The properties of \mathcal{L}_i depend on the actual problem and will be discussed later on in the text.) Notice that \mathcal{L}_0 and \mathcal{L}_1 may still depend on ϵ , but the dominant singularity is as sketched. We seek a perturbative expansion of the solution of (1.6) that has the form

$$\phi^\epsilon = \phi_0 + \epsilon\phi_1 + \epsilon^2\phi_2 + \dots$$

Hence (1.6) can be recast as

$$\frac{1}{\epsilon}\mathcal{L}_1\phi_0 + (\mathcal{L}_1\phi_1 + \mathcal{L}_0\phi_0 - \partial\phi_0) = \mathcal{O}(\epsilon),$$

and equating powers of ϵ yields a hierarchy of equations the first two of which are

$$\begin{aligned} \mathcal{L}_1\phi_0 &= 0 \\ \mathcal{L}_1\phi_1 &= \partial\phi_0 - \mathcal{L}_0\phi_0. \end{aligned}$$

The first equation implies that the lowest-order perturbation approximation of (1.6) lies in the nullspace of \mathcal{L}_1 , which typically entails a condition of the form $\phi_0 = \phi_0(x)$. Averaging or geometric singular perturbation theory now consists in finding an appropriate closure of the second equation subject to $\phi_0 \in \ker \mathcal{L}_1$. This results in an effective equation for $\phi \approx \phi_0$, namely,

$$\partial\phi(x, t) = \bar{\mathcal{L}}\phi(x, t).$$

Once the effective linear operator $\bar{\mathcal{L}}$ has been computed from \mathcal{L}_0 and \mathcal{L}_1 , the result can be reinterpreted in terms of the corresponding differential equation to give

$$\dot{x} = \bar{f}(x), \quad x(0) = x_0.$$

2 Linear systems

Consider the linear system of ordinary differential equations

$$\dot{u}^\epsilon = \mathcal{L}^\epsilon u^\epsilon, \quad u^\epsilon(0) = v \quad (2.1)$$

where $u \in \mathbf{R}^{n+m}$, and \mathcal{L}^ϵ is a real-valued singularly perturbed $(n+m) \times (n+m)$ matrix that reads

$$\mathcal{L}^\epsilon = \mathcal{L}_0 + \frac{1}{\epsilon}\mathcal{L}_1.$$

2.1 First-order perturbation expansion

Our presentation of the linear problem follows essentially the textbook [14]. For the sake of the following argument, let us assume that the nullspace of \mathcal{L}_1 is one-dimensional, i.e., $\ker \mathcal{L}_1 = \text{span}\{\phi\}$, and so is $\ker \mathcal{L}_1^* = \text{span}\{\psi\}$. Let us further assume that $\langle \phi, \psi \rangle \neq 0$. We seek a perturbative expansion of u^ϵ that is of the form

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$$

Plugging the ansatz into (2.1) yields

$$\frac{1}{\epsilon} \mathcal{L}_1 u_0 + (\mathcal{L}_1 u_1 + \mathcal{L}_0 u_0 - \dot{u}_0) + \epsilon (\mathcal{L}_1 u_2 + \mathcal{L}_0 u_1 - \dot{u}_1) = \mathcal{O}(\epsilon^2).$$

By equating equal powers of ϵ we find

$$\mathcal{L}_1 u_0 = 0 \tag{2.2}$$

$$\mathcal{L}_1 u_1 = \dot{u}_0 - \mathcal{L}_0 u_0 \tag{2.3}$$

$$\mathcal{L}_1 u_2 = \dot{u}_1 - \mathcal{L}_0 u_1 \tag{2.4}$$

and so on and so forth. The first equation implies that $u_0 \in \ker \mathcal{L}_1$. As we are aiming at the lowest-order approximation $u^\epsilon \approx u_0$, the time evolution of u_0 is due to the second equation. By the assumption above, the nullspace of \mathcal{L}_1 is one-dimensional, hence the approximation will have the form $u_0(t) = \alpha(t)\phi$. As will become clear later on it is convenient to multiply the second equation by $\psi \in \ker \mathcal{L}_1^*$ from the left,

$$\langle \psi, \mathcal{L}_1 u_1 \rangle = \langle \psi, \dot{u}_0 \rangle - \langle \psi, \mathcal{L}_0 u_0 \rangle.$$

Since $\langle \psi, \mathcal{L}_1 u_1 \rangle = \langle \mathcal{L}_1^* \psi, u_1 \rangle$ and $\mathcal{L}_1^* \psi = 0$ the latter is equivalent to

$$\dot{\alpha} = \bar{\mathcal{L}} \alpha, \quad \bar{\mathcal{L}} = \frac{\langle \psi, \mathcal{L}_0 \phi \rangle}{\langle \psi, \phi \rangle} \tag{2.5}$$

where we have taken advantage of the identity $u_0 = \alpha\phi$. Notice that the ‘‘averaged’’ coefficient $\bar{\mathcal{L}}$ is independent of how ϕ, ψ are normalised. As yet we have not specified the initial conditions for α ; in order to keep the discussion lucid and simple we suppose that the initial conditions in (2.1) are consistent with the lowest-order approximation, that is, we suppose that $v \in \ker \mathcal{L}_1$. In this case we have

$$\alpha_0 = \pm \frac{|v|}{|\phi|}$$

where the sign is determined by the orientation of v with respect to ϕ (i.e., whether the two vectors are parallel or antiparallel). To lowest order, we have the approximation $u^\epsilon \approx u_0$ with

$$u_0 = \pm |v| \exp(\bar{\mathcal{L}}t) \frac{\phi}{|\phi|}$$

which is independent of the normalisation of ϕ . As our problem is linear it can be readily seen that

$$\sup_{0 \leq t \leq T} \|u^\epsilon - u_0\| = C\epsilon$$

for all $T < \infty$ with C depending exponentially on T .

2.2 The Fredholm alternative

Before we come to the next-order perturbation result, let us briefly revisit the essential steps that have led to an effective equation for u_0 . To this end recall that the closure of equation (2.3) that determined the time dependence of u_0 was obtained by a projection onto the nullspace of \mathcal{L}_1^* (i.e., left multiplication with $\psi \in \ker \mathcal{L}_1^*$ where $\mathcal{L}_1^* = \mathcal{L}_1^T$). Generally speaking, this closure consisted in solving an equation of the form $\mathcal{L}_1 u_1 = f$. Its solvability conditions are provided by the following important theorem of which we state only the finite-dimensional version.

Theorem 2.1 (Fredholm alternative) *Let $\mathcal{L} \in \mathbf{R}^{n \times n}$. Then*

1. *either the equation $\mathcal{L}u = f$ has a unique solution for all $f \in \mathbf{R}^n$, or*
2. *the homogeneous equation $\mathcal{L}u = 0$ has at least one nontrivial solution and*

$$1 \leq \dim(\ker \mathcal{L}_1) = \dim(\ker \mathcal{L}_1^*) < \infty.$$

In this case the inhomogeneous equation $\mathcal{L}u = f$ has a solution if and only if

$$\langle v, f \rangle = 0 \quad \forall v \in \ker \mathcal{L}^*.$$

Proof. The first statement is trivial, so we give only a justification of the second. Suppose that $\ker \mathcal{L} \neq \emptyset$. To see that solvability of $\mathcal{L}u = f$ implies $\langle v, f \rangle = 0$ for all $v \in \ker \mathcal{L}^*$ consider $u \in \mathbf{R}^n$ that solves $\mathcal{L}u = f$ for $f \neq 0$. Since

$$\langle v, \mathcal{L}u \rangle = \langle \mathcal{L}^*v, u \rangle \quad \forall u, v \in \mathbf{R}^n$$

and $\langle \mathcal{L}^*v, u \rangle = 0$ for all $v \in \ker \mathcal{L}^*$ it follows that $f \in (\ker \mathcal{L}^*)^\perp$ is a necessary condition for $\mathcal{L}u = f$ to have a solution. Conversely, suppose that $\langle v, f \rangle = 0$ for all $v \in \ker \mathcal{L}^*$. To show that the equation $\mathcal{L}u = f$ has a non-trivial solution for $f \neq 0$ we multiply the equation by \mathcal{L}^* from the left which yields

$$\mathcal{L}^*\mathcal{L}u = b, \quad b = \mathcal{L}^*f.$$

As $f \in (\ker \mathcal{L})^\perp$ entails that $b \in \mathcal{R}(\mathcal{L}^*)$, $b \neq 0$ with $\mathcal{R}(\mathcal{L}^*)$ denoting the range of \mathcal{L}^* , we conclude that $\mathcal{L}^*\mathcal{L}: \mathbf{R}^n \rightarrow \mathcal{R}(\mathcal{L}^*)$ is surjective. Hence $\mathcal{L}u = f$ has a solution and the assertion follows. \square

Remark 2.2 The Fredholm alternative carries over to the infinite-dimensional case when \mathcal{L} is a compact perturbation of the identity, i.e., $\mathcal{L} = \text{Id} - K$ for K being compact. (A linear operator K is called compact when the closure of $K(B)$ is compact for all bounded subsets B of the domain of K .) For details see, e.g., [15, 19].

2.3 Second-order perturbation expansion

We shall study the case that the first-order expansion yields the trivial result

$$\dot{u}_0 = 0, \quad t \in [0, T].$$

That is, we have $\langle \psi, \mathcal{L}_0\phi \rangle = 0$ which implies $\bar{\mathcal{L}} = 0$ in equation (2.5). In this case nontrivial dynamics will occur only on essentially longer time intervals of length $\mathcal{O}(1/\epsilon)$ or even $\mathcal{O}(\exp(-1/\epsilon))$ which amounts to higher-order corrections in the perturbation expansion. In order to understand this phenomenon, we speed up time by scaling the free variable t according to $t \mapsto \epsilon t$, $\epsilon t = \tau$ (diffusive scaling). Using that

$$\frac{d}{dt} = \epsilon \frac{d}{d\tau},$$

our original problem (2.1) now reads

$$\frac{du^\epsilon}{d\tau} = \mathcal{L}^\epsilon u^\epsilon, \quad u^\epsilon(0) = v \tag{2.6}$$

where $u^\epsilon = u^\epsilon(\tau)$, and \mathcal{L}^ϵ is the $n \times n$ matrix

$$\mathcal{L}^\epsilon = \frac{1}{\epsilon} \mathcal{L}_0 + \frac{1}{\epsilon^2} \mathcal{L}_1.$$

Suppose again that $\ker \mathcal{L}_1 = \text{span}\{\phi\}$ and $\ker \mathcal{L}_1^* = \text{span}\{\psi\}$ are one-dimensional with $\langle \phi, \psi \rangle \neq 0$. Additionally, we assume that the so-called centering condition

$$\langle \psi, \mathcal{L}_0\xi \rangle = 0 \quad \forall \xi \in \mathbf{R}^n \tag{2.7}$$

holds true for $\psi \in \mathcal{L}_1^*$; in particular the centering condition implies $\bar{\mathcal{L}} = 0$ in (2.5). We seek a perturbative expansion for (2.6) that is of the form

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$$

Equating powers of ϵ yields again a hierarchy of equations the first three of which are

$$\mathcal{L}_1 u_0 = 0 \tag{2.8}$$

$$\mathcal{L}_1 u_1 = -\mathcal{L}_0 u_0 \tag{2.9}$$

$$\mathcal{L}_1 u_2 = \dot{u}_0 - \mathcal{L}_0 u_1. \tag{2.10}$$

As before, the first equation entails that $u_0 \in \ker \mathcal{L}$ which yields lowest-order approximation $u^\epsilon(\tau) \approx \beta(\tau)\phi$, $\tau \in [0, T]$ we are aiming at. (In terms of the original time t this becomes an approximation on $[0, T/\epsilon]$.)

Since $\langle \psi, \mathcal{L}_0 u_0 \rangle = 0$ by the centering condition, the Fredholm alternative applies and we can solve equation (2.9). Let $\eta \in \mathbf{R}^n$ be the solution

$$\mathcal{L}_1 \eta = -\mathcal{L}_0 \phi. \quad (2.11)$$

The last equation is called the *cell problem* where the word *cell* typically refers to the scale of the fast variables. By the Fredholm alternative, solvability of (2.10) requires that $\langle \psi, \dot{u}_0 - \mathcal{L}_0 u_1 \rangle = 0$. Together with (2.11) this results in an effective equation for β ,

$$\dot{\beta} = -\bar{\mathcal{L}}\beta, \quad \beta_0 = \pm \frac{|v|}{|\phi|} \quad (2.12)$$

with the coefficient

$$\bar{\mathcal{L}} = -\frac{\langle \psi, \mathcal{L}_0 \eta \rangle}{\langle \psi, \phi \rangle}. \quad (2.13)$$

A slightly sloppy but instructive way to write $\bar{\mathcal{L}}$ is

$$\bar{\mathcal{L}} = -\frac{\langle \psi, \mathcal{L}_0 \mathcal{L}_1^{-1} \mathcal{L}_0 \phi \rangle}{\langle \psi, \phi \rangle}$$

as can be found by formally solving (2.9) upon noting that the right hand side of the equation has no component in the kernel of \mathcal{L}_1^* (centering condition). Rescaling back to the original time $t = \tau/\epsilon$ the correction to the constant $\mathcal{O}(1)$ solution $u^\epsilon \approx u_0$ is

$$u^\epsilon - u_0 \approx \pm |v| \exp(\epsilon \bar{\mathcal{L}} t) \frac{\phi}{|\phi|}$$

which now yields an approximation on the interval $[0, T/\epsilon]$. When ϵ is small, the refined approximation entails the original one as $u^\epsilon - u_0 \approx 0$ for times of order 1.

In addition to computing the effective coefficient $\bar{\mathcal{L}}$, the second-order perturbation result that is often termed *homogenised* equation requires to solve a cell problem. Although the solution of the cell problem (2.11) is not unique the effective equation (2.12)–(2.13) is the same for all solutions of (2.11). This can be seen as follows: since \mathcal{L}_1 has a nontrivial nullspace, the solution of

$$\mathcal{L}_1 \eta = f, \quad f = -\mathcal{L}_0 u_0 \in (\ker \mathcal{L}_1^*)^\perp,$$

is unique up to additive multiples of vectors $\zeta \in \ker \mathcal{L}_1$. Equation (2.13) thus becomes

$$\bar{\mathcal{L}} = -\frac{\langle \psi, \mathcal{L}_0(\eta + \zeta) \rangle}{\langle \psi, \phi \rangle}.$$

However the centering condition (2.7) implies $\langle \psi, \mathcal{L}_0 \zeta \rangle = 0$, and therefore $\bar{\mathcal{L}}$ is unambiguously defined.

Remark 2.3 If the initial conditions lie in the nullspace of \mathcal{L}_1 the described perturbation expansions will break down in the neighbourhood of $t = 0$. In this case it is necessary to separately account for the relaxation of the solution to the nullspace in which the approximation is sought. Under suitable dissipativity assumptions regarding \mathcal{L}_1 the relaxation will typically occur in some initial layer $t \in [0, \epsilon]$ or $t \in [0, \sqrt{\epsilon}]$. We will come back to this point at a later stage in the text.

2.4 An example

We shall conclude the discussion of linear systems with a little example from classical mechanics. For this purpose we consider oscillating particles in $\mathbf{R}^d = \mathbf{R}^n \times \mathbf{R}^m$ that are governed by the second-order differential equations

$$\begin{aligned} \ddot{x}^\epsilon &= -(L_{11}x^\epsilon + L_{12}y^\epsilon), & x^\epsilon(0) &= x_0, \dot{x}^\epsilon(0) = v_0 \\ \epsilon^2 \ddot{y}^\epsilon &= -(L_{12}^T x^\epsilon + L_{22}y^\epsilon), & y^\epsilon(0) &= y_0, \dot{y}^\epsilon(0) = w_0. \end{aligned} \quad (2.14)$$

Equations (2.14) describe the oscillation of heavy particles of unit mass that are coupled to light particles of mass ϵ . The equations are Hamiltonian with the energy

$$H(x, y, v, w) = \frac{1}{2} (|v|^2 + |w|^2) + \frac{1}{2} (x^T L_{11} x + 2x^T L_{12} y + y^T L_{22} y)$$

with $L_{22} = L_{22}^T > 0$ (positive definite) and the symplectic form

$$\omega = dx \wedge dv + \frac{1}{\epsilon} dy \wedge dw.$$

The equations of motion (2.14) equivalently read

$$\begin{aligned} \dot{x}^\epsilon &= v^\epsilon, & x^\epsilon(0) &= x_0 \\ \dot{v}^\epsilon &= -(L_{11}x^\epsilon + L_{12}y^\epsilon), & v^\epsilon(0) &= v_0 \\ \epsilon \dot{y}^\epsilon &= w^\epsilon, & y^\epsilon(0) &= y_0 \\ \epsilon \dot{w}^\epsilon &= -(L_{12}^T x^\epsilon + L_{22}y^\epsilon), & w^\epsilon(0) &= \frac{1}{\epsilon} w_0 \end{aligned} \tag{2.15}$$

which is of the form (2.1) with $u = (x, v, y, w)$ and

$$\mathcal{L}_0 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -L_{11} & 0 & -L_{12} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{L}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -L_{12}^T & 0 & -L_{22} & 0 \end{pmatrix}.$$

We want to argue along the lines of Section 2. To this end, we have to adapt the considerations therein to the case $\dim(\ker \mathcal{L}_1) = \dim(\ker \mathcal{L}_1^*) = 2$. Specifically, we seek an effective solution of (2.15) that is of the form $u^\epsilon \approx u_0$ and evolves in the nullspace of \mathcal{L}_1 , viz.,

$$u_0 = \sum_{i=1}^2 \alpha_i \phi_i, \quad \mathcal{L}_1 \phi_1 = \mathcal{L}_1 \phi_2 = 0.$$

Imposing the nullspace requirement on the initial conditions yields $y_0 = -L_{22}^{-1} L_{12}^T x_0$ and $w_0 = 0$ for the fast dynamics. Hence the effective equation turns out to be

$$\begin{aligned} \dot{x} &= v, & x(0) &= x_0 \\ \dot{v} &= -\bar{L}x, & v(0) &= v_0 \end{aligned} \tag{2.16}$$

where $\bar{L} = L_{11} - L_{12} L_{22}^{-1} L_{12}^T$ is the Schur complement of L . Notice that the restriction of the initial conditions (y_0, w_0) entails stationarity of the fast subsystem in equation (2.15), i.e., $\dot{y}^\epsilon = 0$ and $\dot{w}^\epsilon = 0$. In other words,

$$M(x) = \{(y, w) \mid y = -L_{22}^{-1} L_{12}^T x, w = 0\} \subset \mathbf{R}^{2m}$$

are invariant sets of the dynamical system (2.15). Consequently the dynamics satisfying the effective equation (2.16) are exact in the sense that $x^\epsilon(t) = x(t)$ holds independently of ϵ provided that $(y_0, w_0) \in M(x)$.

3 The generator

We shall study the ordinary differential equation

$$\dot{z} = f(z), \quad z(0) = z_0 \tag{3.1}$$

for $z \in \mathcal{Z} \subseteq \mathbf{R}^n$. The actual choice of state space (phase space) \mathcal{Z} will depend on the problem; typically $\mathcal{Z} = \mathbf{R}^n$, or we will choose $\mathcal{Z} = \mathbf{T}^n$ to be the n -dimensional flat torus (periodic boundary conditions). If the vector field $f: \mathcal{Z} \rightarrow T\mathcal{Z}$ is globally Lipschitz, equation (3.1) has a unique solution

$$\varphi^t: \mathcal{Z} \rightarrow \mathcal{Z}, \quad z(t) = \varphi^t(z_0).$$

Now consider the linear operator $\mathcal{L}: C^1(\mathcal{Z}) \rightarrow C^1(\mathcal{Z})$ defined by

$$\mathcal{L}u = f(z) \cdot \nabla u(z). \tag{3.2}$$

For any continuously differentiable function $u \in C^1(\mathcal{Z}, \mathbf{R})$ (observable) the operator \mathcal{L} “generates” the time evolution of u under the flow φ^t . To see this, compute

$$\begin{aligned} \frac{d}{dt}u(\varphi^t(z)) &= \nabla u(\varphi^t(z)) \cdot \frac{d}{dt}\varphi^t(z) \\ &= \nabla u(\varphi^t(z)) \cdot f(\varphi^t(z)) \\ &= \mathcal{L}u(\varphi^t(z)). \end{aligned}$$

Formally, we can view the evolution equation

$$\frac{du}{dt} = \mathcal{L}u$$

as an ordinary differential equation on a function space (here: $C^1(\mathcal{Z}, \mathbf{R})$). Defining the usual scalar product in the Hilbert space $L^2(\mathcal{Z})$,

$$\langle u, v \rangle_{L^2} = \int_{\mathcal{Z}} u(z)v(z) dz,$$

we can introduce the formal adjoint of \mathcal{L} by means of $\langle \mathcal{L}u, v \rangle_{L^2} = \langle u, \mathcal{L}^*v \rangle_{L^2}$, that is,

$$\int_{\mathcal{Z}} (f \cdot \nabla u) v dz = - \int_{\mathcal{Z}} \nabla \cdot (vf) u dz$$

where we impose either periodic boundary conditions for $\mathcal{Z} = \mathbf{T}^n$ or growth conditions at infinity in case of $\mathcal{Z} = \mathbf{R}^n$ such that no boundary terms appear. Hence

$$\mathcal{L}^*v = -f(z) \cdot \nabla v(z) - v(z) \operatorname{div} f(z). \quad (3.3)$$

3.1 The backward equation

Consider the Cauchy problem (initial value problem)

$$\begin{aligned} \partial_t u(z, t) &= \mathcal{L}u(z, t), \quad (z, t) \in \mathcal{Z} \times]0, \infty[\\ u(z, 0) &= \phi(z), \quad z \in \mathcal{Z} \end{aligned} \quad (3.4)$$

the formal solution of which is given by

$$u(z, t) = (\exp(t\mathcal{L})\phi)(z).$$

The last identity can be readily verified by differentiation with respect to time. The operator $T_t = \exp(t\mathcal{L})$ is referred to as the *semigroup* generated by \mathcal{L} , or, simply, the semigroup of \mathcal{L} . It is easy to see that T_t satisfies $T_0 = \operatorname{Id}$ and $T_{t+s} = T_t \circ T_s$; an inverse does not necessarily exist, hence T_t does not form a group in general.

An obvious question concerns the relation between the semigroup T_t and the solutions of (3.1). This issue is addressed by the following theorem:

Theorem 3.1 (see, e.g., Pavliotis & Stuart, 2008) *Let $\varphi^t: \mathcal{Z} \rightarrow \mathcal{Z}$ be the one-parameter group of solutions to (3.1), and suppose that the partial differential equation (3.4) has a (strong) solution (i.e., the initial data ϕ are sufficiently smooth). Then*

$$u(z, t) = \phi(\varphi^t(z))$$

is the solution of (3.4) for all $t > 0$ and $z \in \mathcal{Z}$.

