4.4 Dynamics on Networks

So far, we simply identified the topology of connections between the nodes of a network. In many cases the connectivity is merely the prelude to describing the different states of the network that may arise from the coordinated evolution of its elements. Let us assign a variable $x_i(t)$ to each node, whose time evolution is governed by

$$\frac{dx_i}{dt} = F_i(\text{values of } x_j \text{ on sites connected to } i)\,. \tag{4.20}$$

Despite its apparent generality, the underlying assumption that the dynamics is governed by a set of coupled *first order* in time ordinary differential equations is itself a (potentially drastic) approximation. The concentrations of chemical species vary is space as well as time, necessitating partial differential equations; and the rates dx_i/dt may not be instantaneous functions of other variables requiring higher time derivatives or time delayed kernels. Also various forms of noise are also present requiring a stochastic (e.g. by Langévin or Master equation) rather than deterministic treatment. Nonetheless, Eqs. (4.20) provide a quite useful first approximations in many biological problems. For example, the average densities of participants in a network of chemical reactions, or of proteins and mRNA in a transcription network, can be described (in the mean-field limit, and when well mixed) by a set of rate equations for the concentrations $C_i(t)$, such that

$$\begin{aligned}\frac{dC_i}{dt} = \quad & + \quad \text{Flux from chemical reactions creating } i \\ & - \quad \text{Flux from chemical reactions destroying } i\,.\end{aligned}$$

For example, in the simple reaction A+B ${}^{k_-}\!\rightleftharpoons_{k_+}$ C, the concentration of A varies as

$$\frac{d[\mathrm{A}]}{dt} = -k_+[\mathrm{A}][\mathrm{B}] + k_-[\mathrm{C}]\,. \tag{4.21}$$

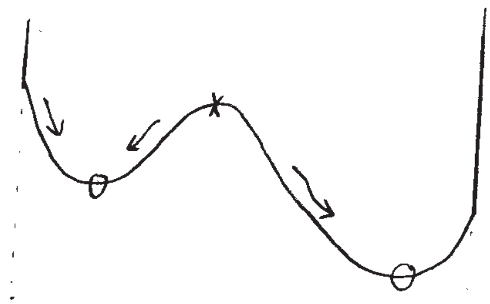
Such systems of equations can encode a variety of interesting dynamical behaviors. We shall discuss stationary fixed points and cycles as common examples of possible outcomes.

4.4.1 Attractive fixed points

With only one variable, the generic outcome is for it to approach an attractive fixed point. This is because the one dimensional equation can be regarded as describing descent in a potential $V(x)$, as

$$\frac{dx}{dt} = F(x) = -\frac{\partial V}{\partial x}\,, \quad \text{where} \quad V(x) = -\int^x dx'\, F(x')\,. \tag{4.22}$$

The coordinate x will descend in this potential, settling down to possible fixed points that are solutions to $F(x^*) = 0$. Note that a general function $F(x)$ does not necessarily have a zero. However, in most physically relevant situations the variable x is constrained to a finite interval; for example, the concentration of a chemical has to be positive and less than some maximal value. In such cases $V(x)$ is effectively infinite outside the allowed interval, and the potential will have a minimum, possibly at the limits of the interval. The function $V(x)$ is also relevant to the stochastic counterpart of Eq. (4.22): The addition of uncorrelated noise $\eta(t)$ to this equation (with $\langle\eta(t)\rangle = 0$ and $\langle\eta(t)\eta(t')\rangle = 2D\delta(t - t')$) results in a Langévin equation with steady steady probability density $p^*(x) \propto \exp[-V(x)/D]$.



The above conclusions continue to hold for coupled equations with many variables, if they correspond to gradient descent in a multi-variable potential $V(x_1, x_2, \cdots, x_N)$, i.e. for

$$\frac{dx_i}{dt} = -\frac{\partial\mathcal{V}(x_1, x_2, \cdots, x_N)}{\partial x_i} \equiv F_i\,. \tag{4.23}$$

The equality of second derivatives then immediately implies that

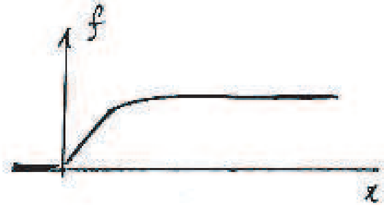
$$\frac{\partial F_i}{\partial x_j} = \frac{\partial F_j}{\partial x_i}\,. \tag{4.24}$$

This condition is too constraining and not generically satisfied. For example, in a linear system with $F_i = \sum_j W_{ij}x_j$ it requires symmetric interactions with $W_{ij} = W_{ji}$.