Proof. First of all notice that $\varphi^0 = \operatorname{Id}$. Hence the function $u(z, 0) = \phi(\varphi^0(z)) = \phi(z)$ satisfies the initial condition in (3.4). As for $t > 0$, recall that φ^{-t} is the inverse of φ^t . Therefore $u(\varphi^{-t}(z), t) = \phi(z)$ by which we conclude that

$$\frac{d}{dt}u(\varphi^{-t}(z), t) = 0.$$

Using chain rule, the last equation entails

$$\frac{\partial}{\partial t}u(\varphi^{-t}(z), t) + \nabla u(\varphi^{-t}(z), t) \cdot \frac{d}{dt}\varphi^{-t}(z) = 0.$$

Since φ^{-t} is the solution of (3.1) with reversed time,

$$\frac{d}{dt}\varphi^{-t}(z) = -f(\varphi^{-t}(z)),$$

the above equation is equal to

$$\frac{\partial}{\partial t}u(\varphi^{-t}(z), t) - \nabla u(\varphi^{-t}(z), t) \cdot f(\varphi^{-t}(z)) = 0.$$

Upon replacing $\varphi^{-t}(z)$ by z this is equivalent to (3.4), and so the assertion follows. \square

Theorem 3.1 states that the solution of the partial differential equation (3.4) is obtained by following the initial condition ϕ along the solution curves of the ordinary differential equation (3.1). This can be rephrased by saying that $u(z, t) = \phi(\varphi^t(z))$ yields the solution of the transport equation (3.4) using the method of characteristics.

Infinitesimal generator So far we have defined the generator \mathcal{L} acting on functions that are differentiable. Setting

$$T_t: L^\infty(\mathcal{Z}) \rightarrow L^\infty(\mathcal{Z}), \quad (T_t\phi)(z) = \phi(\varphi^t(z))$$

we may nonetheless extend the semigroup $T_t = \exp(t\mathcal{L})$ to functions ϕ that are bounded on \mathcal{Z} . In this case, we can define the *infinitesimal generator* of T_t by

$$\mathcal{L}\phi = \lim_{h \rightarrow 0} \frac{T_h\phi - \phi}{h} \quad (3.5)$$

provided that the limit exists in $L^\infty(\mathcal{Z})$. The set of functions for which (3.5) exists is called the domain of definition of \mathcal{L} and is denoted by $\mathcal{D}(\mathcal{L})$. Notice that on $C^1 \subset L^\infty$ (i.e., assuming differentiability) the definition of the generator coincides with (3.2).

3.2 The forward equation (Liouville equation)

Let us study how the situation changes, when we place a probability measure on \mathcal{Z} . That is, rather than solving the initial value problem (3.1) we look at the solutions of

$$\dot{z} = f(z), \quad z(0) \sim \rho_0$$

where ρ_0 is any given probability distribution for $z_0 \in \mathcal{Z}$. The randomness in the initial conditions z_0 implies that the solutions $z(t) = \varphi^t(z_0)$ are now random variables for each $t \geq 0$. The law of $z = z(t, \omega)$ where $\omega \in \Omega$ denotes the possible outcomes of z that are drawn from a sample space Ω is governed by the forward equation

$$\begin{aligned} \partial_t \rho(z, t) &= \mathcal{L}^* \rho(z, t), \quad (z, t) \in \mathcal{Z} \times]0, \infty[\\ \rho(z, 0) &= \rho_0(z), \quad z \in \mathcal{Z} \end{aligned} \quad (3.6)$$

which is the adjoint to the backward equation (3.4) and is often termed the *Liouville equation*. On the Hilbert space $L^2(\mathcal{Z})$, the operator \mathcal{L}^* is given by (3.3), supposing that ρ is differentiable. It has the formal solution

$$\rho(z, t) = (\exp(t\mathcal{L}^*)\rho_0)(z)$$

where $T_t^* = \exp(t\mathcal{L}^*)$ is the adjoint of the semigroup T_t . To see that $\exp(t\mathcal{L}^*)$ indeed is the same as $\exp(t\mathcal{L})^*$, we first of all notice that $T_t\mathcal{L} = \mathcal{L}T_t$, for

$$\begin{aligned} \mathcal{L}T_t\phi &= \lim_{h \rightarrow 0} \frac{T_h(T_t\phi) - T_t\phi}{h} \\ &= T_t \lim_{h \rightarrow 0} \frac{T_h\phi - \phi}{h} \\ &= T_t\mathcal{L}\phi \end{aligned}$$

where we have used the semigroup property $T_h \circ T_t = T_{t+h} = T_t \circ T_h$ in the second equality. The fact that the semigroup commutes with its generator can be used to show that $\partial_t T_t \phi = \mathcal{L} T_t \phi = T_t \mathcal{L} \phi$. Now consider a function g that lies in the domain of \mathcal{L}^* . Clearly, the function $t \mapsto \langle g, T_t \phi \rangle$ is differentiable, and thus

$$\begin{aligned} \partial_t \langle g, T_t \phi \rangle &= \langle T_t^* g, \mathcal{L} \phi \rangle \\ &= \langle \mathcal{L}^* T_t^* g, \phi \rangle \end{aligned}$$

by which it follows that $T_t^* = \exp(t\mathcal{L}^*)$ is the solution operator to (3.6).

Typically, $T_t^*: L^1(\mathcal{Z}) \rightarrow L^1(\mathcal{Z})$ which is the formal adjoint of $T_t: L^\infty(\mathcal{Z}) \rightarrow L^\infty(\mathcal{Z})$ in $L^2(\mathcal{Z})$. As we will see below the adjoint semigroup T_t^* has the interpretation of transporting densities on phase space, so it makes sense to let T_t^* act on functions that are integrable (i.e., normalisable). In accordance with the previous considerations, we can define the infinitesimal generator of the adjoint semigroup by

$$\mathcal{L}g = \lim_{h \rightarrow 0} \frac{T_h^* g - g}{h}$$

provided the limit exists in $L^1(\mathcal{Z})$. Note that on C^1 which is a dense subset of L^1 (i.e., we can approximate any integrable function by a finite number of continuous ones) the definition of \mathcal{L}^* coincides with (3.3). Now we can state the next theorem.

Theorem 3.2 (Propagation of densities) *Let $\varphi^t: \mathcal{Z} \rightarrow \mathcal{Z}$ the solution of (3.1) with random initial conditions $z(0) = z_0$ that are distributed according to some probability distribution ρ_0 . Then $z(t) = \varphi^t(z_0)$ is a random variable with law $\rho_t(z) = \rho(z, t)$.*

Proof. It basically suffices to show that φ^t preserves expectation values. For a function $\phi: \mathcal{Z} \rightarrow \mathbf{R}$, define the expectation with respect to ρ_0 by

$$\mathbf{E}_{\rho_0} \phi(z) = \int_{\mathcal{Z}} \phi(z) \rho_0(z) dz.$$

Now consider $(T_t \phi)(z) = \phi(\varphi^t(z))$, and note that for $\phi \in L^2(\mathcal{Z})$ we can write

$$\mathbf{E}_{\rho_0} \phi = \langle \phi, \rho_0 \rangle_{L^2}.$$

Hence

$$\begin{aligned} \mathbf{E}_{\rho_0} \phi(\varphi^t(z)) &= \int_{\mathcal{Z}} (T_t \phi)(z) \rho_0(z) dz \\ &= \int_{\mathcal{Z}} \phi(z) (T_t^* \rho_0)(z) dz \\ &= \int_{\mathcal{Z}} \phi(z) \rho(z, t) dz \\ &= \mathbf{E}_{\rho_t} \phi(z). \end{aligned}$$

This implies that, for any measurable set $A \subset \mathcal{Z}$,

$$\mathbf{P}(z \in A) = \mathbf{E}_{\rho_t} \chi_A(z)$$

with χ_A being the characteristic function of A by which the assertion is proved. \square

Remark 3.3 The identity $\mathbf{E}_{\rho_0} \phi(z) = \mathbf{E}_{\rho_t} \phi(z)$ is the classical analogue of the famous dichotomy of Schrödinger and Heisenberg picture in quantum mechanics. It states that we can represent the time evolution of expectation values by either letting the observables evolve while keeping the initial densities fixed or letting the densities evolve while keeping the observables fixed. Both viewpoints are in fact equivalent.

3.3 Invariant measures

An important notion is that of an invariant measure: recall that a set $A \subset \mathcal{Z}$ is called invariant if $\varphi^t(A) \subseteq A$. Accordingly, a probability measure μ is called invariant if

$$\mu(\varphi^t(A)) = \mu(A).$$

Let us suppose that μ is absolutely continuous with respect to Lebesgue measure on \mathcal{Z} , i.e., we may write $d\mu = \rho dz$. In this case invariance means

$$\partial_t \int_A \rho(z, t) dz = 0 \quad \Leftrightarrow \quad \mathcal{L}^* \rho = 0.$$

Therefore invariant densities are stationary solutions $\rho = \rho_\infty$ of the forward equation (3.6). A particular instance of a stationary solution in case of divergence-free vector fields f is the constant function $\rho_\infty = 1$. If $\operatorname{div} f = 0$, the adjoint generator satisfies $\mathcal{L}^* = -\mathcal{L}$, hence $\mathcal{L}^* 1 = 0$ and Lebesgue measure $d\mu = dz$ is preserved.²

For the sake of illustration we shall discuss a couple of examples.

Example 3.4 (Hamiltonian system) Let $\mathcal{Z} = \mathbf{R}^{2d}$ be even-dimensional. A prominent example of a divergence-free vector field is the Hamiltonian system

$$\dot{z} = J \nabla H(z), \quad z(0) = z_0$$

where $H: \mathcal{Z} \rightarrow \mathbf{R}$ is called the system's Hamiltonian (total energy), and $J = -J^T \in \mathbf{R}^{2n \times 2n}$ is a constant skew-symmetric matrix. On the space of continuously differentiable functions the infinitesimal generator reads

$$\mathcal{L} = J \nabla H(z) \cdot \nabla.$$

As following from the skew-symmetry of J , Hamiltonian vector-fields are divergence-free, i.e., $\nabla \cdot J \nabla H = 0$, and so the adjoint generator is simply given by $\mathcal{L}^* = -\mathcal{L}$. Moreover it can be readily checked that any smooth function of the Hamiltonian is a stationary solution of the Hamiltonian,

$$\mathcal{L}^* g(H) = -J \nabla H \cdot \nabla H g'(H) = 0,$$

for $Jv \cdot v = -v \cdot Jv = 0$ holds true for all $v \in \mathbf{R}^{2d}$.

Example 3.5 (Harmonic oscillator) Consider the harmonic oscillator in 1D

$$m\ddot{q} = -\omega q, \quad q(0) = q, \quad v(0) = v$$

which is Hamiltonian with

$$H(q, p) = \frac{1}{2m} p^2 + \frac{\omega}{2} q^2, \quad p = m\dot{q}$$

and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Thus the equation above can be recast in

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p}, & q(0) &= q \\ \dot{p} &= -\frac{\partial H}{\partial q}, & p(0) &= mv. \end{aligned}$$

Since Hamiltonian vector fields are divergence-free, the Lebesgue measure $d\lambda = dqdp$ is preserved, but there are infinitely many other invariant measures as we conclude from the considerations in the last example.

Furthermore the system admits a one-parameter family of invariant sets that are ellipses and which are parametrised by the Hamiltonian. To see this, note that the energy H is an integral of motion, i.e.,

$$\frac{d}{dt} H(q(t), p(t)) = - \left. \frac{\partial H}{\partial q} \frac{\partial H}{\partial p} \right|_t + \left. \frac{\partial H}{\partial p} \frac{\partial H}{\partial q} \right|_t = 0.$$

² However, for $\mathcal{Z} = \mathbf{R}^n$ the constant density $\rho_\infty = 1$ is clearly not normalisable, i.e., $\rho_\infty \notin L^1(\mathcal{Z})$.

Equivalently, we have $\mathcal{L}H = 0$. Hence for all $E > 0$ the solution curves of the one-dimensional harmonic oscillator are the level sets $H = E$ which given by

$$H^{-1}(E) = \left\{ (q, p) \in \mathbf{R}^2 : \frac{\omega q^2}{2} + \frac{p^2}{2m} = E \right\}.$$

Example 3.6 (Stable linear system) Let $A \in \mathbf{R}^{n \times n}$ be such that all its eigenvalues have strictly negative real part. In this case the linear system

$$\dot{z} = Az, \quad z(0) = z_0$$

has a unique asymptotically stable fixed point $z = 0$. The corresponding unique invariant measure μ is the point measure located at zero, i.e., $\mu(z) = \delta(z)$ where δ denotes the Dirac measure. The measure μ is normalisable since, by definition,

$$\int_{\mathcal{Z}} \delta(z) dz = 1,$$

but it is singular with respect to Lebesgue measure. In particular there is no density function $\rho_\infty \in L^1(\mathcal{Z})$ that would satisfy $\mathcal{L}^* \rho_\infty = 0$.

4 Invariant manifolds: geometric singular perturbation theory

Consider the following system of singularly perturbed ordinary differential equation

$$\begin{aligned} \dot{x} &= f(x, y), & x(0) &= x_0 \\ \epsilon \dot{y} &= g(x, y), & y(0) &= y_0 \end{aligned} \tag{4.1}$$

for $(x, y) \in \mathbf{R}^n \times \mathbf{R}^m$ and $0 < \epsilon \ll 1$. Here and in the following we omit the parameter ϵ , i.e., we write $x = x^\epsilon$, $y = y^\epsilon$ and so on; the meaning should be always clear from the context and we indicate otherwise when not. We let $\varphi_\xi^t : \mathbf{R}^m \rightarrow \mathbf{R}^m$, $y(t) = \varphi_\xi^t(y_0)$ denote the solution of the associated system

$$\dot{y} = g(\xi, y), \quad y(0) = y_0 \tag{4.2}$$

and recall that the first (i.e., slow) equation in (4.1) can be approximately viewed as an equation of the form

$$\dot{x} = f(x, \varphi_x^{t/\epsilon}(y_0)), \quad x(0) = x_0.$$

Let us suppose that

$$\lim_{t \rightarrow \infty} \varphi_\xi^t(y_0) = m(\xi)$$

exists independently of the initial value $y(0) = y_0$ and uniformly in $x = \xi$, i.e., the rate of convergence is independent of the slow variable. In particular,

$$\lim_{\epsilon \rightarrow 0} \varphi_x^{t/\epsilon}(y_0) = m(x)$$

for fixed t , and, by the above argument, we may replace (4.1) by the equation

$$\dot{x} = f(x, m(x)), \quad x(0) = x_0$$

whenever ϵ is sufficiently small. We shall give an example.

Example 4.1 Consider the linear system

$$\begin{aligned} \dot{x} &= A_{11}x + A_{12}y, & x(0) &= x_0 \\ \epsilon \dot{y} &= A_{21}x + A_{22}y, & y(0) &= y_0. \end{aligned}$$

We suppose that $\sigma(A_{22}) \subset \mathbf{C}^-$, i.e., all eigenvalues of A_{22} lie in the open left complex half-plane. As we shall see this is equivalent to the statement that the fast subsystem is asymptotically stable. The associated system

$$\dot{y} = A_{22}(y + A_{22}^{-1}A_{21}\xi), \quad y(0) = y_0$$

is easily solvable using variation of constants, viz.,

$$\varphi_{\xi}^t(y_0) = \exp(tA_{22})(y + A_{22}^{-1}A_{21}\xi) - A_{22}^{-1}A_{21}\xi.$$

Note that A_{22} is invertible by the stability assumption above. Furthermore

$$\varphi_{\xi}^t(y_0) \rightarrow -A_{22}^{-1}A_{21}\xi \quad \text{as } t \rightarrow \infty.$$

The vector field for a planar linear system with $A_{11} = A_{22} = -1$ and $A_{12} = A_{21} = -1/2$ is shown in Figure 2 below. The leftmost plot shows various solutions for ϵ whereas the right figure depicts solutions (blue curves) for $\epsilon = 0.05$. It turns out that the solutions quickly converge to the nullcline $\dot{y} = 0$ (fast dynamics) before converging to the asymptotically stable fixed point $(x, y) = (0, 0)$ along the nullcline (slow dynamics). Note that the nullcline corresponds to the invariant subspace that is defined by the equation $A_{21}x + A_{22}y = 0$. If $A_{22} < 0$, the subspace is attractive (i.e., asymptotically stable).

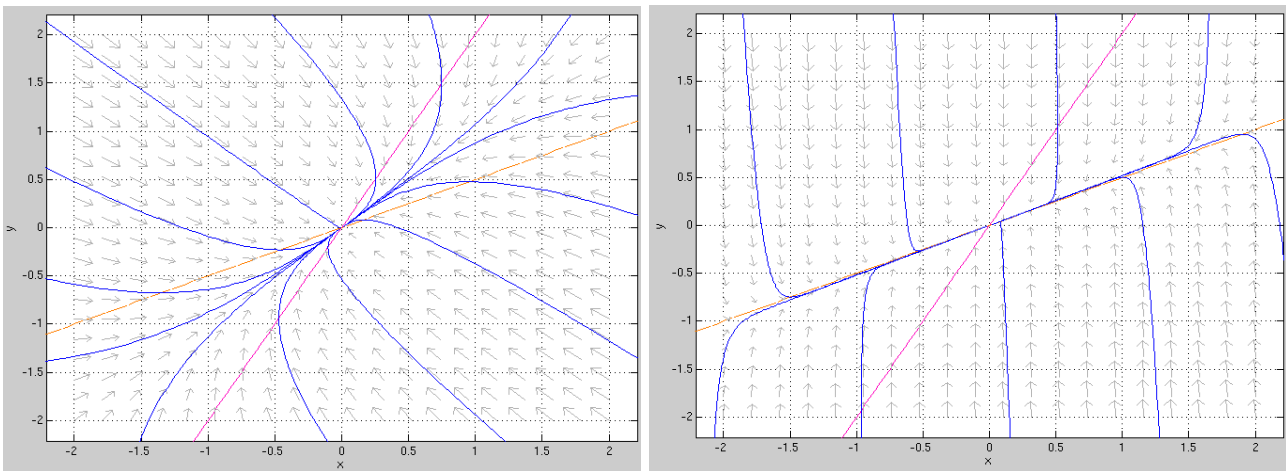


Fig. 2 Planar linear system $A_{11} = A_{22} = -1$, $A_{12} = A_{21} = -1/2$ for $\epsilon = 1$ (left panel) and $\epsilon = 0.05$ (right panel). The orange line shows the nullcline $\dot{y} = 0$.

4.1 Effective equations of motion

Let $\varphi^t : \mathbf{R}^{n+m} \rightarrow \mathbf{R}^{n+m}$ be the solution (flow map) of (4.1). A set $M \subseteq \mathbf{R}^{n+m}$ is called invariant under the flow map φ^t , or, for short, an *invariant manifold* if $\varphi^t(M) \subseteq M$. Setting $\epsilon = 0$ in (4.1) assuming that the right hand sides of the equations remain bounded, our slow/fast system degenerates to the differential-algebraic equation

$$\begin{aligned} \dot{x} &= f(x, y), & x(0) &= x_0 \\ 0 &= g(x, y), & y(0) &= y_0. \end{aligned} \tag{4.3}$$

Equation (4.3) is called differential-algebraic for the evolution of the variables. The variables $y \in \mathbf{R}^m$ are undetermined but linked to the evolution of the dependent variables $x \in \mathbf{R}^n$ by the algebraic equation $g(x, y) = 0$ (slaving principle). As a consequence the set

$$M = \{(x, y) \in \mathbf{R}^{n+m} : g(x, y) = 0\} \subset \mathbf{R}^{n+m}$$

is invariant under the flow of (4.1). If moreover $\det(\partial g / \partial y|_M) \neq 0$, we can invert the equation $g(x, y) = 0$ in a small neighbourhood of M and solve for the undetermined variables. Calling $y = m(x)$ the local solution of $g(x, y) = 0$ such that M can be represented as the graph $(x, m(x))$, we can replace (4.3) by the effective equation

$$\dot{\bar{x}} = f(\bar{x}, m(\bar{x})), \quad x(0) = x_0 \tag{4.4}$$

where consistency requires that the initial conditions in (4.1) are chosen such that $y(0) = m(x(0))$.

4.2 Perturbation expansion

We shall give a formal derivation of the effective equation (4.4) using a perturbative approach. To this end we follow Fenichel (1979) and suppose that, for $\epsilon > 0$ being sufficiently small, the dynamics of (4.1) admit a family of invariant manifolds

$$M_\epsilon = \{(x, y) \in \mathbf{R}^{n+m} : y = m^\epsilon(x)\} \subset \mathbf{R}^{n+m}$$

that can be represented as the graphs $y = m^\epsilon(x)$ over x . Accordingly, we may refine (4.4) as follows

$$\dot{\bar{x}} = f(\bar{x}, m^\epsilon(\bar{x})), \quad \bar{x}(0) = x. \quad (4.5)$$

Taking the time derivative, we see that the "slaved" variables y satisfy the differential equation

$$\dot{y} = \nabla m^\epsilon(x) \cdot \dot{x}.$$

Inserting the governing vector fields g, f for the leftmost and the rightmost term gives rise to a nonlinear partial differential equation for $m^\epsilon : \mathbf{R}^n \rightarrow \mathbf{R}^m$, namely,

$$\nabla m^\epsilon(x) f(x, m(x)) = \frac{1}{\epsilon} g(x, m(x)). \quad (4.6)$$

We seek a perturbative solution to (4.6) that is of the form

$$m^\epsilon(x) = m_0(x) + \epsilon m_1(x) + \epsilon^2 m_2(x) + \dots$$

By substitution and Taylor expansion about $\epsilon = 0$ we find

$$\begin{aligned} & (\nabla m_0 + \epsilon \nabla m_1 + \dots) \left(f(x, m_0) + \epsilon \left(\frac{\partial f}{\partial y} \Big|_M \right) m_1 + \dots \right) \\ &= \frac{1}{\epsilon} \left(g(x, m_0) + \epsilon \left(\frac{\partial g}{\partial y} \Big|_M \right) m_1 + \dots \right) \end{aligned}$$

where we omitted the arguments in $m_i = m_i(x)$. Equating powers of ϵ yields a hierarchy of equations the first three of which read

$$0 = g(x, m_0) \quad (4.7)$$

$$\nabla m_0 f(x, m_0) = \left(\frac{\partial g}{\partial y} \Big|_M \right) m_1 \quad (4.8)$$

$$\frac{1}{2} m_2^T \left(\frac{\partial^2 g}{\partial y^2} \Big|_M \right) m_2 = \nabla m_1 f(x, m_0) + \nabla m_0 \left(\frac{\partial f}{\partial y} \Big|_M \right) m_1. \quad (4.9)$$

To lowest order we recover the guessed effective equation (4.4) which does not come as a surprise. Note, however, that, the condition on the initial condition is now entailed by the lowest order term, i.e., the validity of the perturbation expansion relies on the property $\varphi_x^{t/\epsilon}(y) \rightarrow m(x)$ with $m = m_0$. As we will see later on this behaviour is related to certain contractivity properties of the fast flow or the invariant manifold, respectively. Proceeding in the hierarchy we find the first-order correction

$$m_1 = \left(\frac{\partial g}{\partial y} \Big|_M \right)^{-1} \nabla m_0 f(x, m_0).$$

Setting $m^\epsilon \approx m_0 + \epsilon m_1$ in (4.5) and doing a Taylor expansion around $\epsilon = 0$, equation (4.4) can be refined according to

$$\dot{\bar{x}} = f_0(\bar{x}) + \epsilon f_1(\bar{x}), \quad \bar{x}(0) = x_0 \quad (4.10)$$

with

$$f_0(x) = f(x, m_0(x)), \quad f_1(x) = \left(\frac{\partial f}{\partial y} \Big|_M \right) \left(\frac{\partial g}{\partial y} \Big|_M \right)^{-1} \nabla m_0(x).$$

Equation (4.10) is the result of a formal perturbation expansion of (4.1) in the neighbourhood of the invariant manifold $M = \{g(x, y) = 0\}$. Nonetheless the formal expansion should not be taken as an assertion regarding convergence to (4.4) in the limit of ϵ going to zero. Bounding the first-order term f_1 presupposes bounds on the vector fields f, g thereby imposing certain regularity conditions (e.g., global Lipschitz continuity). Moreover invertibility of the Jacobian $(\partial g / \partial y|_M)$ and well-posedness of m_0 requires that its eigenvalues are bounded away from zero. In fact, the typical scenarios in which invariant manifolds occur are systems for which the spectrum of $(\partial g / \partial y|_M)$ lies entirely in the open left complex half-plane, i.e., the systems are hyperbolic (contractive) in the fast variables.

Remark 4.2 A final remark is in order. Consider the generator

$$\mathcal{L}^\epsilon = \mathcal{L}_0 + \frac{1}{\epsilon} \mathcal{L}_1$$

of (4.1). The backward equation of the associated system (4.2) reads

$$\partial u(y, t) = \mathcal{L}_1 u(y, t), \quad u(y, 0) = \phi(y).$$

Given the flow $y(t) = \varphi_\xi^t(y)$ of the associated system the solution to the backward equation assumes the form

$$u(y, t) = \phi(\varphi_\xi^t(y)).$$

By the assumption $\varphi_\xi^t \rightarrow m(\xi)$ it therefore follows that

$$u(y, t) \rightarrow \phi(m(\xi)) \quad \text{as } t \rightarrow \infty$$

uniformly on $\mathbf{R}^m \ni y$. Denoting $\phi_\infty = \phi(m(\xi))$, the convergence property $u \rightarrow \phi_\infty$ amounts to a sort of *ergodicity property* or *law of large numbers*, for

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \phi(\varphi_\xi^t(y)) dt \rightarrow \mathbf{E}_\xi \phi$$

for almost all initial conditions $y(0) = y$ and with the conditional expectation

$$\mathbf{E}_\xi \phi = \int \phi(y) \delta(y - m(\xi)) dy$$

where the Dirac measure $\delta(y - m(\xi))$ is invariant under the flow φ_ξ^t .

4.3 Invariant manifolds: convergence issues

Consider the following system of a singularly perturbed ordinary differential equation

$$\begin{aligned} \dot{x} &= f(x, y), & x(0) &= x_0 \\ \epsilon \dot{y} &= g(x, y), & y(0) &= y_0 \end{aligned} \tag{4.11}$$

for $(x, y) \in \mathbf{R}^n \times \mathbf{R}^m$ and $0 < \epsilon \ll 1$. We shall prove that in the limit $\epsilon \rightarrow 0$ the slow component $x(t)$ converges uniformly to $X(t)$ that is governed by the effective equation

$$\dot{X} = f(X, m(X)), \quad X(0) = x_0$$

where $y = m(x)$ is the graph representation of the limiting invariant manifold

$$M = \{(x, y) \in \mathbf{R}^{n+m} : g(x, y) = 0\} \subset \mathbf{R}^{n+m}$$

that the fast dynamics approach as $\epsilon \rightarrow 0$.

Exponential convergence to the invariant manifold We suppose that, for all $\xi \in \mathbf{R}^n$, the solution $\varphi_\xi^t : \mathbf{R}^m \rightarrow \mathbf{R}^m$, $y(t) = \varphi_\xi^t(y_0)$ of the associated (fast) system

$$\dot{y} = g(\xi, y), \quad y(0) = y_0 \quad (4.12)$$

has a unique exponentially attracting fixed point, i.e.,

$$\lim_{t \rightarrow \infty} \varphi_\xi^t(y_0) = m(\xi)$$

uniformly in x and independently of the initial condition $\varphi_\xi^0(y_0) = y_0$. For this purpose, we suppose $g(\xi, m(\xi)) = 0$ with g meeting the following *contractivity condition*: for $\xi \in \mathbf{R}^n$, $y, y' \in \mathbf{R}^m$ and $\alpha > 0$, we have

$$\langle g(\xi, y) - g(\xi, y'), y - y' \rangle \leq -\alpha |y - y'|^2. \quad (4.13)$$

Lemma 4.3 *The contraction condition implies that*

$$|\varphi_\xi^t(y) - m(\xi)| < \exp(-\alpha t) |y - m(\xi)|.$$

Proof. By construction, $\varphi_\xi^t(y)$ solves the initial value problem

$$\frac{d}{dt} \varphi_\xi^t(y) = g(\xi, \varphi_\xi^t(y)), \quad \varphi_\xi^0(y) = y$$

and

$$0 = \frac{d}{dt} m(\xi) = g(\xi, m(\xi)).$$

Hence

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\varphi_\xi^t(y) - m(\xi)|^2 &= \langle g(\xi, \varphi_\xi^t(y)) - g(\xi, m(\xi)), \varphi_\xi^t(y) - m(\xi) \rangle \\ &\leq -\alpha |\varphi_\xi^t(y) - m(\xi)|^2. \end{aligned}$$

The last equation is a differential inequality of the form

$$\frac{d\eta}{dt} \leq -2\alpha\eta, \quad \eta = |\varphi_\xi^t(y) - m(\xi)|^2,$$

and Gronwall's Lemma yields

$$\eta \leq \exp(-2\alpha t) \eta(0).$$

Taking the square root on either side of the last equation gives the assertion. \square

Effective motion The last statement is concerned with the convergence of the fast dynamics to the invariant manifold when the slow variable is fixed, i.e., for $x(t) \equiv \xi$. We shall now relax this assumption and allow for slow variations of x on time intervals of order 1. For the sake of simplicity we implement the following standing assumptions: we suppose that there exists a uniform (Lipschitz) constant $L > 0$ such that

$$\begin{aligned} |f(x, y)| &\leq L \forall (x, y) \in \mathbf{R}^{n+m} \\ |\nabla_x f(x, y)|, |\nabla_y f(x, y)| &\leq L \quad \forall (x, y) \in \mathbf{R}^{n+m} \\ |\nabla m(x)| &\leq L \quad \forall x \in \mathbf{R}^n. \end{aligned} \quad (4.14)$$

Latter property is related to the smoothness of the invariant manifold M and essentially follows from the contraction condition (4.13) on the vector field $g(\cdot, y)$.

Theorem 4.4 *Let X denote the solution of the lowest-order perturbation equation*

$$\dot{X} = \bar{f}(X), \quad X(0) = x_0$$

with $\bar{f}(x) = f(x, m(x))$. Then we can find a constant $C > 0$ such that the solution of the singularly perturbed problem (4.11) satisfies

$$|x - X|^2 \leq C \exp(Lt) (\epsilon |y_0 - m(x_0)| + \epsilon^2)$$

uniformly for all $t \in [0, T]$, $T < \infty$.

Proof. We let (x, y) denote the solution of (4.11), and we define the deviations of the fast variable from the invariant manifold as

$$y = m(x) + \eta.$$

Clearly $\eta \rightarrow 0$ as $\epsilon \rightarrow 0$. In first part of the proof we shall estimate the rate at which η goes to zero. Since

$$\dot{\eta} = \dot{y} - \nabla m(X) \dot{X},$$

the augmented set of variables (X, η, y) is governed by the joint system of equations

$$\begin{aligned} \dot{X} &= \bar{f}(X) \\ \dot{\eta} &= \frac{1}{\epsilon} g(X, m(X) + \eta) - \nabla m(X) \bar{f}(X) \\ \dot{y} &= \frac{1}{\epsilon} g(X, m(X) + \eta) \end{aligned}$$

that is fully equivalent to (4.11). Note that the second equation is the same as

$$\dot{\eta} = \frac{1}{\epsilon} (g(X, m(X) + \eta) - g(X, m(X))) - \nabla m(X) \bar{f}(X)$$

as following from the identity $g(X, m(X)) = 0$. Equation (4.13) now entails that

$$\langle g(X, m(X) + \eta) - g(X, m(X)), \eta \rangle \leq -\alpha |\eta|^2.$$

Taking advantage of the Lipschitz continuity (4.14) and the Cauchy-Schwarz inequality,

$$\langle \nabla m(X) \bar{f}(X, m(X)), \eta \rangle \leq L^2 |\eta|,$$

we obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\eta|^2 &= \langle \eta, \dot{\eta} \rangle \\ &= \frac{1}{\epsilon} \langle g(X, m(X) + \eta) - g(X, m(X)), \eta \rangle - \langle \nabla m(X) \bar{f}(X), \eta \rangle \\ &\leq -\frac{\alpha}{\epsilon} |\eta|^2 + L^2 |\eta|. \end{aligned}$$

Completing the square yields

$$\frac{1}{2} \left(\delta L^2 - \frac{|\eta|}{\delta} \right) > 0 \quad \Rightarrow \quad \frac{1}{2} \left(\delta^2 L^4 + \frac{|\eta|^2}{\delta^2} \right) > L^2 |\eta|$$

for any $\delta \in \mathbf{R}$. By setting $\delta = \sqrt{\epsilon/\alpha}$, we therefore find

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\eta|^2 &\leq -\frac{\alpha}{\epsilon} |\eta|^2 + \frac{1}{2} \left(\delta^2 L^4 + \frac{|\eta|^2}{\delta^2} \right) \\ &\leq -\frac{\alpha}{2\epsilon} |\eta|^2 + \frac{\epsilon}{2\alpha} L^4. \end{aligned}$$

The last equation is again a differential inequality for the squared deviations $|\eta|^2$ and we may employ Gronwall's Lemma to obtain the following bound

$$|\eta(t)|^2 \leq \exp\left(-\frac{\alpha}{2\epsilon} t\right) \left(|\eta(0)|^2 + \frac{\epsilon L^4}{2\alpha} \int_0^t \exp\left(\frac{\alpha}{2\epsilon} s\right) ds \right)$$

or, equivalently,

$$|\eta(t)|^2 \leq \exp\left(-\frac{\alpha}{2\epsilon} t\right) |\eta(0)|^2 + \frac{\epsilon^2 L^4}{\alpha^2} \left(1 - \exp\left(-\frac{\alpha}{2\epsilon} t\right)\right). \quad (4.15)$$

This implies $\eta(t) \rightarrow 0$ as

$$\lim_{\epsilon \rightarrow 0} |\eta(t)|^2 = 0$$

for all $t \in [0, T]$ with $T < \infty$ fixed which completes the first part of the proof. In order to show that this implies convergence $x \rightarrow X$, we note that

$$\dot{x} = f(X, m(X) + \eta)$$

by definition of η . Hence, using the Cauchy-Schwarz and Lipschitz continuity of f ,

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |x - X|^2 &= \langle x - X, f(X, m(X) + \eta) - f(X, m(X)) \rangle \\ &\leq |x - X| |f(X, m(X) + \eta) - f(X, m(X))| \\ &\leq L |x - X| |\eta|. \end{aligned}$$

By completing the square we obtain the inhomogeneous differential inequality

$$\frac{d}{dt} |x - X|^2 \leq L^2 |x - X|^2 + |\eta|^2$$

with $|\eta|^2$ as given by (4.15) above. For $x(0) = X(0)$, Gronwall's Lemma yields

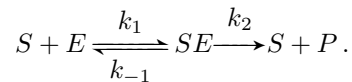
$$|x - X|^2 \leq \int_0^t \exp(L(t-s)) |\eta(s)|^2 ds.$$

The assertion follows upon inserting the upper bound for $|\eta|^2$ in the last inequality and integrating. \square

Remark 4.5 The error bound for $|x - X|^2$ consists of two parts the first of which depends on the deviation of the initial condition $y(0) = y_0$ from the invariant manifold. That is, the first term is due to the initial exponential relaxation of the fast dynamics to the invariant manifold whereas the second term describes the actual approximation error that arises from replacing $f(x, y)$ by $f(x, m(x))$. Notice further that for $\epsilon > 0$ fixed, the approximation error grows exponentially with t , i.e., the for $t = \mathcal{O}(-\ln \epsilon)$ the quadratic approximation error becomes essentially of order 1.

4.4 A problem from enzyme kinetics

As an illustrative example we consider an enzyme-catalysed reactions with single-substrate mechanisms that is due to Michaelis and Menten. The reaction involves a substrate S that is irreversibly converted into a product P by means of an enzyme E ; the back reaction is negligible. The reaction can be systematically written as



The law of mass action states that the rate of concentration change of a specific substrate is proportional to the concentrations of the substrates that are involved in the reaction. Calling C_1, C_2, C_3, C_4 the respective concentrations of S, E, SE and P , the law of mass action yields the nonlinear system of equations

$$\begin{aligned} \dot{C}_1 &= -k_1 C_1 C_2 + k_{-1} C_3, & C_1(0) &= c_1 \\ \dot{C}_2 &= -k_1 C_1 C_2 + (k_{-1} + k_2) C_3, & C_2(0) &= c_2 \\ \dot{C}_3 &= k_1 C_1 C_2 - (k_{-1} + k_2) C_3, & C_3(0) &= 0 \\ \dot{C}_4 &= -k_2 C_3, & C_4(0) &= 0 \end{aligned} \tag{4.16}$$

where the initial conditions are assumed to be non-negative. It is easy to see that

$$\frac{d}{dt} (C_2 + C_3) = \frac{d}{dt} (C_1 + C_3 + C_4) = 0.$$

Consequently the system admits the two constants of motion

$$c_2 = C_2 + C_3 \quad \text{and} \quad c_1 = C_1 + C_3 + C_4$$

which upon substitution allows to simplify (4.16) to the following system of equations

$$\begin{aligned} \dot{C}_1 &= -k_1 C_1 c_2 + (k_1 C_1 + k_{-1}) C_3, & C_1(0) &= c_1 \\ \dot{C}_3 &= k_1 C_1 c_2 - (k_1 C_1 + k_{-1} + k_2) C_3, & C_3(0) &= 0. \end{aligned} \quad (4.17)$$

The chemical picture now is as follows: if the concentration C_1 of the substrate S is high, the enzyme E is entirely saturated and exists only in its complex form ES with concentration C_3 which entails that, after a short relaxation time, the concentration of both the enzyme and the complex quickly converge to a steady-state. In the chemical literature the typical reasoning proceeds by assuming $dC_2/dt \approx 0$. As $C_2 + C_3 = \text{const}$ this entails $dC_3/dt \approx 0$, and the *steady-state approach* consists in solving the second equation in (4.17) for the remaining time-dependent unknown C_1 .

To make this intuitive argument mathematically precise, it is necessary to make equation (4.17) dimensionless. Otherwise it is not possible to distinguish between different time scales as the “smallness” of either dC_1/dt or dC_3/dt depends on the physical dimensions in the equations. (Note that the equation is still nonlinear; hence changing the physical dimension from, say, litres to millilitres affects each term in a different way.) We therefore introduce the dimensionless quantities

$$\tau = k_1 c_2 t, \quad x = \frac{C_1}{c_1}, \quad y = \frac{C_3}{c_2}$$

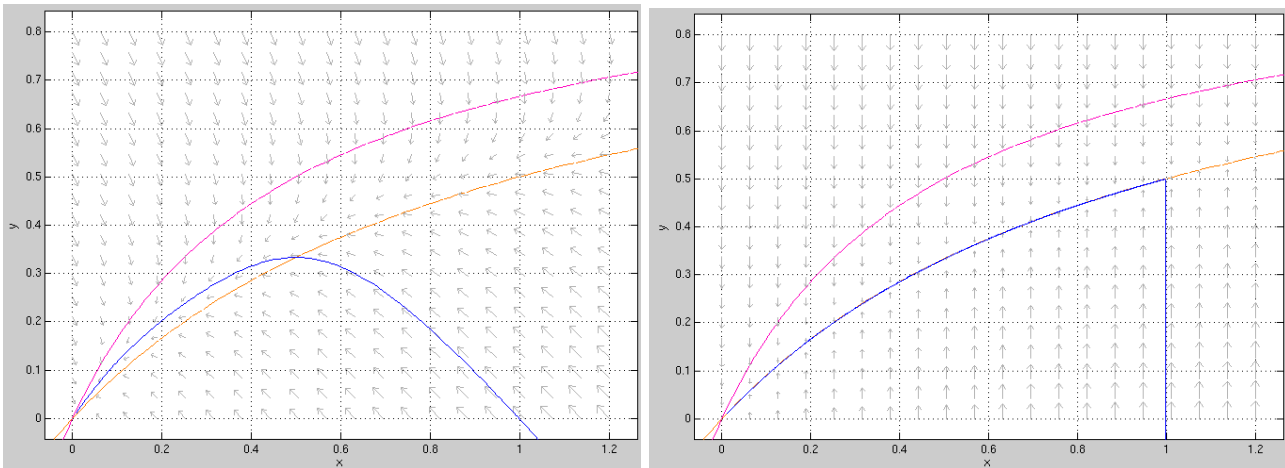


Fig. 3 Michaelis-Menten system for $\epsilon = 1$ (left panel) and $\epsilon = 10^{-4}$ (right panel) and the respective solutions of the initial value problem (blue lines). The orange lines show the nullcline $\dot{y} = 0$.

Using the shorthands

$$\lambda = \frac{k_2}{k_1 c_1}, \quad \mu = \frac{k_{-1} + k_2}{k_1 c_1},$$

equation (4.17) turns out to be equivalent to the dimensionless equation

$$\begin{aligned} \frac{dx}{d\tau} &= -x + (x + \mu - \lambda)y, & x(0) &= 1 \\ \epsilon \frac{dy}{d\tau} &= x - (x + \mu)y, & y(0) &= 0. \end{aligned} \quad (4.18)$$

The small parameter $\epsilon = c_2/c_1$ that is typically of the order $\epsilon \sim 10^{-6}$. Letting ϵ go to zero, (4.18) reduces to the differential-algebraic equation

$$\begin{aligned} \frac{dX}{d\tau} &= -X + (X + \mu - \lambda)Y, & X(0) &= 1 \\ 0 &= X - (X + \mu)Y. \end{aligned} \quad (4.19)$$

Solving the second equation for $Y = m(X)$ immediately reveals

$$m(X) = \frac{X}{X + \mu}. \quad (4.20)$$

However we have picked the initial condition $Y(0) = 0$ in (4.18) which does not satisfy $Y(0) = m(X(0))$. That is, the initial conditions do not lie on the invariant manifold $Y = m(X)$, and we expect the solution for $\epsilon > 0$ to exhibit some initial layer behaviour due to the relaxation to equilibrium. Replacing Y by $m(X)$ in equation (4.19) finally yields the reduced system for $\epsilon = 0$,

$$\frac{dX}{d\tau} = -\lambda \frac{X}{X + \mu}, \quad X(0) = 1. \quad (4.21)$$

Figure 3 below shows phase portraits of (4.18) for two different values of ϵ . It turns out that for $\epsilon = 1$ the solution reaches the invariant manifold just before it eventually collapses to the unique fixed point $(x, y) = (0, 0)$. For $\epsilon = 10^{-4}$, however, the initial value problem converges almost instantaneously to the invariant manifold $Y = m(X)$ and then evolves to its rest point along the nullcline (i.e., its invariant manifold).

5 Averaging: eliminating fast degrees of freedom

As an example let us consider a particle of mass m on the real line that is moving in a harmonic well (see Figure 4 below). The total energy of the particle is given by the Hamiltonian $H = T + V$ that is the sum of kinetic and potential energy, i.e.,

$$H: \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}, \quad H = \frac{1}{2m}p^2 + \frac{k}{2}(r - r_0)^2$$

where $k > 0$ is the spring constant (Hooke's law). It is convenient to introduce the new variable $q = r - r_0$. Letting v denote the particle's velocity, Hamilton's equations boil down to the system of equations

$$\begin{aligned} \dot{q} &= \frac{1}{m}p, & q(0) &= q_0 \\ \dot{p} &= -kq, & p(0) &= mv_0. \end{aligned} \quad (5.1)$$

Inconsistent limit equations For any nonzero initial condition the solution will describe oscillations of the particle around $q = 0$ and $v = 0$, and we may ask what happens if we let the mass go to zero. Obviously the system (5.1) is equivalent to

$$m\ddot{q} = -kq, \quad q(0) = q_0, \quad \dot{q}(0) = v_0. \quad (5.2)$$

Say, we choose initial values $q_0 \neq 0$ and $v_0 = 0$. For all $m > 0$, the solutions of the last equation are linear combinations of sine and cosine functions, hence uniformly bounded at all times. Consequently $q(t) \rightarrow 0$ as $m \rightarrow 0$ uniformly for all $t \in]0, \infty[$. Note, however, that we have assumed that $q_0 \neq 0$, i.e., the limit dynamics are inconsistent with the initial condition. Indeed given our choice of initial conditions, the solution for $\epsilon = \sqrt{m} > 0$ and $\omega = \sqrt{k} > 0$ is given by

$$q(t) = q_0 \sin\left(\frac{\omega t}{\epsilon}\right),$$

so neither q nor \dot{q} converge as ϵ goes to zero; instead, the solutions wildly oscillate around zero. Notice that $p = \epsilon^2 \dot{q} \rightarrow 0$ uniformly on $[0, \infty[$, including convergence of the initial value. Together with the limit equation $q = 0$ above this suggests that the particle is completely at rest, i.e., has zero energy $H = 0$. Still, we know that Hamiltonian flows preserve energy, i.e.,

$$\frac{d}{dt}H(q(t), p(t)) = 0$$

for all values of $\epsilon = \sqrt{m}$ as can be readily checked upon using chain rule and inserting (5.1); see Example 3.4 for details. For nonzero initial condition $q_0 \neq 0$, we have $H \neq 0$ which yields a contradiction. So, what is wrong with the above reasoning?

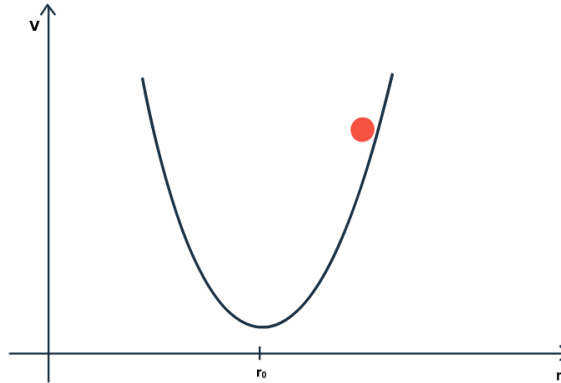


Fig. 4 Particle oscillating in a parabolic potential V .

5.1 Action-angle variables

We shall find appropriate coordinates by which we can represent (5.1) or (5.2) as a slow/fast system. Clearly, the total energy H is conserved by the flow which makes it (or functions thereof) a good candidate for a slow variable. We introduce

$$I = H(q, p)/\omega, \quad \varphi = \arctan\left(\frac{p}{\epsilon q}\right). \quad (5.3)$$

as new variables where $I > 0$ and $\varphi \in S^1$ is periodic. The new variables (I, φ) can be considered a form of specifically scaled polar coordinates and are known by the name of action-angle variables. In terms of (I, φ) the equations of motion (5.1) assume a particularly simple form, namely,

$$\begin{aligned} \dot{I} &= 0, & I(0) &= \frac{1}{2\omega} q_0^2 \\ \dot{\varphi} &= -\frac{\omega}{\epsilon}, & \varphi(0) &= 0 \end{aligned} \quad (5.4)$$

where we have used that $v_0 = 0$ and remind the reader that $\omega = \sqrt{k}$. Up to time rescaling $t \mapsto \epsilon t$, the system (5.4) is Hamiltonian with the energy

$$H : \mathbf{R}_+ \times S^1 \rightarrow \mathbf{R}, \quad H = I\omega.$$

It is an instance of an integrable system with the trivial solution

$$I \equiv \frac{1}{2\omega} q^2, \quad \varphi(t) = -\frac{\omega t}{\epsilon} \bmod 2\pi.$$

Hence the fast variable turns out to be the periodic fast angle which, coming back to our original problem (5.1), amounts to fast oscillations around the equilibrium position $q = 0$. Since the solution of (5.2) can be recast in

$$q(t) = q_0 \cos \varphi(t),$$

and as the angle moves around the circle S^1 at constant angular velocity ω/ϵ , taking the limit $\epsilon \rightarrow 0$ results in averaging over the fast angle. That is, we have

$$\lim_{\epsilon \rightarrow 0} q(t) = \frac{q_0}{2\pi} \int_0^{2\pi} \cos \varphi d\varphi$$

which vanishes identically for $t > 0$ and arbitrary initial conditions $q(0) = q_0$. The last formula describes the application of the averaging principle for highly-oscillatory systems and agrees with the intuitive idea that infinitely fast oscillations around an equilibrium point effectively result in a quasi-stationary state with nonzero energy.