A less constraining version of approach to a fixed point is a dynamics that minimizes a *Lyapunov function*. An important example of such is provided by Hopfield's model of a 'neural network' with graded response, which is capable of storing and recalling 'associative memories.' In this model the activity of each neuron is indicated by a variable x_i (related to the spiking rate of the neuron) that evolves in time according to

$$\frac{dx_i}{dt} = -\frac{x_i}{\tau} + f\left(\sum_j W_{ij}x_j + b_i\right)\,. \tag{4.25}$$

In Eq. (4.25), τ is a natural time constant for decay of activity in the absence of stimuli, and for simplicity we set it to unity; b_i represents external input to the network, say from sensory cells; and W_{ij} is a matrix encoding the strength of synaptic connections from neuron j to neuron i. (Synaptic connections between real neurons pass information only in one direction, and the corresponding connectivity matrix will not be symmetric, with $W_{ij} \neq W_{ji}$.) The function f captures the input/output characteristics of the neuron's response; it is assumed to be a monotonic function of its argument, typically a sigmoidal form that switches between a low and a high value at a threshold input (which can be folded into the parameter b_i). A simplified version of the neural network assigns discrete binary values (say -1 and +1) to each neuron, and a randomly selected neuron i asynchronously switches depending on the sign of $\sum_j W_{ij}x_j + b_i$. Hopfield in fact introduced the model with continuous variables $\{x_i(t)\}$ to address criticism that the binary model was too removed from biological neurons.[1]



Even with symmetric connections $W_{ij} = W_{ji}$,

$$\frac{\partial F_i}{\partial x_j} = -\delta_{ij} + f'\left(\sum_k W_{ik}x_k + b_i\right) W_{ij} \neq \frac{\partial F_j}{\partial x_i} = -\delta_{ij} + f'\left(\sum_k W_{jk}x_k + b_j\right) W_{ji}\,,$$

the Hopfield model does not correspond to gradient descent in a potential, as the arguments of f', corresponding to net inputs into i or j are different. Nonetheless, we can still demonstrate the existence of fixed points by introducing a *Lyapunov function*,

$$\mathcal{L}(x_1, x_2, \cdots, x_N) = \sum_{i=1}^{N} \left[G(x_i) - b_i x_i\right] - \frac{1}{2}\sum_{i,j} W_{ij}x_i x_j\,, \tag{4.26}$$

where the function G shall be defined shortly. The time derivative of $\mathcal{L}$ is given by

$$\begin{aligned}\frac{d\mathcal{L}}{dt} &= \sum_i \frac{\partial \mathcal{L}}{\partial x_i}\cdot\frac{dx_i}{dt}\\ &= \sum_i \left[G'(x_i) - b_i - \sum_j W_{ij}x_j\right]\cdot\left[-x_i + f\left(b_i + \sum_j W_{ij}x_j\right)\right]\,.\end{aligned}$$

Note that for simplicity we have assumed a symmetric connection, as otherwise the derivative of $\mathcal{L}$ leads to $x_j(W_{ij} + W_{ji})/2$.

With appropriately chosen G, we can show that $\mathcal{L}$ is always either decreasing or stationary. To achieve this goal, let us set

$$G'(x) \equiv f^{-1}(x)\,, \tag{4.27}$$

[1] J.J. Hopfiled, Proc. Nat. Acad. Sci. **81**, 3088 (1984).

where $f^{-1}(x)$ is the inverse function such that $f^{-1}[f(x)] = x$. This definition implies that

$$\frac{d\mathcal{L}}{dt} = \sum_i [\alpha_i - \beta_i] \cdot [-f(\alpha_i) + f(\beta_i)] \ , \tag{4.28}$$

where we have made the auxiliary definitions

$$\alpha_i \equiv G'(x_i) = f^{-1}(x_i) \, , \quad \text{and} \quad \beta_i \equiv b_i + \sum_j W_{ij} x_j \, . \tag{4.29}$$

Note that since $f(x)$ is monotonically increasing, the two factors in Eq. (4.28) always have opposite signs, unless they happen to be zero, and thus

$$\frac{d\mathcal{L}}{dt} \leq 0 \, . \tag{4.30}$$

The proof of Eq. (4.30) is similar in spirit to that for the Boltzmann H-theorem in Statistical Physics. A similar proof exists for the discrete (binary) version of the network.