5.2 Averaging of highly-oscillatory systems

Typically, highly-oscillatory systems assume the more general form

$$\begin{aligned} \dot{I} &= f(I, \varphi), & I(0) &= I_0 \\ \dot{\varphi} &= -\frac{\omega(I)}{\epsilon} + g(I, \varphi), & \varphi(0) &= \varphi_0 \end{aligned} \quad (5.5)$$

for $(I, \varphi) \in \mathbf{R}_+^n \times \mathbf{T}^n$, $\mathbf{T}^n = S^1 \times \dots \times S^1$ and $0 < \epsilon \ll 1$ where f, g are smooth 2π -periodic functions. Upon rescaling of time, equation (5.5) is Hamiltonian with

$$H : \mathbf{R}_+^n \times \mathbf{T}^n \rightarrow \mathbf{R}, \quad H = \langle I, \omega(I) \rangle + \epsilon H_1(I, \varphi)$$

where we suppose that $f = \partial H_1 / \partial \varphi$ and $g = -\partial H_1 / \partial I$. Equation (5.5) describes a rapidly oscillating multi-frequency system: on times of order 1 (note that we have rescaled time), the action variables are effectively constants of motion whereas on times of order $1/\epsilon$ the action variables slowly drift with superimposed oscillations (see Figure 5). We assume that the unperturbed oscillation frequencies $\omega_i(I)$ are all strictly larger than zero and moreover meet the following *diophantine condition*

$$|\langle \omega(I), \mathbf{k} \rangle| \geq \delta \quad \forall \mathbf{k} \in \mathbf{Z}^n \setminus 0. \quad (5.6)$$

The reason for this technical assumption will become clear in a moment. Roughly speaking the diophantine condition reflects the requirement that the frequencies are rationally independent which excludes periodic or quasi-periodic orbits. In other words, the unperturbed fast dynamics will cover the whole torus rather than a low-dimensional subset of measure zero as it would the case for periodic motion.

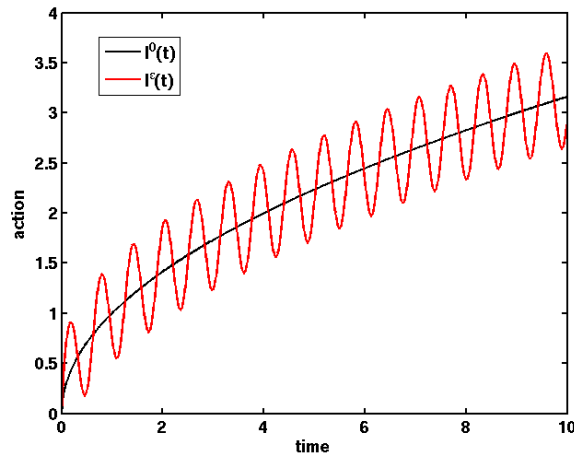


Fig. 5 Slowly evolving action with rapid oscillation

In order to derive an effective equation for the singularly perturbed system (5.5) we follow the general strategy and consider the corresponding backward Liouville equation. Letting $X_H = (\partial H / \partial \varphi, -\partial H / \partial I)$ denote the Hamiltonian vector field above, the infinitesimal generator $\mathcal{L}^\epsilon = \epsilon^{-1} X_H \cdot \nabla$ can be split according to

$$\mathcal{L}^\epsilon = \mathcal{L}_0 + \frac{1}{\epsilon} \mathcal{L}_1$$

with

$$\mathcal{L}_0 = f(I, \varphi) \cdot \frac{\partial}{\partial I} + g(I, \varphi) \cdot \frac{\partial}{\partial \varphi}, \quad \mathcal{L}_1 = -\omega(I) \cdot \frac{\partial}{\partial \varphi}.$$

Thus, we seek a perturbative solution to the linear operator equation

$$\partial_t u^\epsilon(I, \varphi, t) = \mathcal{L}^\epsilon u^\epsilon(I, \varphi, t), \quad u^\epsilon(I, \varphi, 0) = \phi(I, \varphi) \quad (5.7)$$

that is of the form

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$$

Inserting the ansatz into (5.7) and equating equal powers of ϵ yields a hierarchy of equations the first three of which read

$$\mathcal{L}_1 u_0 = 0 \tag{5.8}$$

$$\mathcal{L}_1 u_1 = \partial_t u_0 - \mathcal{L}_0 u_0 \tag{5.9}$$

$$\mathcal{L}_1 u_2 = \partial_t u_1 - \mathcal{L}_0 u_1. \tag{5.10}$$

Stepping through the equations, the first one implies that $u_0 \in \ker \mathcal{L}_1$ subject to the requirement that $u_0 = u_0(I, \varphi)$ is 2π -periodic in each of its angular arguments $\varphi_i \in S^1$. Since \mathcal{L}_1 is a differential operator acting in φ only, functions that are constant in φ are obviously in the nullspace of \mathcal{L}_1 . As we will argue below, the diophantine condition (5.6) guarantees that no other periodic functions solve the stationary equation $\mathcal{L}_1 u = 0$.

The time evolution of u_0 is due to the second equation, and we are aiming at the lowest-order approximation $u^\epsilon \approx u_0$. By the Fredholm alternative, equation (5.9) has a solution if and only if the right hand side is orthogonal to the kernel of \mathcal{L}_1^* . As $\mathcal{L}_1^* = -\mathcal{L}_1$ is the formal adjoint with respect to the $L^2(\mathbf{T}^n)$ scalar product

$$\langle u, v \rangle_{L^2} = \int_{\mathbf{T}^n} uv \, d\varphi,$$

the stationary densities, i.e., the nontrivial solutions of $\mathcal{L}_1^* \rho = 0$ are constant on the torus. Hence $\rho_\infty = \mathbf{1}(\varphi)$ is the unique stationary probability density of the fast dynamics.³ Specifically, the normalized Lebesgue measure on the torus,

$$d\mu(\varphi) = (2\pi)^{-n} d\varphi,$$

is the unique invariant measure of the oscillatory fast dynamics. If we integrate the right hand side of equation (5.9) with respect to $d\mu = \rho_\infty d\varphi$, the solvability condition (Fredholm alternative with $\rho_\infty \in \ker \mathcal{L}_1^*$ and L^2 scalar product) implies that

$$\int_{\mathbf{T}^n} (\partial_t u_0 - \mathcal{L}_0 u_0) d\mu(\varphi) = 0.$$

Since u_0 does not depend upon φ , it follows that

$$\mathcal{L}_0 u_0 = f(I, \varphi) \cdot \frac{\partial u_0}{\partial I},$$

and so the solvability condition reduces to the backward equation

$$\partial_t u_0(I, t) = \bar{\mathcal{L}} u_0(I, t), \quad u_0(I, 0) = \phi_0(I) \tag{5.11}$$

with the averaged Liouvillian

$$\bar{\mathcal{L}} = \frac{1}{(2\pi)^n} \int_{\mathbf{T}^n} f(I, \varphi) d\varphi \cdot \frac{\partial}{\partial I}. \tag{5.12}$$

The derivation is complete upon noting that (5.11)–(5.12) is equivalent to the ordinary differential equation

$$\dot{I} = \bar{f}(I), \quad I(0) = I \tag{5.13}$$

with the averaged drift

$$\bar{f}(I) = \frac{1}{(2\pi)^n} \int_{\mathbf{T}^n} f(I, \varphi) d\varphi. \tag{5.14}$$

³ The notation $\mathbf{1}(\cdot)$ is used for functions that are constant in the respective argument.

5.3 Diophantine condition and the law of large numbers

labelsec:lln

It remains to show that the diophantine condition (5.6) entails uniqueness of the solution of the stationary problem $\mathcal{L}_1^* \rho = 0$. We suppose that \mathcal{L}_1^* is given by

$$\mathcal{L}_1^* = \omega(I) \cdot \frac{\partial}{\partial I}$$

and we consider \mathcal{L}_1^* to act on a suitable subset of $L^1(\mathbf{T}^n)$, i.e., we consider functions that are 2π -periodic in each of its arguments and that are integrable over the torus. Since the space of continuously differentiable functions $C^1(\mathbf{T}^n)$ is a dense subspace of $L^1(\mathbf{T}^n)$ we can approximate any such function (i.e., any periodic density) by a finite set of continuously differentiable functions, which therefore allows us to write the forward generator as we did (see also the remark below). As we confine ourselves to periodic functions ρ it is convenient to expand ρ into a Fourier series, i.e.,

$$\rho(\varphi) = \sum_{\mathbf{k} \in \mathbf{Z}^n} a_{\mathbf{k}} \exp(-i \langle \mathbf{k}, \varphi \rangle).$$

The functions $e_{\mathbf{k}} = \exp(-i \langle \mathbf{k}, \varphi \rangle)$ form an orthonormal basis of $L^2(\mathbf{T}^n)$ which is a dense subspace of $L^1(\mathbf{T}^n)$. Using the expression for \mathcal{L}_1^* above any solution to the eigenvalue problem $\mathcal{L}_1^* \psi = \lambda \psi$ is obviously of the form

$$\psi_{\mathbf{k}} = e_{\mathbf{k}}, \quad \lambda_{\mathbf{k}} = -i \langle \mathbf{k}, \varphi \rangle.$$

Hence the diophantine condition

$$|\langle \omega(I), \mathbf{k} \rangle| \geq \delta \quad \forall \mathbf{k} \in \mathbf{Z}^n \setminus 0$$

trivially implies that the eigenvalue $\lambda_0 = 0$ (i.e., $\mathbf{k} = 0$) is simple and is separated from the rest of the L^2 spectrum by a gap δ . This does not imply anything for the spectrum in L^1 , though, but as the $e_{\mathbf{k}}$ are linearly independent we cannot find any other periodic function $\rho \in L^1$ that solves $\mathcal{L}_1^* \rho = 0$. But the corresponding eigenfunction for $\mathbf{k} = 0$ is the constant function $\psi_0 = \mathbf{1}(\varphi)$, which proves that

$$\ker \mathcal{L}_1^* = \text{span}\{\mathbf{1}(\varphi)\}$$

is one-dimensional.

Remark 5.1 Recall that we have introduced the forward generator \mathcal{L}_1^* as the formal adjoint of \mathcal{L}_1 that is typically assumed to act on functions $u \in L^\infty(\mathbf{T}^n)$. But, of course, boundedness does not entail differentiability, and so the usual integration by parts argument does not apply. Nonetheless we can unambiguously define the adjoint generator employing the definition of the infinitesimal generator, viz.,

$$\mathcal{L}_1 \phi = \lim_{h \rightarrow 0} \frac{T_h \phi - \phi}{h}, \quad \phi \in L^\infty(\mathbf{T}^n)$$

where T_h denotes the strongly continuous semigroup associated with the solution of

$$\dot{\varphi} = -\omega(I), \quad \varphi(0) = \varphi_0. \tag{5.15}$$

For details we refer to Section 3. Letting $\langle \cdot, \cdot \rangle_{1, \infty}$ denote the pairing between the dual spaces L^1 and L^∞ and exploiting the strong continuity, we find

$$\begin{aligned} \langle \mathcal{L}_1 u, v \rangle_{1, \infty} &= \lim_{h \rightarrow 0} \frac{\langle T_h u - u, v \rangle_{1, \infty}}{h} \\ &= \lim_{h \rightarrow 0} \frac{\langle u, T_h^* v - v \rangle_{1, \infty}}{h} \\ &= \langle u, \mathcal{L}_1^* v \rangle_{1, \infty} \end{aligned}$$

for any two functions $u \in L^1(\mathbf{T}^n)$ and $v \in L^\infty(\mathbf{T}^n)$.

Law of large numbers Before we conclude, we shall briefly explain in which sense the diophantine condition implies ergodicity. In the formal derivation above, the condition of the dimensionality of the nullspaces of \mathcal{L}_1 and \mathcal{L}_1^* appeared as a solvability (closure) condition that eventually led to the effective equation (5.11)–(5.12). However, the fact that the eigenvalue zero is simple even implies that we can replace the time average of the slow dynamics over the fast oscillations φ by the respective spatial average over the torus (compare the discussion at the beginning of the last section). This can be seen as follows: define

$$\mathbf{E}f = \frac{1}{(2\pi)^n} \int_{\mathbf{T}^n} f(\varphi) d\varphi$$

for $f \in L^1(\mathbf{T}^n)$ and consider the linear operator equation

$$\mathcal{L}_1\Phi = f - \mathbf{E}f.$$

By the Fredholm alternative and since $\dim \ker \mathcal{L}_1 = 1$ the equation has a solution that is unique up to constants. If $\varphi(t)$ denotes the solution of the associated equation (5.15), $\Phi(t) = \Phi(\varphi(t))$ solves the differential equation

$$\dot{\Phi} = \mathcal{L}_1\Phi,$$

by which it follows that

$$\begin{aligned} \Phi(t) - \Phi(0) &= \int_0^t \mathcal{L}_1\Phi(s) ds \\ &= \int_0^t f(\varphi(s)) ds - \int_0^t \mathbf{E}f ds. \end{aligned}$$

Hence

$$\frac{1}{T} (\Phi(t) - \Phi(0)) = \frac{1}{T} \int_0^T f(\varphi(t)) dt - \mathbf{E}f.$$

But as $\Phi \in L^\infty$ and $\varphi \in \mathbf{T}^n$ for all $t \in \mathbf{R}_+$ the left hand side vanishes as T goes to infinity and we obtain the law of large numbers

$$\lim_{T \rightarrow \infty} \int_0^T f(\varphi(t)) dt = \mathbf{E}f.$$

5.4 Averaging of highly-oscillatory systems, cont'd

A standard problem in classical mechanics consists in confining a particle to a submanifold of its configuration space; see, e.g., the seminal work by Rubin and Ungar [17], the article by van Kampen [7], or the standard textbook of Arnold [1] to mention just a few. We shall give an example: consider a smooth curve $\Gamma \subset \mathbf{R}^2$ in the plane. Say, we impose a strong force acting perpendicular to the curve that forces a particle to stay close to it (see Figure 6 below). In the limit of infinitely strong forcing, the particle will remain on the curve.

To make this precise, we introduce a curve parameter coordinates $x \in \mathbf{R}$ and a normal coordinate $y \in \mathbf{R}$ measuring the distance to Γ , and we consider the singularly perturbed Hamiltonian

$$H: \mathbf{R}^2 \times \mathbf{R}^2 \rightarrow \mathbf{R}, \quad H(x, y, u, v) = \frac{1}{2} (u^2 + v^2) + V(x, y/\epsilon)$$

with the potential

$$V(x, y) = U(x) + \frac{1}{2} \omega(x)^2 y^2.$$

The corresponding equations of motion read

$$\begin{aligned} \dot{x} &= u, & x(0) &= x_0 \\ \dot{u} &= -U'(x) - \frac{1}{\epsilon^2} \omega'(x) \omega(x) y^2, & u(0) &= u_0 \\ \dot{y} &= v, & y(0) &= y_0 \\ \dot{v} &= -\frac{1}{\epsilon^2} \omega(x)^2 y, & v(0) &= v_0. \end{aligned} \tag{5.16}$$

By skew-symmetry, Hamilton's equation (5.16) preserve the energy $E_\epsilon = H(x, y, u, v)$, but the form of the singularity implies that $E_\epsilon \rightarrow \infty$ as $\epsilon \rightarrow 0$. In order to prevent this blow-up of the total energy, it is convenient to scale the initial conditions in such a way that the initial energy remains finite for all ϵ . Noting that $E_1 = H(x, \epsilon y, u, v)$ is independent of ϵ , we replace (5.16) by the scaled initial value problem

$$\begin{aligned} \dot{x} &= u, & x(0) &= x_0 \\ \dot{u} &= -U'(x) - \frac{1}{\epsilon^2} \omega'(x) \omega(x) y^2, & u(0) &= u_0 \\ \dot{y} &= v, & y(0) &= \epsilon y_0 \\ \dot{v} &= -\frac{1}{\epsilon^2} \omega(x)^2 y, & v(0) &= v_0. \end{aligned} \tag{5.17}$$

We suppose that the potential U is bounded from below by a positive constant and that $\omega(x) \geq c > 0$ for all $x \in \mathbf{R}$. This, together with the conservation of the total energy $H = E_1$ implies that $y \rightarrow 0$ as $\epsilon \rightarrow 0$ which can be seen by

$$\begin{aligned} y^2 &= \frac{2\epsilon^2}{\omega(x)^2} \left(H - \frac{1}{2} (u^2 + v^2) - U(x) \right) \\ &= \frac{2\epsilon^2}{\omega(x)^2} \left(E_1 - \frac{1}{2} (u^2 + v^2) - U(x) \right) \\ &\leq \frac{2E_1\epsilon^2}{c}. \end{aligned}$$

Hence $y = \mathcal{O}(\epsilon)$ for the solutions of (5.17). The same, however, is not true for the velocities (compare the example at the beginning of Section 5). Equation (5.17) is not very transparent regarding the assignment of fast and slow scales; in particular, the scaling argument above suggests that the term that is formally $\mathcal{O}(1/\epsilon^2)$ in the equation for u is actually of order 1; it is therefore convenient to introduce the scaled variable $\xi = y/\epsilon$. In terms of the new variables (x, ξ, u, v) , equation (5.17) takes the form

$$\begin{aligned} \dot{x} &= u, & x(0) &= x_0 \\ \dot{u} &= -U'(x) - \omega'(x) \omega(x) \xi^2, & u(0) &= u_0 \\ \dot{\xi} &= \frac{1}{\epsilon} v, & \xi(0) &= y_0 \\ \dot{v} &= -\frac{1}{\epsilon} \omega(x)^2 \xi, & v(0) &= v_0. \end{aligned} \tag{5.18}$$

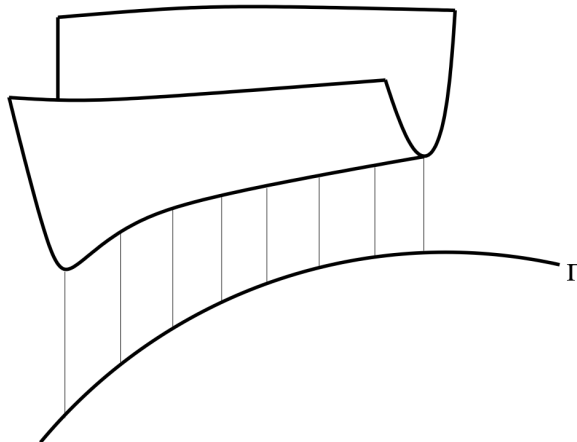


Fig. 6 Particle oscillating in a parabolic potential.

Note that the initial condition for the normal component scales according to $\xi_0 = y_0/\epsilon$, such that $\xi_0 = \mathcal{O}(1)$ is independent of ϵ . The thus scaled equations now clearly reveal the two dominant time scales; rather than

converging to the limiting set $\Gamma \times \mathbf{R}$ as ϵ goes to zero, the fast dynamics now rapidly oscillate around it. For frozen slow variables, the associated system is given by the harmonic oscillator

$$\begin{aligned}\dot{\xi} &= v, & \xi(0) &= y_0 \\ \dot{v} &= -\omega(x)^2 \xi, & v(0) &= v_0\end{aligned}\tag{5.19}$$

or, equivalently,

$$\ddot{\xi} = -\omega(x)^2 \xi, \quad \xi(0) = y, \quad \dot{\xi}(0) = v.\tag{5.20}$$

As we know from the previous paragraph, the last equation describes harmonic oscillations with frequency $\omega(x)$ and the (normal) energy

$$H_x^\perp = \frac{1}{2}v^2 + \frac{1}{2}\omega(x)^2 \xi^2.$$

Given initial conditions (x, y, u, v) of the full system (5.18), the instantaneous normal energy can be expressed in terms of the slow variables as

$$H_x^\perp = E_1 - \frac{1}{2}u^2 - U(x)$$

where $E_1 = H(x_0, \epsilon y_0, u_0, x_0)$ denotes the total energy of the system. Again, the result from the previous lecture suggests that we can approximate the slow dynamics by simply replacing the fast components in (5.18) by their time averages. Other than before, however, we want to avoid the explicit transformation to action-angle variables and, instead, average directly over the fast variable ξ . We need the following lemma that is known by the name of *Virial Theorem* in statistical mechanics.

Lemma 5.2 *Let $\psi_x^t : \mathbf{R}^2 \rightarrow \mathbf{R}^2$ be the solution (flow map) of the associated equation (5.19) with $\pi : (\xi, v) \mapsto \xi$ being the projection onto the first component. Then*

$$\lim_{T \rightarrow \infty} \frac{1}{2} \int_0^T \omega(x)^2 ((\pi \circ \psi_x^t)(y_0, v_0))^2 dt = \frac{1}{2} E_x^\perp,$$

i.e., the average potential energy of the fast oscillator equals half the instantaneous normal energy $E_x^\perp = H_x^\perp$. By symmetry, the same is true for the kinetic energy.

Proof. Using the shorthand $\xi_x(t) = (\pi \circ \psi_x^t)(y_0, v_0)$, we have

$$\xi_x(t) = \lambda \sin(\omega(x)t) + \mu \cos(\omega(x)t)$$

with constants λ, μ depending on x and the initial conditions $\xi_x(0) = y_0$ and $\dot{\xi}_x(0) = v_0$. Notice that

$$\begin{aligned}H_x^\perp &= \frac{1}{2}(\dot{\xi}_x)^2 + \frac{1}{2}\omega(x)^2(\xi_x)^2 \\ &= \frac{1}{2}\omega(x)^2(\lambda^2 + \mu^2)\end{aligned}$$

is constant in time. Using the trigonometric identity

$$\begin{aligned}(\xi_x(t))^2 &= \lambda^2 \sin^2(\omega(x)t) + \lambda\mu \sin(\omega(x)t) \cos(\omega(x)t) + \mu^2 \cos^2(\omega(x)t) \\ &= \frac{1}{2}(\lambda^2 + \mu^2) + \lambda\mu \sin(2\omega(x)t) + \frac{1}{2}(\lambda^2 - \mu^2) \cos(2\omega(x)t),\end{aligned}$$

it follows that

$$\begin{aligned}\lim_{T \rightarrow \infty} \frac{1}{2} \int_0^T \omega(x)^2 (\xi_x(t))^2 dt &= \frac{1}{4}\omega(x)^2(\lambda^2 + \mu^2) \\ &= \frac{1}{2}H_x^\perp.\end{aligned}$$

□

In fact the last statement covers only a special case of the Virial Theorem that allows for much more general assertions; see, e.g., the textbook of Bornemann [3]. Replacing the fast term ξ^2 in the second equation of (5.18) by the respective average expression, we obtain the limit dynamics on $\Gamma \times \mathbf{R}$,

$$\begin{aligned} \dot{x} &= u, & x(0) &= x_0 \\ \dot{u} &= -U'(x) - \frac{\omega'(x)}{\omega(x)} E_x^\perp, & u(0) &= u_0. \end{aligned} \quad (5.21)$$

Employing the arguments from the previous section, the last equation ought to yield the lowest-order approximation of the original oscillatory equation (5.17) for sufficiently small ϵ .

Remark 5.3 If the limiting set $\Gamma \times \mathbf{R}$ is given as the level set $\varphi^{-1}(0)$ of some smooth function $\varphi: \mathbf{R}^2 \rightarrow \mathbf{R}$, confinement to Γ is achieved by replacing $V(x, y/\epsilon)$ in (5.16) by

$$V_\epsilon(x, y) = U(x) + \frac{1}{2\epsilon^2} (\varphi(x, y))^2.$$

Since the normal variable y points in the direction normal to Γ , Taylor expansion of φ around $y = 0$ yields

$$(\varphi(x, y))^2 = |\nabla\varphi(x, 0)|^2 y^2 + \mathcal{O}(y^4).$$

Noting that $y = \mathcal{O}(\epsilon)$ it is easy to see that only the quadratic term remains in the limit $\epsilon \rightarrow 0$, so that we end up with the limit equation (5.21) for $\omega(x) = |\nabla\varphi(x, 0)|$.

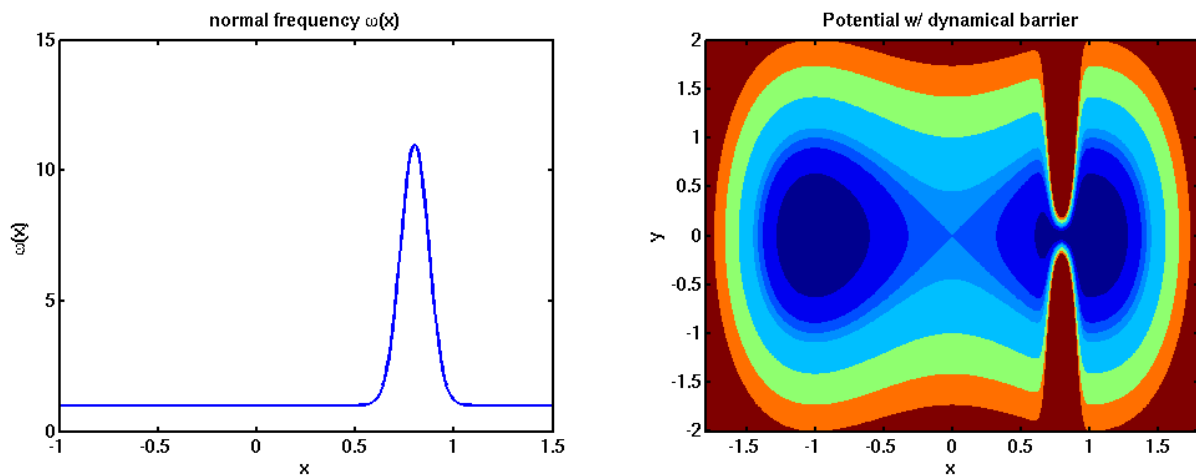


Fig. 7 Potential with a dynamical barrier. Left panel: normal frequency. Right panel: potential energy.

5.5 Adiabatic invariance

We shall now highlight the relation between the confinement approach and the oscillatory action-angle equations. To this end recall that we have defined the action of an unperturbed harmonic oscillator with frequency ω and energy H as the ratio $I = H/\omega$. For a single unperturbed oscillator, the action is trivially a “slow” variable, for the energy H is an integral of motion, i.e., $dH/dt = 0$. But if the system is perturbed by a slowly-varying parameter, e.g. an additional slow variable, it may happen that H is no longer a slow variable whereas I still is. This is expressed in the following lemma that is an instance of the famous *Adiabaticensatz* (adiabatic theorem) for quantum mechanical systems that has been stated first as a hypothesis by Ehrenfest in 1916 [4].

Lemma 5.4 (Adiabatic invariance of the action) *The quantity*

$$I = \frac{E_x^\perp}{\omega(x)}$$

is a constant of motion under the dynamics (5.21).

Proof. Recall that the instantaneous energy of the normal oscillations is given by

$$E_x^\perp = E_1 - \frac{1}{2}u^2 - U(x)$$

with $E_1 = H(x, \epsilon y, u, v)$ being a constant. A straightforward calculation shows that

$$\begin{aligned} \frac{d}{dt} \left(\frac{E_x^\perp}{\omega(x)} \right) &= \frac{d}{dt} \left(\frac{E_1 - \frac{1}{2}u^2 - U(x)}{\omega(x)} \right) \\ &= \frac{E_1 - \frac{1}{2}u^2 - U(x)}{\omega(x)^2} \dot{x} \\ &\quad - \frac{(\dot{u}u + U'(x)\dot{x})\omega(x)}{\omega(x)^2}. \end{aligned}$$

Substituting the expression for the normal energy E_x^\perp , the momentum $u = \dot{x}$ and \dot{u} by the respective expressions from the equations of motion (5.21), it follows immediately that the numerator is zero, for

$$(\dot{u}u + U'(x)\dot{x})\omega(x) = E_x^\perp \omega'(x).$$

Hence

$$\frac{d}{dt} \left(\frac{E_x^\perp}{\omega(x)} \right) = 0$$

which proves that $I = E_x^\perp/\omega(x)$ is a constant of motion. \square

The adiabatic invariance of the ratio $E_x^\perp/\omega(x)$ allows us to further simplify the averaged equation (5.21). Calling

$$I_0 = \frac{1}{\omega(x)} \left(\frac{1}{2}v^2 + \frac{1}{2}\omega(x)^2 y^2 \right)$$

the initial action $I_0 = I(x(0), \xi(0), v(0))$, the limit equation (5.21) can be recast as

$$\begin{aligned} \dot{x} &= u, & x(0) &= x_0 \\ \dot{u} &= -U'(x) - I_0 \omega'(x), & u(0) &= u_0. \end{aligned} \tag{5.22}$$

It can be readily seen that the last equation is Hamiltonian with the effective energy

$$\bar{H} = \frac{1}{2}u^2 + U(x) + I_0 \omega(x).$$

Example 5.5 (Potential with a dynamical barrier) We wrap up the section with a simple example. To this end, consider the Hamiltonian

$$H: \mathbf{R}^2 \times \mathbf{R}^2 \rightarrow \mathbf{R}, \quad H(x, y, u, v) = \frac{1}{2}(u^2 + v^2) + V(x, y/\epsilon)$$

with the perturbed double-well potential

$$V(x, y) = \frac{1}{2}(x^2 - 1)^2 + \frac{1}{2}\omega(x)^2 y^2$$

where the normal frequency be given by the formula

$$\omega(x) = 1 + Ce^{-\alpha(x-x_b)^2},$$

with C, α positive constants. The frequency has a sharp peak at $x = x_b$ that induces a large force pointing towards the constraint set $y = 0$. This has the effect that a particle which approaches x_0 with a large oscillation (i.e., normal) energy will bounce off the *dynamical barrier* that arises from the frequency peak, although the potential is almost flat in this direction. The normal frequency together with the resulting potential are shown

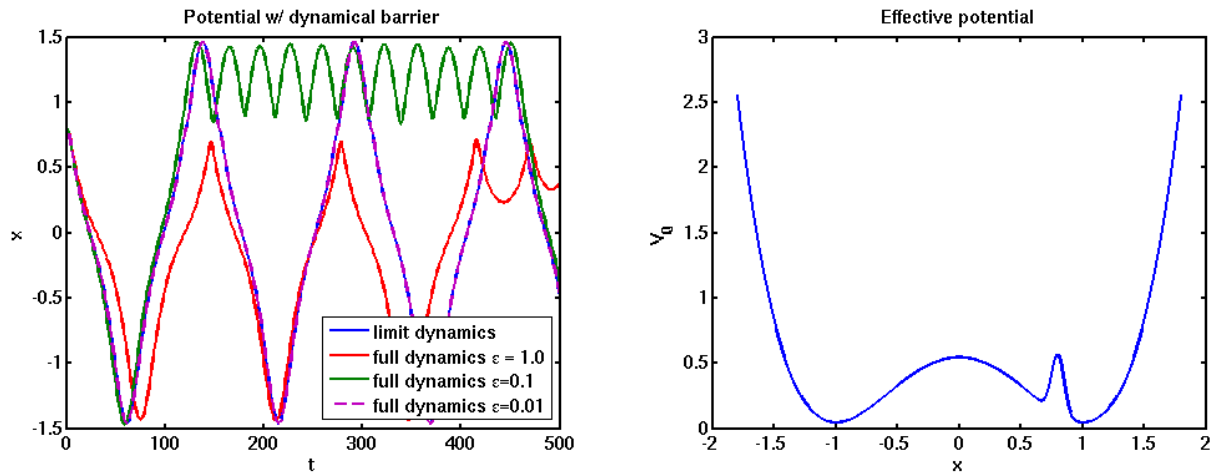


Fig. 8 Limiting dynamics of the system with dynamical barrier. Left panel: convergence of the slow configuration variable. Right panel: averaged potential.

in Figure 7 for $C = 10$, $\alpha = 200$ and $x_b = 0.8$. In order to demonstrate the effect of the dynamical (or entropic) barrier we fix initial values $(x_0, y_0, u_0, v_0) = (0.8, 0, -0.5, 1.0)$ and compute the resulting effective potential

$$\bar{V}(x) = \frac{1}{2}(x^2 - 1)^2 + I_0 \omega(x)$$

which is shown in the left panel of Figure 8. Apparently the *dynamical* barrier in the full potential shows up as an additional potential barrier in the effective potential. Nevertheless it is not a potential barrier in the usual sense: it becomes harder to cross as the initial normal energy $E_x^\perp = I_0 \omega(x)$ with $I_0 = I(x_0, y_0, v_0)$ increases.

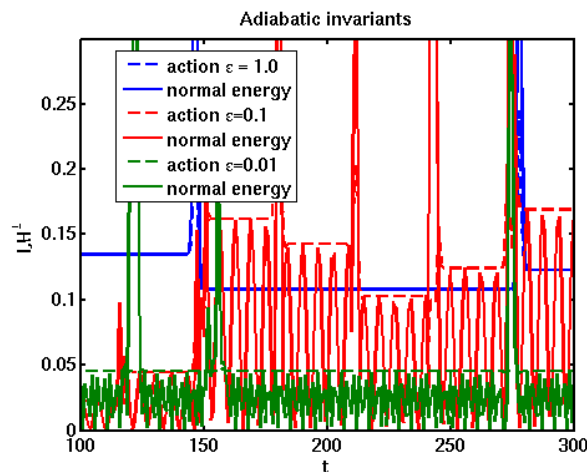


Fig. 9 Action variable $I = E_x^\perp / \omega$ and the normal energy E_x^\perp for $\epsilon > 0$.

The left panel of Figure 8 depicts the convergence of the slow position variable $x = x^\epsilon$ in the limit of strong confinement to the real axis. Notice that although the confinement limit eventually leads to restriction of the system to the x -axis, the effective potential exhibits an additional barrier that vanishes only when $I_0 = 0$, i.e., when the initial positions lie exactly on the real axis and the initial momenta are tangential to the real axis. In other words, the confinement is *intrinsically* defined by the dynamics on the constraint set if the system is initialised with zero normal energy (or if the normal frequency ω is constant).

We conclude by comparing the action variable $I = E_x^\perp / \omega(x)$ with the instantaneous normal energy E_x^\perp for $\epsilon > 0$. It turns out that E_x^\perp is rapidly oscillating for all values of ϵ , although it depends only on the slowly varying variables x and u and the associated system preserves the normal energy $E_x^\perp = H_x^\perp$. In turn, the action variable

is almost constant except for jumps that occur whenever the system crosses the dynamical barrier at $x = x_b$; see Figure 9. As ϵ goes to zero, the jumps vanish.

6 Random perturbations

We shall now come to the case of differential equations that are subject to noise. More precisely, we consider the scenario of (fast) random perturbations to the dynamics. A brief introduction to stochastic differential equations and Brownian motion will be given in the appendix.

6.1 Kolmogorov and Fokker-Planck equations

Recall from Section 3 that to any ODE we could associate two partial differential equations, forward and the backward equations, that were defined in terms of the infinitesimal generator of the dynamics. As we will now explain, stochastic differential equations (SDE) allow for an analogous construction. Consider the SDE

$$dz = b(z)dt + \sigma(z)dW_t, \quad z(0) = x \quad (6.1)$$

for $z \in \mathcal{Z} \subseteq \mathbf{R}^n$, $b: \mathcal{Z} \rightarrow \mathbf{R}^n$ locally Lipschitz and $\sigma: \mathcal{Z} \rightarrow \mathbf{R}^{n \times n}$ invertible. As before, $\mathcal{Z} = \mathbf{R}^n$ if the vector field satisfies certain growth conditions (e.g., see [16]), or $\mathcal{Z} = \mathbf{T}^n$ being the n -dimensional flat torus otherwise (periodic boundary conditions).

Clearly $Z = (z(t))_{t \in \mathbf{R}_+}$ is a Markov process and comes with a (smooth) transition kernel $\rho_x(z, t, s)$. The kernel specifies the transition probabilities of the process and is defined by

$$\mathbf{P}[z(t+s) \in A | z(s) = x] = \int_A \rho_x(z, t) dz$$

where we have already taken advantage of the fact that the coefficients in (6.1) are time-homogeneous which implies that ρ_x is independent of s . An evolution equation for ρ_x can be obtained in the following way: For any smooth function $f: \mathcal{Z} \rightarrow \mathbf{R}$, Itô's formula implies (see the appendix)

$$f(z(t)) - f(x) = \int_0^t \nabla f(z(s)) \cdot dz(s) + \frac{1}{2} \int_0^t a(z(s)) : \nabla^2 f(z(s)) ds$$

with the shorthand $a(z) = \sigma(z)\sigma(z)^T$. Taking expectations over all realization of $Z = (z(t))_{t \in \mathbf{R}_+}$ starting at $z(0) = x$ on both sides of the equation yields

$$\mathbf{E}_x f(z(t)) - f(x) = \mathbf{E}_x \int_0^t \nabla f(z(s)) \cdot dz(s) + \frac{1}{2} \mathbf{E}_x \int_0^t a(z(s)) : \nabla^2 f(z(s)) ds$$

which, by using the first Itô isometry and the definition of the transition kernel ρ_x , can be recast as

$$\int_{\mathcal{Z}} f(z) \rho_x(dz, t) = \int_0^t \int_{\mathcal{Z}} \nabla f(z) \cdot b(z) \rho_x(dz, s) ds + \frac{1}{2} \int_0^t \int_{\mathcal{Z}} a(z) : \nabla^2 f(z) \rho_x(dz, s) ds.$$

Finally integrating by parts and pulling off the integral over \mathcal{Z} (since f is arbitrary), it follows by differentiation with respect to t that the transition density $\rho(z, t) := \rho_x(z, t)$ solves the *Fokker-Planck* or *forward Kolmogorov equation*

$$\partial_t \rho(z, t) = \frac{1}{2} \nabla^2 : (a(z) \rho(z, t)) - \nabla \cdot (b(z) \rho(z, t)), \quad \lim_{t \rightarrow 0^+} \rho(z, t) = \delta(z - x) \quad (6.2)$$

where we have used the notation

$$\nabla^2 : (a\rho) = \sum_{i,j} \frac{\partial^2}{\partial z_i \partial z_j} (a_{ij} \rho).$$

Given an initial value $z(0) = x$ the forward equation describes the dynamics of (6.1) in terms of z and t . Conversely, we may ask what is the respective evolution equation for x and t . By the Markov property we have

$$\mathbf{P}[z(t+s) \in A | \{z(\tau), 0 \leq \tau \leq s\}] = \mathbf{P}[z(t+s) \in A | z(s)]$$

which entails the Chapman-Kolmogorov equation

$$\rho_x(z, s+t) = \int_{\mathcal{Z}} \rho_y(t, z) \rho_x(y, s) dy.$$

The latter implies

$$\begin{aligned} \rho_x(z, t + \Delta t) - \rho_x(z, t) &= \int_{\mathcal{Z}} \rho_y(t, z) \rho_x(y, \Delta t) dy - \rho_x(z, t) \\ &= \int_{\mathcal{Z}} \rho_y(t, z) (\rho_x(y, \Delta t) - \delta(x-y)) dy. \end{aligned}$$

If we divide the last equation by Δt and let $\Delta t \rightarrow 0$, we obtain

$$\partial_t \rho_x(z, t) = \int_{\mathcal{Z}} \rho_y(t, z) \left(\frac{1}{2} \nabla^2 : (a(y) \delta(x-y)) - \nabla \cdot (b(y) \delta(x-y)) \right) dy.$$

Integration by parts yields the *backward Kolmogorov equation* for $u(x, t) := \rho_x(\cdot, t)$, namely,

$$\partial_t u(x, t) = \frac{1}{2} a(x) : \nabla^2 u(x, t) + b(x) \cdot \nabla u(x, t), \quad u(x, 0) = \phi(x). \quad (6.3)$$

6.2 Forward-backward dichotomy

The two equations (6.2) and (6.3) are dual to each other in the sense that forward and backward Liouville equations were dual. To make this statement a bit more precise, we introduce the *infinitesimal generator* of the diffusion process Z as the elliptic second-order operator

$$\mathcal{L} = \frac{1}{2} a(z) : \nabla^2 + b(z) \cdot \nabla \quad (6.4)$$

Its meaning is completely analogous to the semigroup definition (3.5) of the Liouvilian in Section 3, but for the sake of simplicity we confine our attention to functions that twice continuously differentiable in the spatial argument, i.e., we assume $\mathcal{D}(\mathcal{L}) \subseteq C^{2,1}(\mathcal{Z}, [0, \infty))$ to be the domain of definition of \mathcal{L} . Then the formal definition (3.5) coincides with (6.4).

Now using the definition of \mathcal{L} we may write backward Kolmogorov equation as the Cauchy problem

$$\begin{aligned} \partial_t u(z, t) &= \mathcal{L}u(z, t), \quad (z, t) \in \mathcal{Z} \times]0, \infty[\\ u(z, 0) &= \phi(z), \quad z \in \mathcal{Z} \end{aligned} \quad (6.5)$$

the formal solution of which is given by

$$u(z, t) = (\exp(t\mathcal{L})\phi)(z).$$

As before, the last identity can be readily verified by differentiation with respect to time where the operator $T_t = \exp(t\mathcal{L})$ denotes the semigroup of \mathcal{L} . The operator

$$\mathcal{L}^* v = \frac{1}{2} \nabla^2 : (a(z)v(z)) + \nabla \cdot (b(z)v(z)) \quad (6.6)$$

is that is assumed to act on a suitable subspace of $C^{2,1}(\mathcal{Z}, [0, \infty)) \cap L^1(\mathcal{Z})$ is the formal of \mathcal{L} that is defined by the inner product $\langle \mathcal{L}u, v \rangle_{L^2} = \langle u, \mathcal{L}^*v \rangle_{L^2}$. Hence we may recast the (forward) Fokker-Planck equation as

$$\begin{aligned} \partial_t \rho(z, t) &= \mathcal{L}^* \rho(z, t), \quad (z, t) \in \mathcal{Z} \times]0, \infty[\\ \rho(z, 0) &= \rho_0(z), \quad z \in \mathcal{Z}, \end{aligned} \quad (6.7)$$

having the formal solution

$$\rho(z, t) = (\exp(t\mathcal{L}^*)\rho_0)(z).$$

Again, $T_t^* = \exp(t\mathcal{L}^*)$ with $T_t = \exp(t\mathcal{L})$ denoting the semigroup of \mathcal{L} (cf. Section 3.2).

Particle-interpretation of Kolmogorov and Fokker-Planck equations Recall that in the ODE case we could interpret the trajectories of the differential equation as the characteristics of the corresponding backward Liouville equation. Roughly speaking, we could express the solution to the backward PDE in terms of the trajectories as $u(z, t) = \phi(z(t))$. Here the situation is slightly different because the trajectories (realizations) of (6.1) are noisy, in other words, Z is a random process, whereas $u(z, t)$ is deterministic.

Nonetheless we may express the solution to the backward equation in a similar fashion: Define $u(z, t) = \mathbf{E}_z \phi(z(t))$ where \mathbf{E}_z denotes the expectation over all realizations of $Z = (z(t))_{t \in \mathbf{R}_+}$ starting at $z(0) = z$. Then u solves the backward equation (6.5) as can be readily verified by noting that u can be expressed by

$$u(z, t) = \int_{\mathcal{Z}} \phi(y) \rho_z(y, t) dy$$

with $\rho_z(\cdot, t)$ denoting the transition kernel of the process Z . The assertion then follows by writing out the Chapman-Kolmogorov equation for $u(z, t + \Delta t) - u(z, t)$ and repeating the derivation of the backward equation.⁴

For the forward equation we may prove the following Lemma.

Lemma 6.1 *Let $z(t)$ be the solution of the SDE*

$$dz = b(z)dt + \sigma(z)dW_t, \quad z(0) \sim \rho_0$$

with initial conditions $z(0)$ that are drawn from the probability distribution ρ_0 . Then the solution $\rho(z, t)$ of the forward equation (6.7) with initial condition $\rho(z, 0) = \rho_0(z)$ is the law of Z at time $t > 0$.

Proof. We have to show that we may express any expectation of a smooth function f with respect to the time-dependent probability distribution ρ by an average over the realizations of Z (cf. Theorem 3.2). To this end consider the backward equation

$$\begin{aligned} \partial_t u(z, t) &= \mathcal{L}u(z, t), \quad (z, t) \in \mathcal{Z} \times]0, \infty[\\ u(z, 0) &= f(z), \quad z \in \mathcal{Z} \end{aligned}$$

Given that $f \in L^1$ is sufficiently differentiable, it suffices to show that

$$\int_{\mathcal{Z}} f(z) \rho(z, t) dz = \int_{\mathcal{Z}} \mathbf{E}_z f(z(t)) \rho_0(z) dz.$$

But as $u(z, t) = \mathbf{E}_z f(z(t))$ solves the backward equation for $z(0) = z$ we have

$$\begin{aligned} \int_{\mathcal{Z}} \mathbf{E}_z f(z(t)) \rho_0(z) dz &= \int_{\mathcal{Z}} (\exp(t\mathcal{L})f)(z) \rho_0(z) dz \\ &= \int_{\mathcal{Z}} f(z) (\exp(t\mathcal{L}^* \rho_0))(z) \\ &= \int_{\mathcal{Z}} f(z) \rho(z, t) dz. \end{aligned}$$

It follows that, for any measurable set $A \subset \mathcal{Z}$,

$$\mathbf{P}[z(t) \in A] = \int_{\mathcal{Z}} \chi_A(z) \rho(z, t) dz$$

by which the assertion is proved. □

Invariant measures By the last lemma, the stationary solutions of the the Fokker-Planck equation (6.2) are the stationary probability distributions of the stochastic process governed by (6.1). The following case is of particular importance: in (6.1), suppose that $\sigma(z) = \sqrt{2\zeta}$ is constant with $\zeta > 0$ denoting the “temperature” of the system. Further assume that the vector field b has gradient form, i.e., $b = -\nabla V$ with $V: \mathcal{Z} \rightarrow \mathbf{R}$ being a smooth potential that is bounded below and has the property $V(z) \rightarrow \infty$ as $|z| \rightarrow \infty$. Then the SDE

$$dz = -\nabla V(z)dt + \sqrt{2\zeta}dW$$

⁴ Alternatively, one might write down Itô’s formula for $f(z)$. The expectation then solves the backward equation.

has the unique stationary probability distribution

$$\mu(dz) = I^{-1} \exp(-\varsigma^{-1}V(z))dz, \quad I = \int_{\mathcal{Z}} \exp(-\varsigma^{-1}V(z)) dz.$$

that is known as the *Boltzmann distribution* in the literature. To see that μ is indeed stationary, note that the formal L^2 adjoint to the infinitesimal generator \mathcal{L} reads

$$\mathcal{L}^* = \Delta + \nabla V(z) \cdot \nabla + \Delta V(z)$$

with the rightmost term acting as a multiplication operator. Defining the stationary Boltzmann density by $\mu(dz) = \rho_{\infty}(z)dz$ or $\rho_{\infty} \propto \exp(-\varsigma^{-1}V)$, it is easy to check that $\mathcal{L}^*\rho_{\infty} = 0$ which proves that μ is an invariant measure of (6.1).

Proving that μ is in fact *the* invariant measure is more involved and requires the application of the maximum principle for elliptic second-order PDEs given that V grows at least quadratically in z as $|z| \rightarrow \infty$. We refer to [14] for a discussion and conclude the subsection by some examples.

Example 6.2 (Heat equation) Let $Z = W$, $W(0) = 0$ be standard Brownian motion in $\mathcal{Z} = \mathbf{R}^n$. The corresponding infinitesimal generator is now simply half the Laplacian,

$$\mathcal{L} = \frac{1}{2}\Delta.$$

As the Laplacian is essentially self-adjoint (i.e., symmetric), we have $\mathcal{L} = \mathcal{L}^*$, and the solution to the Fokker-Planck equation (6.2) with sharp initial condition $\rho(z, 0) = \delta(z)$ is given by the Gaussian heat kernel

$$\rho(z, t) = \frac{1}{(2\pi t)^{n/2}} \exp\left(-\frac{1}{2t}|z|^2\right).$$

Conversely $\rho(z, t)dz$ determines the probability to find a Brownian particle in an infinitesimal volume element dz around z . Note, however, that the stationary solution to the Fokker-Planck equation, the constant function $\rho_{\infty} = \mathbf{1}$, cannot be a probability density since it is not normalizable. Moreover $\rho(z, t) \rightarrow 0$ as $t \rightarrow \infty$, hence n -dimensional Brownian motion does not admit an ergodic probability distribution.

Example 6.3 (Multidimensional Ornstein-Uhlenbeck process) Consider the gradient system

$$dz = -\nabla V(z; m)dt + \sqrt{2\varsigma}dW$$

on $\mathcal{Z} = \mathbf{R}^n$ with the quadratic potential

$$V(z; m) = \frac{1}{2}(z - m)^T A(z - m)$$

and $A = A^T \in \mathbf{R}^{n \times n}$ positive definite. The unique stationary distribution is the Gaussian distribution

$$\mu(dz) = \frac{\sqrt{\det A}}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2\varsigma}(z - m)^T A(z - m)\right) dz.$$

Example 6.4 (Double-well potential) For V being the double-well potential

$$V(z) = (z^2 - 1)^2,$$

the Boltzmann distribution $\exp(-\varsigma^{-1}V)$ for various ς is depicted in Figure 10.

6.3 Averaging of random perturbations

We will now consider the problem of fast random perturbations to an ODE where the fast dynamics are given by an SDE. More precisely, we consider the coupled system of equations

$$\begin{aligned} \dot{x} &= f(x, y, \epsilon), & x(0) &= x_0 \\ dy &= \frac{1}{\epsilon}g(x, y, \epsilon)dt + \frac{1}{\sqrt{\epsilon}}\sigma(x, y)dW, & y(0) &= y_0 \end{aligned} \tag{6.8}$$

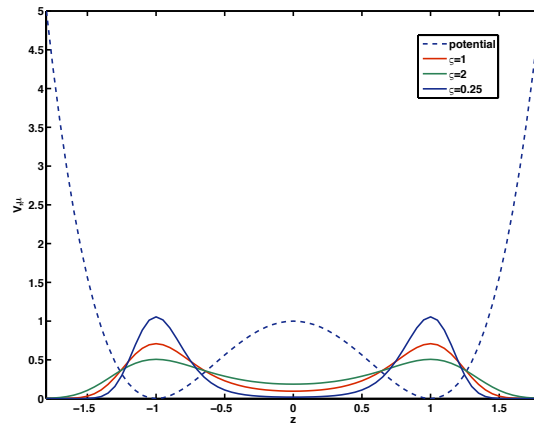


Fig. 10 Stationary distributions $\mu \propto \exp(-\zeta^{-1}V)$ for the double-well potential.

that is the natural generalisation of the slow-fast system (1.1) to the case of stochastic perturbations. As before $(x, y) \in \mathbf{R}^n \times \mathbf{R}^m$ and $0 < \epsilon \ll 1$ is a small parameter. If $f(\cdot, \cdot, \epsilon)$ and $g(\cdot, \cdot, \epsilon)$ are globally Lipschitz and uniformly bounded in ϵ , then y will be of order $1/\epsilon$ faster than x . To see that W is in fact living on a fast time scale $\tau = t/\epsilon$ it is helpful to recall that $dW \sim \sqrt{dt}$ and note that $\alpha W(t/\alpha^2)$ has the same law as $W(t)$; hence $\epsilon^{-1/2}W(\epsilon\tau)$ is a standard Wiener process living on the microscopic (fast) time scale.

To average (6.8) over the fast perturbation we proceed essentially as in the deterministic case: Since the slow dynamics hardly move on the time scale of the fast variables, the fast dynamics decouple from the slow ones whenever ϵ is sufficiently small. Hence we may replace the coupled system (6.8) by the equation

$$\dot{x} = f(x, y_x, \epsilon), \quad x(0) = x_0 \quad (6.9)$$

where $y_x(t)$ is the solution of the associated SDE

$$dy_\xi = g(\xi, y_\xi, 0)dt + \sigma(\xi, y_\xi)dW, \quad y_\xi(0) = y_0 \quad (6.10)$$

for frozen slow variable $x = \xi$. Provided that the process $Y_x = (y_x(t))_{t \in \mathbf{R}_+}$ has the unique (ergodic) stationary probability distribution $\mu_x(dy) = \rho(y; x)dy$, we may replace (6.9) by the averaged equation

$$\dot{x} = \bar{f}(x), \quad x(0) = x_0 \quad (6.11)$$

with the averaged vector field

$$\bar{f}(x) = \int_{\mathbf{R}^m} f(x, y, 0) \mu_x(dy). \quad (6.12)$$

Perturbation expansion To systematically derive the averaged equations (6.11)–(6.12) we follow the general strategy and proceed as in Section 5.2. For simplicity, we assume that both f and g are independent of ϵ . The generator \mathcal{L}^ϵ associated with the slow-fast system (6.8) then reads

$$\mathcal{L}^\epsilon = \mathcal{L}_0 + \frac{1}{\epsilon} \mathcal{L}_1$$

with

$$\mathcal{L}_0 = f(x, y) \cdot \frac{\partial}{\partial x}, \quad \mathcal{L}_1 = \frac{1}{2} a(x, y) : \frac{\partial}{\partial y} \otimes \frac{\partial}{\partial y} + g(x, y) \cdot \frac{\partial}{\partial y} \quad (\text{here: } a = \sigma\sigma^T).$$

Just as in the deterministic case, we seek a perturbative solution to the backward equation

$$\partial_t u^\epsilon(x, y, t) = \mathcal{L}^\epsilon u^\epsilon(x, y, t), \quad u^\epsilon(x, y, 0) = \phi(x, y),$$

given the ansatz

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$$

Substituting the series and equating equal powers of ϵ yields a hierarchy of equations the first three of which are

$$\mathcal{L}_1 u_0 = 0 \tag{6.13}$$

$$\mathcal{L}_1 u_1 = \partial_t u_0 - \mathcal{L}_0 u_0 \tag{6.14}$$

$$\mathcal{L}_1 u_2 = \partial_t u_1 - \mathcal{L}_0 u_1. \tag{6.15}$$

The first equation, equation (6.13), says that $u_0 \in \ker \mathcal{L}_1$. By the strong maximum principle this implies that $u_0 = u_0(x, t)$ is constant in y and is the unique eigenfunction to the eigenvalue zero (using ergodicity). The time evolution of u_0 is then due to the second equation, and we are aiming at the lowest-order approximation $u^\epsilon \approx u_0$. By the Fredholm alternative, equation (5.9) has a solution if and only if the right hand side is orthogonal to the kernel of \mathcal{L}_1^* . To define the adjoint of the generator of the fast dynamics, \mathcal{L}_1 , it is helpful to note that we may treat x as a parameter. Accordingly we define \mathcal{L}_1^* with respect to the L^2 scalar product for fixed x , i.e.,

$$\langle u, v \rangle_{x, L^2} = \int_{\mathcal{Z}_x} uv \, dy$$

where we exploit the fact that $\mathcal{Z} = \mathcal{Z}_y \times \mathcal{Z}_x \subseteq \mathbf{R}^n \times \mathbf{R}^m$ has a trivial structure with \mathcal{Z}_x denoting the fibre of the fast variables over the base space $x \in \mathcal{Z}_y$. Then the stationary densities ρ that are the nontrivial solutions of the elliptic equation $\mathcal{L}_1 \rho$ are of the form $\rho(y; x)$, provided they exist and assuming that we equip \mathcal{L}_1 with suitable boundary conditions (e.g., periodic).

Now, setting $\mu_x(dy) = \rho_\infty(y; x)dy$ the Fredholm alternative for (6.14) requires that

$$\int_{\mathcal{Z}_x} (\partial_t u_0 - \mathcal{L}_0 u_0) \mu_x(dy) = 0.$$

But since u_0 the solvability condition reduces to the averaged backward equation

$$\partial_t u_0(x, t) = \bar{\mathcal{L}} u_0(x, t), \quad u_0(x, 0) = \phi_0(x)$$

with the averaged Liouville operator

$$\begin{aligned} \bar{\mathcal{L}} &= \int_{\mathcal{Z}_x} f(x, y) \mu_x(dy) \cdot \frac{\partial}{\partial x} \\ &= \bar{f}(x) \cdot \frac{\partial}{\partial x}. \end{aligned} \tag{6.16}$$

The derivation is complete upon noting that (6.16) is the generator of the averaged SDE (6.11)–(6.12).

Remark 6.5 Consistency of the averaged equation with the full dynamics for all $t \in [0, T]$ requires that the initial condition $u^\epsilon(x, y, 0) = \phi(x, y)$ is independent of y , i.e., $\phi(x, y) = \phi_0(x) \mathbf{1}(y)$. If, however, the initial condition is not independent of the fast variable, the perturbation ansatz $u^\epsilon = u_0 + \epsilon u_1 + \dots$ must be replaced by a suitable *2-scale expansion* of $u^\epsilon = u^\epsilon(x, y, t, \tau)$ that involves the microscopic time scale $\tau = t/\epsilon$ on which the initial relaxation of the fast dynamics to the (ergodic) stationary distribution $\rho(y; x)$ takes place, similarly to the initial relaxation to an attractive invariant manifold as described in Section 4.3.

Convergence result For the approximation of the randomly perturbed slow dynamics by the deterministic averaged equation we have the following strong convergence result (for details on stochastic convergence see the appendix).

Theorem 6.6 *Let $x(t) = \varphi^t(x_0)$ denote the solution of the averaged equation*

$$\dot{x} = \bar{f}(x), \quad x(0) = x_0$$

with

$$\bar{f}(x) = \int_{\mathbf{R}^m} f(x, y) \mu_x(dy)$$

and μ_x being the invariant measure of the fast stochastic dynamics (6.10) for fixed x . The slow component x^ϵ of the solution of the coupled system (6.8) converges to the averaged solution in the mean square as $\epsilon \rightarrow 0$, viz.,

$$\mathbf{E} \left[\sup_{t \in [0, T]} |x^\epsilon(t) - x(t)| \right] \leq C \sqrt{\epsilon}$$

for a constant $C > 0$ independent of ϵ that grows exponentially in T .

Proof. We follow the convergence proof given in [14] with some slight modifications. Suppose that both f and g are locally Lipschitz and consider the Poisson equation

$$\begin{aligned}\mathcal{L}_1\phi(x, y) &= f(x, y) - \bar{f}(x) \\ \phi(\cdot, y) &\rightarrow 0 \quad \text{as } |y| \rightarrow \infty.\end{aligned}$$

By construction of \bar{f} being the average of f with respect to μ_x the Fredholm alternative asserts that our Poisson equation has a solution. (Note that $d\mu_x(y) = \rho(y; x)dy$ where $\rho(y; x)$ is the normalized solution of $\mathcal{L}_1^*\rho = 0$.) By requiring that ϕ decays at infinity the solution is also unique and all its derivatives are bounded (assuming smoothness of the coefficients and Lipschitz continuity); alternatively we may equip \mathcal{L}_1 with periodic boundary conditions and ask for a solution ϕ that is periodic in its second argument. Itô's formula then yields

$$d\phi^\epsilon = \mathcal{L}^\epsilon\phi(x^\epsilon, y^\epsilon)dt + \frac{1}{\sqrt{\epsilon}} \left(\frac{\partial}{\partial y}\phi(x^\epsilon, y^\epsilon) \right) \cdot \sigma(x^\epsilon, y^\epsilon)dW.$$

Using that $\mathcal{L}_1\phi = f - \bar{f}$, equation (6.8) can be recast as

$$\begin{aligned}dx^\epsilon &= \bar{f}(x^\epsilon) + \mathcal{L}_1\phi(x^\epsilon, y^\epsilon) \\ &= \bar{f}(x^\epsilon) + \epsilon d\phi(x^\epsilon, y^\epsilon) + \epsilon\mathcal{L}_0\phi(x^\epsilon, y^\epsilon) + \sqrt{\epsilon} \left(\frac{\partial}{\partial y}\phi(x^\epsilon, y^\epsilon) \right) \cdot \sigma(x^\epsilon, y^\epsilon)dW.\end{aligned}$$

By smoothness of ϕ , the two $\mathcal{O}(\epsilon)$ terms are uniformly bounded, i.e.,

$$S^\epsilon(t) - S^\epsilon(0) = \phi(x^\epsilon, y^\epsilon) - \phi(x_0, y_0) + \int_0^t (\mathcal{L}_0\phi)(x^\epsilon(s), y^\epsilon(s)) ds$$

satisfies

$$\sup_{0 \leq t \leq T} |S^\epsilon(t) - S^\epsilon(0)| \leq C_1. \quad (6.17)$$

with probability one and for all $\epsilon > 0$. By the second Itô isometry, the remaining martingale term

$$M^\epsilon(t) = \int_0^t \left(\frac{\partial}{\partial y}\phi(x^\epsilon(s), y^\epsilon(s)) \right) \cdot \sigma(x^\epsilon(s), y^\epsilon(s))dW(s)$$

has bounded quadratic variation, i.e., for all $\epsilon > 0$ and $t < \infty$. In other words,

$$\mathbf{E}|M_t^\epsilon|^2 = \int_0^t \mathbf{E} \left[\left| \sigma(x^\epsilon(s), y^\epsilon(s)) \left(\frac{\partial}{\partial y}\phi(x^\epsilon(s), y^\epsilon(s)) \right) \right|^2 \right] ds$$

is finite which implies that

$$\mathbf{E}|M_t^\epsilon| \leq C_2. \quad (6.18)$$

For the deviations $\xi^\epsilon = x^\epsilon - x$ we therefore obtain

$$\begin{aligned}\xi^\epsilon(t) &= - \int_0^t (\bar{f}(x^\epsilon(s)) - \bar{f}(x(s))) ds + \epsilon(S^\epsilon(t) - S^\epsilon(0)) + \sqrt{\epsilon}M^\epsilon(t) \\ &\leq L \int_0^t |\xi^\epsilon(s)| ds + C_3\sqrt{\epsilon}\end{aligned}$$

with $C_3 = C_1 + C_2$ and on any compact time interval $[0, T]$, employing the Lipschitz continuity of \bar{f} with Lipschitz constant $L < \infty$ and (6.17)–(6.18). Taking expectations on either side of the last equation we find

$$\begin{aligned}\mathbf{E} \left[\sup_{0 \leq t \leq T} |\xi^\epsilon(t)| \right] &\leq C_4 \left(\sqrt{\epsilon} + L \int_0^T \mathbf{E}|\xi^\epsilon(s)| ds \right) \\ &\leq C_5 \left(\sqrt{\epsilon} + \int_0^T \mathbf{E} \left[\sup_{0 \leq t \leq T} |\xi^\epsilon(s)| \right] ds \right)\end{aligned}$$

It finally follows from the integral version of Gronwall's Lemma that

$$\mathbf{E} \left[\sup_{0 \leq t \leq T} |\xi^\epsilon(t)| \right] \leq \sqrt{\epsilon} \exp(C_6 T)$$

which proves Theorem 6.6. □

6.3.1 Averaging of highly-oscillatory systems revisited

We shall come back to the confinement problem that we have discussed in Section 5, thereby slightly extending the previous stochastic averaging scenario to the fully stochastic case. Consider the singularly perturbed SDE

$$dz = -\nabla V^\epsilon(z)dt + \sqrt{2\varsigma}dW, \quad z(0) = z_0 \quad (6.19)$$

with $z = (x, \xi) \in \mathbf{R} \times \mathbf{R}^m$ and the confining potential

$$V^\epsilon(x, \xi) = U(x) + \frac{1}{2\epsilon}\xi^T A(x)\xi, \quad A(\cdot) \in \mathbf{R}^{m \times m} \text{ s.p.d.} \quad (6.20)$$

Splitting the state variables accordingly the equations of motion are

$$\begin{aligned} dx &= -\left(U'(x) + \frac{1}{2\epsilon}\xi^T A'(x)\xi \right) dt + \sqrt{2\varsigma}dW_x, \quad x(0) = x_0 \\ d\xi &= \frac{1}{\epsilon}A(x)\xi dt + \sqrt{2\varsigma}dW_\xi, \quad \xi(0) = 0 \end{aligned}$$

Like in the Hamiltonian case the dynamics become confined to the set $\{\xi = 0\}$ as $\epsilon \rightarrow 0$ where the convergence $\xi \rightarrow 0$ will now be stochastic, i.e., we expect that first and second moments converge with $\mathbf{E}|\xi|^2 = \mathcal{O}(\epsilon)$.⁵ To see this it is convenient to introduce the scaled variables $y = \xi/\sqrt{\epsilon}$ in terms of which our SDE reads

$$\begin{aligned} dx &= -\left(U'(x) + \frac{1}{2}y^T A'(x)y \right) dt + \sqrt{2\varsigma}dW_x, \quad x(0) = x_0 \\ dy &= \frac{1}{\epsilon}A(x)y dt + \sqrt{\frac{2\varsigma}{\epsilon}}dW_y, \quad y(0) = 0 \end{aligned} \quad (6.21)$$

where we have relabeled the noise increments $dW_\xi = dW_y$. Equation (6.21) is again a slow-fast system where the only difference to (6.8) is that also the slow dynamics is governed by an SDE. Therefore the averaging principle applies and we may replace the fast component in the slow equation by the stationary solution of the associated SDE

$$dy_x = A(x)y_x dt + \sqrt{2\varsigma}dW_y, \quad y(0) = 0$$

that is an centred Ornstein-Uhlenbeck process with covariance (for details see the appendix)

$$\begin{aligned} \mathbf{E}[Y_x Y_x^T] &= 2\varsigma \int_0^t \exp(-2A(x)s) ds \\ &\rightarrow \varsigma A(x)^{-1} \text{ as } t \rightarrow \infty. \end{aligned}$$

Let μ_x be the invariant measure of $Y_x = (y_x(t))_{t \in \mathbf{R}^+}$ that has the Gaussian density

$$\rho(y; x) = \frac{\sqrt{\det A(x)}}{(2\pi)^{m/2}} \exp\left(-\frac{1}{2\varsigma}y^T A(x)y\right), \quad \mu_x(dy) = \rho(y; x)dy.$$

Averaging y in the quadratic form above amounts to evaluating an integral of the form

$$\int_{\mathbf{R}^m} y^T B y \mu_x(dy) = \varsigma B : A^{-1},$$

which for the slow equation, using the Jacobi's formula $(\det A)' = \det A A' : A^{-1}$, yields

$$dx = -\frac{\partial}{\partial x} \left(U(x) + \frac{\varsigma}{2} \ln \det A(x) \right) dt + \sqrt{2\varsigma}dW_x, \quad x(0) = x_0.$$

The effective potential

$$F(x) = \frac{\varsigma}{2} \ln \det A(x)$$

⁵ The change of the small parameter from ϵ^2 to ϵ in the confining potential is merely a matter of notational convenience; cf. Section 5.

is called the *Fixman potential* and essentially captured the influence of the random motion orthogonal to the confinement set $\{y = 0\}$ on the dynamics on the set. Note that the appearance of the Fixman potential is different from the situation considered in Section 5 where the correction potential was the sum of the initial normal energies $I_i \omega_i(x)$ with $\omega_i = \sqrt{\lambda_i} \in \text{spec}(A)$ and I_i being identically zero if the dynamics is initially on the confinement set. The fact that the Fixman potential appears independently of the initial conditions is owed to, (i), the ergodicity of the Ornstein-Uhlenbeck process and, (ii), to the white noise that kicks the system off the confinement set with probability one (the first is actually a consequence of the latter).

Example 6.7 (Dynamical barrier) As an example we consider the system from Section 5, i.e., we assume $V: \mathbf{R}^2 \rightarrow \mathbf{R}$ to be the dynamical barrier potential

$$V(x, y) = \frac{1}{2}(x^2 - 1) + \frac{1}{2}\omega(x)^2 y^2, \quad \omega(x) = 1 + C e^{-\alpha(x-x_b)^2}.$$

The Fixman potential then reads

$$F(x) = \varsigma \ln \det \omega(x).$$

Both original potential and Fixman potential are depicted in Figure 11 below. As before in the Hamiltonian we observe that the additional (entropic) barrier that pops up becomes more pronounced as temperature is increased, where the barrier height is only a function of temperature and of the normal frequency $\omega(x)$ that couples slow and fast motion. Pathwise convergence to the limiting solution as $\epsilon \rightarrow 0$ for a single realization of the Brownian motion (i.e., convergence in probability) is shown in Figure 12.

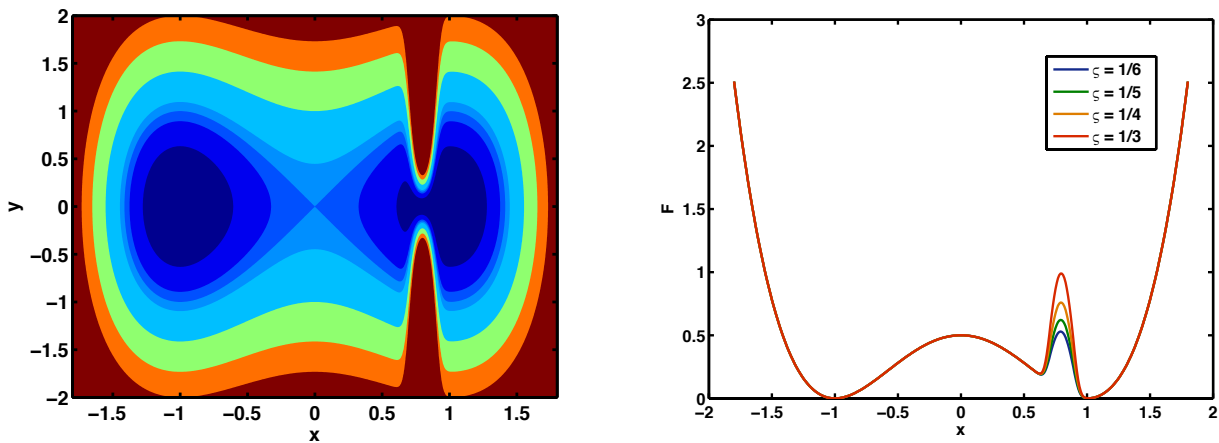


Fig. 11 Potential with an entropic barrier (left panel) and the corresponding Fixman potential for various ς (right panel).

Free energy If in (6.21) the gradient field $-\nabla V = (-\partial V/\partial x, -\partial V/\partial y)$ comes from an arbitrary potential V (smooth, polynomially growing and bounded below), the joint stationary distribution is still the Boltzmann distribution and the invariant measure of the fast dynamics is given by the *conditional* Boltzmann distribution

$$\mu_x(dy) = Z_x^{-1} \exp(-\varsigma^{-1} V(x, y)) dy, \quad Z_x = \int_{\mathbf{R}^m} \exp(-\varsigma^{-1} V(x, y)) dy.$$

In this case, also the averaged force $\overline{\partial V/\partial x}$ is a gradient field, as can be readily checked upon noting that

$$\int_{\mathbf{R}^n} \frac{\partial V}{\partial x} \mu_x(dy) = \frac{\partial}{\partial x} \varsigma \ln Z_x$$

with the so-called partition function (normalization constant) Z_x as given above. Hence $F(x) = -\varsigma \ln Z_x$ is the potential of mean force that is also known as the thermodynamical free energy.

Remark 6.8 For the Ornstein-Uhlenbeck process we have shown in the previous section that it converges almost surely (i.e., with probability one) to a stationary Gaussian process whose covariance is given by the inverse

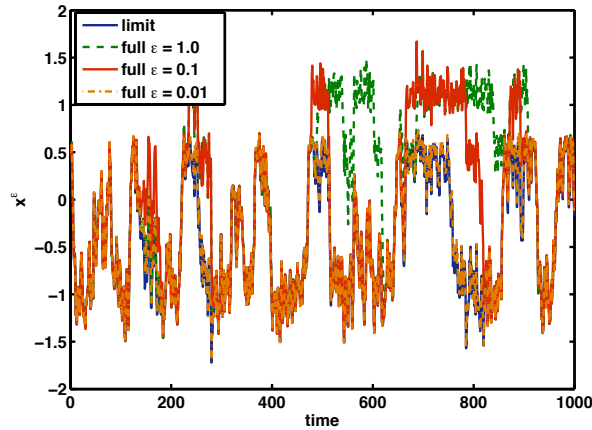


Fig. 12 Convergence of a typical realization of (6.21) with the 2-dimensional dynamical barrier potential to the limiting dynamics that is governed by the Fixman potential.

of the symmetric positive definite (s.p.d.) stiffness matrix. For more general SDEs of non-degenerate diffusion type (i.e., the noise matrix σ has full rank) it is possible to prove a law of large numbers (LLN), similarly to the LLN discussed in Section 5.3 where essentially the strong maximum principle that implies that the generator's kernel is only one-dimensional takes over the role of the diophantine condition (5.6).

6.4 Diffusive limits

It may happen that $\bar{f} = 0$ in which case the averaged dynamics become trivial on the on the time interval of interest, typically $[0, T]$. In this case the interesting dynamics happens on the infinite time interval $[0, \infty)$ and it is desirable to study the effective dynamics there. Suppose one is interested in the effective dynamics of the following coupled system of equations

$$\begin{aligned} \dot{x} &= f(x, y), & x(0) &= x_0 \\ dy &= \frac{1}{\epsilon} g(x, y) dt + \frac{1}{\sqrt{\epsilon}} \sigma(x, y) dW, & y(0) &= y_0 \end{aligned}$$

on the time interval $[0, T]$. For simplicity, we assume that all the coefficients are independent of ϵ — this is not a major restriction, however. Further suppose that the effective drift is zero if averaged against the invariant measure of the fast dynamics, i.e.,

$$\int_{Z_x} f(x, y) \mu_x(dy) = 0.$$

Now we may ask what happens if we derive the next perturbation order for the effective motion (i.e., the first-order correction to $\dot{x} = 0$). It turns out that going to the next perturbation order is equivalent to speeding up time according to $t \rightarrow t/\epsilon$ which yields the system

$$\begin{aligned} \dot{x} &= \frac{1}{\epsilon} f(x, y), & x(0) &= x_0 \\ dy &= \frac{1}{\epsilon^2} g(x, y) dt + \frac{1}{\epsilon} \sigma(x, y) dW, & y(0) &= y_0 \end{aligned} \tag{6.22}$$

Unlike in the averaging case it is now less obvious how the effective equation for x look like. By comparing the different powers of ϵ , however, we may expect that the slow motion will now couple to the Brownian motion that is of the same order of magnitude. Therefore the limiting dynamics on the time interval $[0, T/\epsilon]$, if it exists, will probably be diffusive (hence the name *diffusive limit*).

Derivation of the limit equations To systematically derive effective equations for the slow variable in (6.22) as $\epsilon \rightarrow 0$ we proceed as before and consider the backward equation

$$\partial_t u^\epsilon(x, y, t) = \mathcal{L}^\epsilon u^\epsilon(x, y, t), \quad u^\epsilon(x, y, 0) = \phi(x),$$

where, in accordance with the previous considerations, we assume from the outset that the initial datum ϕ is independent of the fast variables. The generator is now of the form

$$\mathcal{L}^\epsilon = \frac{1}{\epsilon} \mathcal{L}_0 + \frac{1}{\epsilon^2} \mathcal{L}_1$$

with

$$\mathcal{L}_0 = f(x, y) \cdot \frac{\partial}{\partial x}, \quad \mathcal{L}_1 = \frac{1}{2} a(x, y) : \frac{\partial}{\partial y} \otimes \frac{\partial}{\partial y} + g(x, y) \cdot \frac{\partial}{\partial y}$$

as before. Using the ansatz

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$$

in the backward equation and substituting the series, equating equal powers of ϵ yields

$$\mathcal{L}_1 u_0 = 0 \tag{6.23}$$

$$\mathcal{L}_1 u_1 = -\mathcal{L}_0 u_0 \tag{6.24}$$

$$\mathcal{L}_1 u_2 = \partial_t u_0 - \mathcal{L}_0 u_1 \tag{6.25}$$

and so on and so forth. As before, the first equation tells us that $u_0 = u_0(x, t)$. But the time evolution of u_0 is now due to the third equation where the closure is provided by the second one (by solving the equation for u_1).

Closure scheme We define the *cell problem* as the following system of elliptic equations

$$\mathcal{L}_1 \phi(x, y) = -f(x, y) \tag{6.26}$$

with x as a parameter and, say, periodic boundary conditions, i.e., $\mathcal{Z}_x \cong \mathbf{T}^m$. The solution, that is understood component-wise, is unique only up to a constants in y (i.e., functions in $\ker \mathcal{L}_1$); we may fix it by requiring that

$$\int_{\mathcal{Z}_x} \phi(x, y) \rho_\infty(y; x) dy \tag{6.27}$$

for all $x \in \mathcal{Z}_y \subseteq \mathbf{R}^n$ and with ρ_∞ as the unique solution of $\mathcal{L}_1^* \rho_\infty = 0$. As before we assume that $Y_x = (y_x(t))_{t \in \mathbf{R}^+}$ is ergodic, hence the nullspace of its generator \mathcal{L}_1 is one-dimensional. Note that $\bar{f} = 0$ (centering condition), so by the Fredholm alternative (6.26) has a solution. Equating powers of ϵ , equation (6.25) implies that

$$\mathcal{L}_1 u_1 = -f(x, y) \cdot \frac{\partial u_0}{\partial x}$$

where $u_0 = u_0(x, t)$. Since \mathcal{L}_1 contains only derivatives with respect to y , we can split off the rightmost term from which we conclude that u_1 must be of the form

$$u_1(x, y, t) = \phi(x, y) \cdot \nabla u_0(x, t) + \psi(x, t)$$

where $\psi \in \ker \mathcal{L}_1$ so we can ignore it in what follows and set it to zero. If we substitute the ansatz for u_1 we see that ϕ must solve the cell problem (6.26). Inserting the ansatz into (6.25), the solvability condition entails

$$\partial_t u_0 = \int_{\mathcal{Z}_x} \mathcal{L}_0 (\phi \cdot \nabla u_0) \mu_x(dy).$$

Again $\mu_x(dy) = \rho_\infty(y; x) dy$ with ρ_∞ being the unique eigenfunction of \mathcal{L}_1^* for the eigenvalue $\lambda = 0$. Given ϕ , the integrand on the right-hand side of the effective equation reads

$$\mathcal{L}_0 (\phi \cdot \nabla u_0) = f \otimes \phi : \nabla^2 u_0 + \left(\frac{\partial \phi}{\partial x} f \right) \cdot \nabla u_0.$$

Hence the effective equation for u_0 is of the form

$$\partial_t u_0 = \frac{1}{2} A(x) : \nabla^2 u_0 + F(x) \cdot \nabla u_0 \tag{6.28}$$

with the homogenised coefficients for the drift

$$F(x) = \int_{\mathcal{Z}_x} \left(\frac{\partial}{\partial x} \phi(x, y) \right) f(x, y) \rho_\infty(y; x) dy. \quad (6.29)$$

and for the (symmetrised) covariance

$$A(x) = \int_{\mathcal{Z}_x} (f(x, y) \otimes \phi(x, y) + \phi(x, y) \otimes f(x, y)) \rho_\infty(y; x) dy. \quad (6.30)$$

Defining a noise coefficient $\Sigma: \mathbf{R}^n \supseteq \mathcal{Z}_y \rightarrow \mathbf{R}^{n \times n}$ by $A(x) = \Sigma(x)\Sigma(x)^T$, the effective SDE is given by

$$dx = F(x)dt + \Sigma(x)dW, \quad x(0) = x_0 \quad (6.31)$$

which is, clearly, not unique as the Cholesky decomposition of the covariance matrix A is not. Nonetheless for any choice of Σ satisfying $A(x) = \Sigma(x)\Sigma(x)^T$ all the solutions to the SDE (6.31) are equivalent in that their laws coincide. It remains to show that (6.28)–(6.31) define a non-degenerate diffusion process.

Lemma 6.9 *The matrix field $A: \mathbf{R}^n \supseteq \mathcal{Z}_y \rightarrow \mathbf{R}^{n \times n}$ is positive definite.*

Proof. Set $v(x, y) = \xi \cdot \phi(x, y)$ with ϕ being the solution of the cell problem. Then v solves

$$\mathcal{L}_1 v(x, y) = -f(x, y) \cdot \xi$$

and therefore, using (6.30),

$$\begin{aligned} \langle A(x)\xi, \xi \rangle &= \int_{\mathcal{Z}_x} ((f(x, y) \cdot \xi)v(x, y) + v(x, y)(f(x, y) \cdot \xi)) \rho_\infty(y; x) dy \\ &= -2 \int_{\mathcal{Z}_x} (v(x, y)\mathcal{L}_1 v(x, y)) \rho_\infty(y; x) dy. \end{aligned}$$

But the spectrum of \mathcal{L}_1 is entirely on the negative real half-axis with a simple eigenvalue zero. By (6.27), the components of ϕ are orthogonal to the kernel of \mathcal{L}_1^* , hence entirely in the range of \mathcal{L}_1 . Since $\xi \neq 0$ is a constant vector, the same is true for v . Hence we can exclude v to lie in the kernel of \mathcal{L}_1 which implies that

$$\langle A(x)\xi, \xi \rangle > 0 \quad \forall \quad \xi \neq 0$$

and so gives the assertion. \square

Integral representation of the cell problem The cell problem (2.11) may be formally rewritten as

$$\phi(x, y) = -\mathcal{L}_1^{-1} f(x, y)$$

where the inverse of the elliptic operator \mathcal{L}_1 on the right-hand side is well-defined as $f \in (\ker \mathcal{L}_1^*)^\perp$. An explicit integral representation of \mathcal{L}_1^{-1} can be defined as follows: Let $g(x, \cdot)$ be orthogonal to the kernel of \mathcal{L}_1^* . Then

$$G(x, y) = - \int_0^\infty \exp(t\mathcal{L}_1) g(x, y) dt$$

is an integral representation of $\mathcal{L}_1^{-1}g$, for

$$\begin{aligned} \mathcal{L}_1 G &= - \int_0^\infty \mathcal{L}_1 \exp(t\mathcal{L}_1) g dt \\ &= - \int_0^\infty \frac{d}{dt} \exp(t\mathcal{L}_1) g dt \\ &= (1 - \lim_{t \rightarrow \infty} \exp(t\mathcal{L}_1))g, \end{aligned}$$

and \mathcal{L}_1 is negative-definite for all functions $g \in (\ker \mathcal{L}_1^*)^\perp$. Hence $\exp(t\mathcal{L}_1) \rightarrow 0$ and

$$\phi(x, y) = \int_0^\infty \exp(t\mathcal{L}_1) f(x, y) dt.$$

The above integral representation is convenient from a numerical point of view. To see why, bear in mind that \mathcal{L}_1 is the infinitesimal generator of the fast dynamics for fixed x with the semigroup $\exp(t\mathcal{L}_1)$ being the corresponding time evolution operator $\mathbf{E}_y[\cdot]$; cf. the discussion in Section 6.2. Substituting the expression for ϕ in (6.4) and (6.30) and exploiting the semigroup property of $\exp(t\mathcal{L}_1)$, the coefficients become

$$F(x) = \int_{\mathcal{Z}_x} \left(\int_0^\infty \mathbf{E}_y \left[\frac{\partial}{\partial x} f(x, y_x(t)) \right] dt \right) f(x, y) \mu_x(dy)$$

and

$$\begin{aligned} A(x) &= \int_{\mathcal{Z}_x} \left(f(x, y) \otimes \left(\int_0^\infty \mathbf{E}_y f(x, y_x(t)) dt \right) + \left(\int_0^\infty \mathbf{E}_y f(x, y_x(t)) dt \right) \otimes f(x, y) \right) \mu_x(dy) \\ &= \lim_{T \rightarrow \infty} \int_0^T \int_0^T \text{cov}(f(x, y_x(t)), f(x, y_x(s))) dt ds. \end{aligned}$$

Here $y_x(t)$ denotes the fast process at time t starting at $y_x(0) = y$, and $\mathbf{E}_y[\cdot]$ labels the average over all realizations up to time t conditional on the initial value y .

6.4.1 Overdamped limit of the Langevin equation

A classical problem is the high-friction or *overdamped* limit of the second order Langevin equation [10]. The second-order Langevin equation describes the motion of an inertial particle of mass m in a (smooth) potential V that is subject to friction and noise. A common and convenient writing is

$$m\ddot{q} + \gamma\dot{q} + \nabla V(q) = \xi, \quad (6.32)$$

where $q \in Q \subseteq \mathbf{R}^n$, and $\xi \in \mathbf{R}^n$ denotes a Gaussian white noise process with covariance matrix

$$\mathbf{E}\xi(t)\xi(t)^T = 2\gamma.$$

We shall assume throughout that $\gamma = \gamma^T$ is invertible (i.e., positive definite). For our purposes it is convenient to define new variables $x = q$ and $y = \dot{q}$ and recast the Langevin equation as

$$\begin{aligned} \dot{x} &= y \\ m dy &= -(\nabla V(x) + \gamma y) dt + \sigma dW \end{aligned} \quad (6.33)$$

with $\sigma \in \mathbf{R}^{n \times n}$ invertible and defined by the *fluctuation-dissipation relation* $2\gamma = \sigma\sigma^T$. The latter implies that the Boltzmann distribution

$$\rho \propto \exp\left(-\frac{m}{2}|y|^2 - V(x)\right)$$

is an, in fact *the* invariant distribution of the Langevin equation (6.33). (Invariance of ρ under the Langevin dynamics can be easily verified by plugging the expression into the corresponding Fokker-Planck equation.⁶) Suppose we want to study $\gamma \rightarrow \infty$ in the sense that all matrix entries uniformly go to infinity; if we want to preserve the Boltzmann distribution this requires that σ goes to infinity, so that the fluctuation-dissipation relation is preserved. More precisely, we consider the scaled Langevin equation

$$\begin{aligned} \dot{x} &= y \\ m dy &= -\left(\nabla V(x) + \frac{1}{\epsilon}\gamma y\right) dt + \frac{1}{\sqrt{\epsilon}}\sigma dW \end{aligned} \quad (6.34)$$

which is a slow-fast system with $x \in \mathcal{Z}_y \cong Q$ being the slow variable and $y \in \mathcal{Z}_x$ being fast. It is easy to see that the fast process is governed by the associated SDE

$$m dy = -\gamma y dt + \sigma dW \quad (6.35)$$

that is an Ornstein-Uhlenbeck (OU) process on $\mathcal{Z}_x \cong \mathbf{R}^n$ with asymptotic mean zero and covariance $m^{-1}\text{Id}$ as $t \rightarrow \infty$. But since $\mathbf{E}Y = 0$ asymptotically, the averaged equation for x turns out to be

$$\dot{x} = 0.$$

which tells us that the homogenisation principle applies (due to the centering condition). We have:

⁶ Proving uniqueness is a bit more involved and requires to show that the infinitesimal generator is hypo-elliptic and the Langevin dynamics is completely controllable which implies that all trajectories fill the whole phase space; for we details we refer to [9].

Theorem 6.10 (Nelson, 1967) *Let ∇V be globally Lipschitz and let $(X^\epsilon, Y^\epsilon) = (x^\epsilon(t), y^\epsilon(t))_{t \in \mathbf{R}^+}$ be the solution of the time-rescaled Langevin equation*

$$\begin{aligned} \dot{x} &= \frac{1}{\epsilon} y, & x(0) &= x_0 \\ m dy &= - \left(\frac{1}{\epsilon} \nabla V(x) + \frac{1}{\epsilon^2} \gamma y \right) dt + \frac{1}{\epsilon} \sigma dW, & y(0) &= y_0. \end{aligned}$$

Further let $X = (x(t))_{t \in \mathbf{R}^+}$ be the solution of the Smoluchowski equation

$$\gamma dx = -\nabla V(x) dt + \sigma dW, \quad x(0) = x_0. \quad (6.36)$$

Then, for all (x_0, y_0) and for all $\delta > 0$,

$$\lim_{\epsilon \rightarrow 0} \mathbf{P} \left[\sup_{t \in [0, T]} |x^\epsilon(t) - x(t)| > \delta \right] = 0$$

on all compact time intervals $[0, T]$.

We refrain from repeating the proof of Nelson that is very much tied to the specific form of the Langevin equation. A more general proof that uses similar techniques as we used to prove the averaging principle can be found in [13]; cf. also the original work [8] and the weak convergence result in [14].

Derivation of the overdamped equation We may still give some intuition about the high-friction limit by doing a formal derivation (without proving convergence though). To compute the Smoluchowski equation from the overdamped Langevin equation, it would be sufficient to solve the cell problem 6.26 for the fast OU process which is tedious, however (see the remark below). Instead we give an alternative derivation that goes as follows: Firstly note that upon rescaling time according to $t \mapsto t/\epsilon$, the Langevin equation (6.34) becomes

$$\begin{aligned} \dot{x} &= \frac{1}{\epsilon} y \\ m dy &= - \left(\frac{1}{\epsilon} \nabla V(x) + \frac{1}{\epsilon^2} \gamma y \right) dt + \frac{1}{\epsilon} \sigma dW. \end{aligned}$$

The corresponding infinitesimal generator then admits a splitting of the form

$$\mathcal{L}^\epsilon = -\frac{1}{\epsilon} \mathcal{L}_0 + \frac{1}{\epsilon^2} \mathcal{L}_1$$

where

$$\mathcal{L}_0 = y \cdot \frac{\partial}{\partial x} - m^{-1} \nabla V(x) \cdot \frac{\partial}{\partial y}, \quad \mathcal{L}_1 = \frac{1}{2m} \sigma \sigma^T : \frac{\partial}{\partial y} \otimes \frac{\partial}{\partial y} - m^{-1} \gamma y \cdot \frac{\partial}{\partial y}$$

In a slight abuse of notation, let us write the homogenised backward equation as

$$\partial_t u_0 = \int_{\mathbf{R}^n} \mathcal{L}_0 \mathcal{L}_1^{-1} \mathcal{L}_0 u_0 \mu_x(dy)$$

where the stationary distribution μ_x of the fast OU-process is independent of x and has the density

$$\rho_\infty(y) = \left(\frac{m}{2\pi} \right)^{n/2} \exp \left(-\frac{m}{2} |y|^2 \right).$$

In order to compute the effective generator explicitly, we observe that

$$\mathcal{L}_0 u = y \cdot \nabla u$$

for functions $u = u(x, t)$. Hence, upon noting that

$$\mathcal{L}_1 (\gamma^{-1} y) = -m^{-1} y,$$

we find

$$\mathcal{L}_1^{-1} \mathcal{L}_0 u = -m \gamma^{-1} y \cdot \nabla u$$

for the action of \mathcal{L}_1^{-1} on $\mathcal{L}_0 u \in (\ker \mathcal{L}_1^*)^\perp$. Therefore

$$\mathcal{L}_0 \mathcal{L}_1^{-1} \mathcal{L}_0 u = m (\gamma^{-1} y \otimes y) : \nabla^2 u - \gamma^{-1} \nabla V \cdot \nabla u$$

and integrating against μ_x yields

$$\left(\int_{\mathbf{R}^n} \mathcal{L}_0 \mathcal{L}_1^{-1} \mathcal{L}_0 \mu_x(dy) \right) u = \gamma^{-1} : \nabla^2 u - \gamma^{-1} \nabla V \cdot \nabla u.$$

Thus the homogenised backward equation reads

$$\partial_t u(x, t) = \gamma^{-1} : \nabla^2(x, t) - \gamma^{-1} \nabla V(x) \cdot \nabla u(x, t).$$

Using that $2\gamma = \sigma \sigma^T$ it follows that the backward equation is equivalent to the SDE

$$\gamma dx = -\nabla V(x) dt + \sigma dW$$

which is the desired Smoluchowki equation.

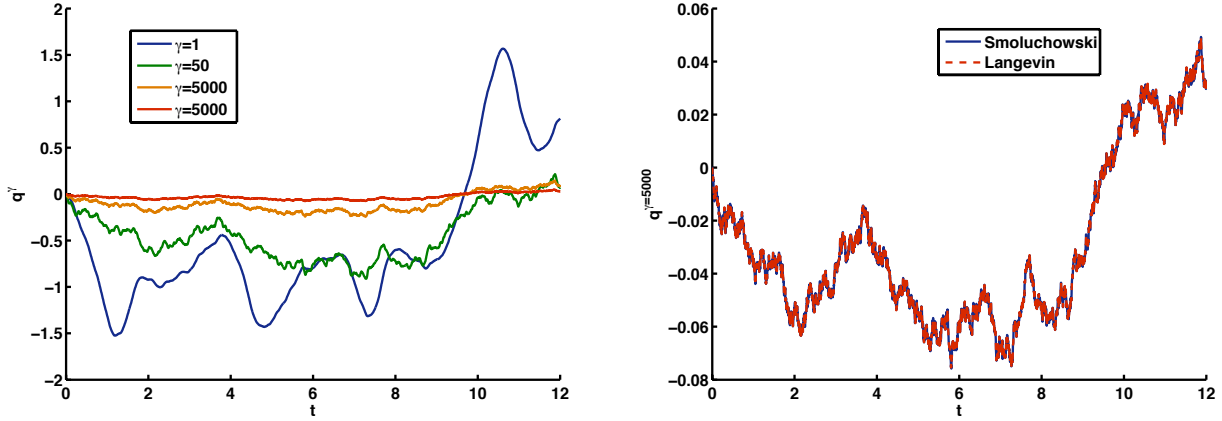


Fig. 13 Behaviour of the Langevin dynamics as the friction coefficient γ goes to infinity. Eventually the large damping lets the dynamics freeze, so that it converges to the initial value $q_0 = 0$ (left panel). The right panel illustrates that the first-order correction to $q(t) \approx q_0$ is indeed given by the overdamped equation (note the scale on the q -axis).

Remark 6.11 We may briefly explain how the cell problem may be solved in 1D. For a function $\phi \in (\ker \mathcal{L}_1^*)^\perp$ the cell problem, equation (6.26), reads

$$\frac{d^2 \phi}{dy^2} - y \frac{d\phi}{dy} + \frac{m}{\gamma} y = 0.$$

Using separation of variables, the solution of the homogeneous problem is found to be

$$\phi_0(y) = C_2 + C_1 \sqrt{\frac{\pi}{2}} \operatorname{erfi} \left[\frac{y}{\sqrt{2}} \right],$$

where C_1, C_2 are integration constants, and $\operatorname{erfi}[z]$ is the *complex error function* that is defined by

$$\operatorname{erfi}[z] = -i \operatorname{erf}[iz] \quad \text{with} \quad \operatorname{erf}[z] = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) d\xi.$$

It can be readily seen that the full solution is now given by

$$\phi(y) = C_2 + C_1 \sqrt{\frac{\pi}{2}} \operatorname{erfi} \left[\frac{y}{\sqrt{2}} \right] + \frac{m}{\gamma} y. \quad (6.37)$$

where the integration constant C_1 is arbitrary, and $C_2 = 0$ is determined by the requirement $\phi \in (\ker \mathcal{L}_1^*)^\perp$, i.e., must ϕ vanish if integrated with respect to $\mu_x(dy) = \rho_\infty(y)dy$.

Example 6.12 (Averaging vs. homogenisation) We consider Langevin dynamics in a double-well potential,

$$\ddot{q} + \gamma \dot{q} + 2q(q^2 - 1) = \sqrt{2\gamma} \eta, \quad q(0) = q_0, \dot{q}(0) = v_0$$

with $q \in \mathbf{R}$ and η being Gaussian white noise with $\mathbf{E}[\eta(t)\eta(s)] = \delta(t - s)$. For simplicity we have set $m = 1$. We shall now probe the dynamics as $\gamma \rightarrow \infty$ and compare it to the solution of the overdamped equation

$$\gamma dq = -2q(q^2 - 1) + \sqrt{2\gamma} \eta, \quad q(0) = q_0$$

where we distinguish two cases: the original equation and the time-rescaled problem on the diffusive time scale $\tau = \gamma t$. For the unscaled problem the left panel of Figure 13 illustrates how an increasing friction coefficient γ damps the dynamics until it eventually freezes completely, i.e.,

$$\lim_{\gamma \rightarrow \infty} q^\gamma(t) = q_0 \quad \forall t \in [0, T].$$

Also observe that the trajectory gets rougher and rougher as γ is increased which illustrates the onset of the diffusive behaviour. As the right panel shows, the Smoluchowski equation provides indeed the correct limit dynamics, but the right-hand side has the prefactor γ^{-1} that damps drift and noise as γ grows large (note the different scales on the q -axes of left and right panel of the figure).

As $\gamma \rightarrow \infty$ the non-trivial dynamics such as convergence to the Boltzmann distribution $\exp(-V)$ happens on the time diverging interval $[0, T/\gamma)$ as can be seen in Figure 14 for $\gamma = 50$: the Smoluchowski equation reproduces the Langevin dynamics very well, but the time interval on which the non-trivial dynamics happens is now dilated by a factor γ (compare the time interval in Figure 13).

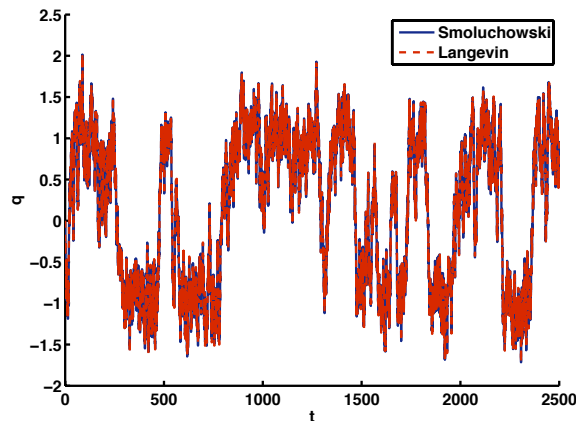


Fig. 14 Long-term behaviour of the Langevin and Smoluchowski dynamics for a large friction coefficient $\gamma = 50$.

Appendices

A Gronwall Lemma

An important result that is prevalently used in the convergence proofs is Gronwall's Lemma. It is an inequality version of the variation of constants formula and typically appears if the right hand side in a differential equation that one is interested is locally Lipschitz with Lipschitz constant L . We state two variants of the lemma.

Lemma A.1 (Differential version) *Let $z(t) = \varphi^t(z_0)$, $\varphi^t: \mathcal{Z} \rightarrow \mathcal{Z}$ satisfy the differential inequality*

$$\dot{z} \leq Lz + u, \quad z(0) = z_0 \quad (\text{A.1})$$

with $L \in \mathbf{R}$ and u being a sufficiently smooth time-dependent function, e.g., $u \in L^1([0, T], \mathcal{Z})$. Then

$$z(t) \leq e^{Lt} \left(z_0 + \int_0^t e^{-Ls} u(s) ds \right) \quad \forall t \in [0, T]. \quad (\text{A.2})$$

Proof. We use variation of constants: multiplying (A.1) by $\exp(-Lt)$ we obtain

$$\dot{z}(t)e^{-Lt} \leq (Lz(t) + u(t))e^{-Lt}.$$

Hence, by chain rule,

$$\frac{d}{dt} (z(t)e^{-Lt}) \leq \exp(-Lt)u(t).$$

Integrating from 0 to t and multiplying both sides by $\exp(Lt)$ gives the desired result. \square

Corollary A.2 (Integral version) *Now, let $\zeta(t)$ satisfy the integral inequality*

$$\zeta(t) \leq L \int_0^t \zeta(s) ds + M. \quad (\text{A.3})$$

for some positive constants L, M . Then

$$\zeta(t) \leq Me^{Lt}. \quad (\text{A.4})$$

Proof. Set

$$z(t) = \int_0^t \zeta(s) ds.$$

Then, by definition, $z(t)$ defines the differential inequality

$$\dot{z} \leq Lz + M, \quad z(0) = 0,$$

so that Lemma A.1 implies

$$z(t) \leq \frac{M}{L} (e^{Lt} - 1).$$

Now replacing the integral in (A.3) by the upper bound for $z(t)$ proves the assertion. \square

B Diffusion processes

Before we introduce the basic concepts of diffusion processes, we shall give some intuition as to what is the major difference between deterministic and stochastic initial value problems; for details regarding stochastic differential equations we refer to the textbook [11]. Firstly, let us consider the solution to a typical initial value problem

$$\dot{x} = b(x), \quad x(0) = x_0$$

which solution may look like the blue curve depicted in Figure 15. On the other hand we may compute solutions of a the generic stochastic differential equation

$$\dot{z} = b(z) + \xi, \quad z(0) = x_0$$

where $\xi = \xi(t, \omega)$ is a stochastic process, i.e., for every $t > 0$ fixed, the $\xi(t, \omega)$ is a random variable with values in \mathcal{Z} which distribution is determined by the unknown sample space $\Omega \ni \omega$ and the probability measure \mathbf{P} defined on it. Since the perturbation is random, every realization of $z(t) = z(t, \omega)$ will be different (whereas we have just one trajectory $x(t)$ for x_0 being fixed). Two typical realizations of $z(t)$ are shown in Figure 15 (dashed curves).

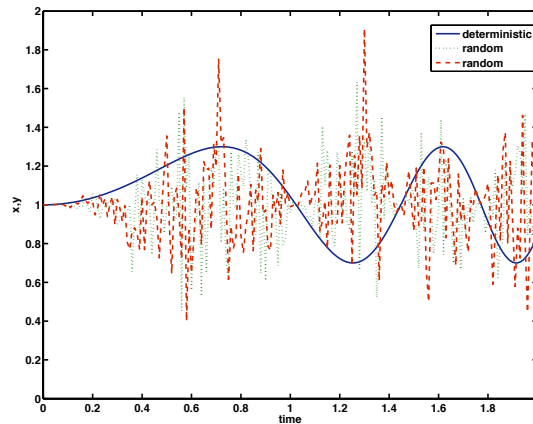


Fig. 15 Typical realizations of a randomly perturbed stochastic differential equation together with its fully deterministic counterpart.

Brownian motion To begin with, we recap some basic definitions from probability. The classic definition of a *stochastic process* goes as follows: a stochastic process with index set $I \subset \mathbf{R}$ on a state space \mathcal{Z} that is equipped with a Borel σ -algebra \mathcal{L} is a family $Z = (z(t))_{t \in I}$ where the $z(t)$ are defined on a common probability space $P = (\Omega, \mathcal{B}, \mathbf{P})$ and assume values in \mathcal{Z} . The expectation of $Z: I \times P$ is defined by

$$\mathbf{E}Z = \int_{\Omega} z(t, \omega) d\mathbf{P}(\omega).$$

Accordingly we define its probability distribution function (law) as

$$\rho(z, t) dz = \mathbf{P} \left[\omega \in \Omega: z(t, \omega) \in \prod_{i=1}^n [z_i, z_i + dz_i] \right].$$

We are now ready to introduce the concept of Brownian motion where, without loss of generality, we confine our attention to the one-dimensional case. Let us begin with a formal definition and then construct a suitable stochastic process that meets all the required properties.

Definition B.1 (Standard Brownian motion, a.k.a. Wiener process) A one-dimensional Brownian motion is a stochastic process $W: P \rightarrow \mathbf{R}$ with the following properties:

1. $W(0) = 0$.
2. $W(t)$ is continuous.
3. The increments $\Delta W(t_k) = W(t_k) - W(t_{k-1})$ are independent random variables for all $1 \leq k \leq n$ with $0 \leq t_0 \leq t_1 \dots t_n$. Moreover $\Delta W(t) = W(t) - W(s)$, $t > s$ is normally distributed with zero mean and variance $t - s$.

It follows directly from the definition that W is a centred Gaussian process with variance t ; its law is

$$\rho(x, t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right).$$

We will introduce Brownian motion as the limiting process of a suitably scaled random walk on \mathbf{Z} . To this end consider the time-discrete stochastic process

$$Z: P \rightarrow \mathbf{R}, \quad z(t) = \Delta z \sum_{i=1}^{t/\Delta t} \eta_i \tag{B.1}$$

with $t/\Delta t \in \mathbf{N}$ and $\eta_i \in \{-1, 1\}$ with equal probability $\mathbf{P}[\eta_i = \pm 1] = 1/2$. Note that

$$\mathbf{E}\eta_i = 0$$

and

$$\text{var}\eta_i = 1.$$

We will show that $Z \rightarrow W$ as $\Delta z, \Delta t \rightarrow 0$ in the sense that their probability distributions are the same (therefore the new symbol “ \rightarrow ”). As W is Gaussian its distribution is completely determined by its mean and its variance, so we need to consider only the first two moments. It suffices that for $z(0) = 0$,

1. $\mathbf{E}Z \rightarrow 0$,
2. $\mathbf{E}Z^2 \rightarrow t$

as $\Delta z, \Delta t \rightarrow 0$. The first property follows independently of Δz ; using the definition of Z , equation (B.1), with $n = t/\Delta t$ and the linearity of the expectation we readily see that

$$\mathbf{E}Z = \Delta z \sum_{i=1}^n \mathbf{E}\eta_i$$

which is zero by the fact that $\mathbf{E}\eta_i = 0$ for all $1 \leq i \leq n$. For the second moment we find

$$\begin{aligned} \mathbf{E}Z^2 &= (\Delta z)^2 \mathbf{E} \left(\sum_{i=1}^n \eta_i \right)^2 \\ &= n(\Delta z)^2 \mathbf{E}\eta_i^2 \\ &= n(\Delta z)^2 \end{aligned}$$

where in the second equality we use the independence of the η_i , i.e., $\mathbf{E}[\eta_i \eta_j] = \delta_{ij}$. Now setting $\Delta z = \sqrt{\Delta t}$ keeping in mind that $n = t/\Delta t$ we conclude that

$$\lim_{\Delta t \rightarrow 0} \mathbf{E}Z^2 \rightarrow t, \quad t \in \mathbf{R}_+$$

as desired. Continuity of Z follows from $\Delta z = (\Delta t)^2 \rightarrow 0$.⁷

Remark B.2 In pretty much the same way as above one can construct generalised variants of W such as

$$B(t) = \mu t + \sigma W(t).$$

which is obtained by simply rescaling Δz and replacing the symmetric random walk by a biased one.

White noise Intimately related to Brownian motion and diffusion processes in general is a process called *Gaussian white noise* or, in brief, *white noise*. We call the process $\xi: P \rightarrow \mathbf{R}$ white noise if

1. $\mathbf{E}\xi(t) = 0$,
2. $\mathbf{E}[\xi(t)\xi(s)] = \delta(t - s)$

where the second property implies that $\xi \sim \mathcal{N}(0, 1)$ for all $t > 0$. White noise can be considered the generalised derivative of Brownian motion (where we leave it open what we understand by “generalised”). To get a rough idea what we mean by that, note that

$$W(t + \Delta t) = W(t) + \sqrt{\Delta t} \xi(t + \Delta t). \quad (\text{B.2})$$

with $\xi(t + \Delta t) \sim \mathcal{N}(0, 1)$. Knowing the law of W and using the independence of its increments, we can easily compute the autocorrelation of ξ , namely, $\mathbf{E}[\xi(t + \Delta t)\xi(t)] = \delta(\Delta t)$. The assertion then follows in the limit $\Delta t \rightarrow 0$.

⁷ The above result is essentially a consequence of the central limit theorem that asserts that the sum of n independent and identically distributed (i.i.d.) random variables divided by \sqrt{n} converges in distribution to a $\mathcal{N}(0, 1)$ random variable.

The generator Before we introduce Itô stochastic differential equations, we shall briefly anticipate the concept of the infinitesimal generator of a diffusion process. To this end, consider the (infinitesimal) difference equation

$$dZ = \xi, \quad z(0) = 0$$

that is essentially (B.2) rephrased. Its solution is given by the Wiener process $Z = W$. The probability distribution function $\mathbf{P}[z(t) \in [z, z + dz]]$ has the Gaussian density

$$\rho(z, t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{z^2}{2t}\right)$$

and solves the one-dimensional Fokker-Planck equation (heat equation)

$$\frac{\partial \rho}{\partial t} = \frac{1}{2} \frac{\partial^2 \rho}{\partial z^2}, \quad \lim_{t \rightarrow 0^+} \rho(z, t) = \delta(z).$$

This statement can be rephrased saying that $\mathcal{L} = 1/2 \partial^2 / \partial z^2$ is the generator of the semigroup $\exp(t\mathcal{L})$ that describes the time-evolution of functions $f = f(z)$ under the stochastic process Z .

Stochastic differential equations Equation (B.1) is a time-discrete version of Brownian motion in terms of a recurrence relation. A natural generalization of this recurrence is

$$z(t + \Delta t) = z(t) + b(z(t))\Delta t + \sigma(z(t))\eta(t + \Delta t)\sqrt{\Delta t}, \quad z(0) = z_0 \quad (\text{B.3})$$

where $\eta(\cdot) \in \{-1, 1\}$ and both $b: \mathcal{Z} \rightarrow \mathbf{R}$ and $\sigma: \mathcal{Z} \rightarrow \mathbf{R} \setminus \{0\}$ are sufficiently smooth. Without the rightmost term, equation (B.3) would simply be the forward Euler discretisation of the ODE

$$\dot{z} = b(z), \quad z(0) = z_0.$$

The continuous version of the stochastic recurrence as $\Delta t \rightarrow 0$ is the Itô stochastic differential equation (SDE)

$$dz = b(z)dt + \sigma(z)dW, \quad z(0) = z_0 \quad (\text{B.4})$$

where, for our purposes, the Brownian increments dW may be interpreted in the sense of (B.2).

Itô's formula and Itô isometries The SDE (B.4) has some remarkable properties that distinguish it from ordinary differential equation. One such property is Itô's formula that can be considered a stochastic generalisation of the standard chain rule.⁸

Lemma B.3 (*Itô's formula*) *Let $z(t)$ be a solution of (B.4). Then $g: \mathcal{Z} \rightarrow \mathbf{R}$ solves the equation*

$$dg(z) = g'(z)dz + \frac{1}{2}g''(z)a(z)dt, \quad a(z) = \sigma(z)^2. \quad (\text{B.5})$$

Proof. We use again the recurrence (B.3); the generalization to the multidimensional case is straightforward. To prove (B.5) we do a Taylor expansion of $g(z)$ up to terms of order Δt . Upon introducing the shorthands $\Delta g(z(t + \Delta t)) = g(z(t + \Delta t)) - g(z(t))$ and $\Delta z(t + \Delta t) = z(t + \Delta t) - z(t)$ we find

$$\begin{aligned} \Delta g(z(t + \Delta t)) &= g(z(t + \Delta t)) - g(z(t)) \\ &= g'(z(t))\Delta z(t + \Delta t) + \frac{1}{2}g''(z(t))(\Delta z(t + \Delta t))^2 + \mathcal{O}(|\Delta z(t + \Delta t)|^3) \\ &= g'(z(t))\Delta z(t + \Delta t) + \frac{1}{2}g''(z(t))a(z(t))\Delta t + \mathcal{O}(|\Delta t|^{3/2}) \end{aligned}$$

where the last equality follows from inserting (B.3) and $\eta^2 = 1$. Letting $\Delta t \rightarrow 0$ yields the result. \square

Note that standard chain rule (i.e., omitting the noise term) would imply that g solves the equation $\dot{g}(z(t)) = g'(z(t))\dot{z}(t)$. The fact that an additional term, the *quadratic variation*, appears can be understood by observing that the Brownian increments dW are formally of order dt and chain rule is an expansion up to dt while omitting all higher order terms.

⁸ In the following we shall not distinguish between the Itô equation (B.4) and its discrete analogue (B.3), the so-called Euler-Maruyama discretization. We refer to either of them as *SDE*.

Lemma B.4 (*Itô isometries*) Consider the SDE

$$dz = f(W, t)dW, \quad z(0) = 0$$

that has the solution

$$z(t) = \int_0^t f(W(s), s)dW(s).$$

Then:

- first Itô isometry

$$\mathbf{E} \int_0^t f(W(s), s)dW(s) = 0$$

- second Itô isometry

$$\mathbf{E} \left(\int_0^t f(W(s), s)dW(s) \right)^2 = \mathbf{E} \int_0^t (f(W(s), s))^2 ds.$$

Proof. Using the discrete scheme (B.3) and introducing the shorthands $Z_n = z(t_n)$, $W_n = W(t_n)$, $\eta_n = \eta(t_n)$ and $t_{n+1} = t_n + \Delta t$, we see that

$$\begin{aligned} \mathbf{E}Z_{n+1} &= \mathbf{E} \sum_{i=1}^n f(W_i, t_i)\eta_{i+1}\sqrt{\Delta t} \\ &= \sum_{i=1}^n \mathbf{E}f(W_i, t_i)\mathbf{E}\eta_{i+1}\sqrt{\Delta t} \\ &= 0 \end{aligned}$$

which is the first isometry where the second above equality is entailed by the independence of the Brownian increments in the second equality (i.e., $\mathbf{E}[W_i\eta_{i+1}] = \mathbf{E}W_i\mathbf{E}\eta_{i+1}$).

The second isometry can be proved in the same way, namely,

$$\begin{aligned} \mathbf{E}Z_{n+1}^2 &= \mathbf{E} \sum_{i,j=1}^n f(W_i, t_i)\eta_{i+1}f(W_j, t_j)\eta_{j+1}\Delta t \\ &= \sum_{i=1}^n \mathbf{E}f(W_i, t_i)\Delta t \end{aligned}$$

where we have (again) taken advantage of the property $\mathbf{E}[\eta_i\eta_j] = \delta_{ij}$. □

Ornstein-Uhlenbeck process An important class of stochastic processes are Gaussian processes that are governed by linear SDEs. One such case is the *Ornstein-Uhlenbeck (OU) process* that, in 1D, assumes the form

$$dz = -\alpha zdt + \sigma dW, \quad z(0) = x \tag{B.6}$$

with $\alpha > 0$. Its solution reads

$$z(t) = x - \alpha \int_0^t z(s) ds + \sigma \int_0^t dW(s).$$

Using Itô's formula we can recast the solution as something more familiar, viz.,

$$\begin{aligned} d(e^{\alpha t}z) &= \alpha e^{\alpha t}z + e^{\alpha t}dz \\ &= e^{\alpha t}\sigma dW. \end{aligned}$$

Rearranging the terms, we recover the well-known variation-of-parameters formula

$$z(t) = e^{-\alpha t}x - \sigma \int_0^t e^{-\alpha(t-s)}dW(s), \tag{B.7}$$

again, with a straightforward generalisation to the multidimensional case.

Properties of the OU process We can demonstrate the usage of the two Itô isometries by computing mean and variance of the OU process $Z = (z(t))_{t \in \mathbf{R}_+}$. As a direct consequence of the first Itô isometry the martingale term (i.e., the one involving dW) has mean zero. Therefore

$$\mathbf{E}Z = e^{-\alpha t} x.$$

By employing the second Itô isometry, it follows that

$$\begin{aligned} \mathbf{E}(Z - \mathbf{E}Z)^2 &= \sigma^2 \mathbf{E} \left(\int_0^t e^{-2\alpha(t-s)} dW(s) \right)^2 \\ &= \mathbf{E} \int_0^t e^{-2\alpha(t-s)} ds \\ &= \frac{\sigma^2}{2\alpha} (1 - e^{-2\alpha t}). \end{aligned}$$

Since Z is Gaussian its law is completely determined by the first two moments. Its stationary distribution is found by letting $t \rightarrow \infty$, i.e.,

$$\mathbf{E}Z \rightarrow 0 \quad \text{and} \quad \text{var}Z \rightarrow \frac{\sigma^2}{2\alpha}$$

as $t \rightarrow \infty$. In other words, $Z \rightarrow \mathcal{N}(0, \sigma^2/(2\alpha))$ in distribution, independently of the initial conditions.

C Stochastic convergence

Let \mathbf{P} be a probability measure on (Ω, \mathcal{B}) , i.e., $\mathbf{P}(\Omega) = 1$ and let z^ϵ be a sequence on $(\mathcal{Z}, \mathcal{Z})$. For our purposes it is sufficient to distinguish to types of (strong) convergence of z^ϵ to z (provided that the limit exists):

1. Convergence in mean:

$$\begin{aligned} \mathbf{E}|z^\epsilon - z| &= \int_{\Omega} |z^\epsilon(\omega) - z(\omega)| d\mathbf{P}(\omega) \\ &\rightarrow 0. \end{aligned}$$

2. Convergence in probability: For all $\delta > 0$,

$$\begin{aligned} \mathbf{P}[|z^\epsilon - z| > \delta] &= \int_{|z^\epsilon - z| > \delta} d\mathbf{P}(\omega) \\ &\rightarrow 0. \end{aligned}$$

Markov inequality Convergence in L^1 implies uniform integrability. This can be restated by saying that convergence in mean implies convergence in probability. The latter can be easily seen by noting that

$$\begin{aligned} \int_{\Omega} |z^\epsilon(\omega) - z(\omega)| d\mathbf{P}(\omega) &\geq \int_{\Omega} |z^\epsilon(\omega) - z(\omega)| \chi_{|z^\epsilon(\omega) - z(\omega)| > \delta}(\omega) d\mathbf{P}(\omega) \\ &\geq \delta \int_{\Omega} \chi_{|z^\epsilon(\omega) - z(\omega)| > \delta}(\omega) d\mathbf{P}(\omega) \\ &= \delta \int_{|z^\epsilon - z| > \delta} d\mathbf{P}(\omega). \end{aligned} \tag{C.1}$$

where χ_B denotes the characteristic function of the set $B \in \mathcal{B}$ and we have used that $0 \leq \mathbf{P}(B) \leq 1$.

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