The activities of neurons in the Hopfield network thus proceed to attractive fixed points which are solutions to $x_i^* = f(b_i + \sum_j W_{ij} x_j^*)$. The fixed points of the Hopfield model can be interpreted as associative, or content addressable memories. The idea is to first imprint a memory in the network by appropriate choice of the couplings W_{ij}. For a particular "memory" represented by $\{x_i^*\}$, the network is trained according to $\Delta W_{ij} = \eta x_i^* x_j^*$. The new network will be described by a Lyaponov function, $\mathcal{L} + \Delta\mathcal{L}$, with a deeper minimum at the encoded memory as

$$\Delta\mathcal{L}(\{x_i^*\}) = -\frac{1}{2} \sum_{i,j} \Delta W_{ij} x_i^* x_j^* = -\frac{\eta}{2} \sum_{i,j} (x_i^* x_j^*)^2 < 0 \, . \tag{4.31}$$

The imprinting procedure is a computational implementation of the so called *Hebbian rule* according to which "neurons that fire together wire together." If the thus trained network is presented with a partial or corrupted version of the stored memory, it is likely to be in the basin of attraction of a minimum of the Lyapunov function representing the original memory. In principle one can store many different memories in the network, each with its own separate basin of attraction. Of course at some point the memories interfere, and the network has a finite capacity dependent on the number of its nodes.

4.4.2 Stability, Bifurcation, and Cycles

Let us consider a bounded set of variables $\{x_i\}$ evolving in time as $\dot{x}_i = F_i(\{x_j\})$. Fixed points are possible solutions to $F_i(\{x_j^*\}) = 0$, but they will correspond to potential outcomes (attractors) of the dynamics, only if all eigenvalues of the matrix

$$M_{ij} = \left. \frac{\partial F_i}{\partial x_j} \right|^* \, , \tag{4.32}$$

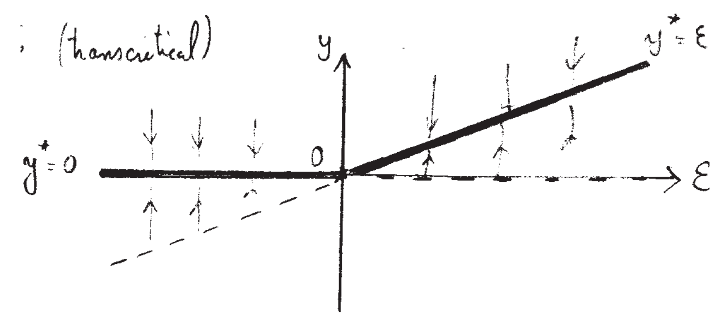
have negative real parts. (This is the condition for *linear stability*. For zero eigenvalues, stability is determined by examining higher derivatives.) We are interested in physical problems where the functions F_i, and hence all elements of the matrix M_{ij}, are real. The eigenvalues $\{\lambda_i\}$ of a real-valued matrix are either real, or come in complex conjugate pairs $u \pm iv$.

In the biological context, the functions F_i may determine the evolution of protein concentrations, and could then include parameters that depend on external stimuli. As such parameters are changed, a fixed point (protein concentrations) may become unstable, causing the system to switch to another state. The initial fixed point becomes unstable at the point where the real part of an eigenvalue changes sign from negative to positive. If this happens for a real eigenvalue, we can focus on the dynamics along the corresponding eigendirection– a one dimensional parametrization is then sufficient to capture the change in behavior near such an instability. If the real part of a complex eigenvalue pair changes sign, we need to analyze the behavior in the corresponding two dimensional surface spanned by the eigenvectors.

Let us first consider a single eigenvalue $\lambda(\epsilon)$ that changes sign as a control parameter ϵ goes through zero. Indicating deviations along the corresponding eigendirection by y, at linear level we have $\dot{y} = \epsilon y$. The fixed point at $y^* = 0$ is stable for $\epsilon < 0$, and unstable for $\epsilon > 0$. Higher order terms in the expansion in y are then necessary to determine the fate of the fixed point. The most generic stabilization is provided by addition of a quadratic term, leading to

$$\dot{y} = \epsilon y - y^2 \,. \tag{4.33}$$

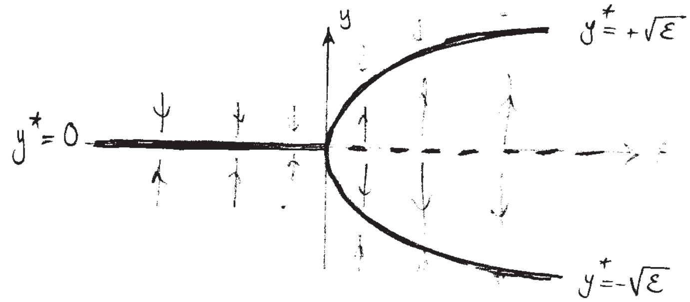
(The coefficient of the quadratic term can be set to 1 with proper scaling of y.) This model then admits a stable fixed point at $y^* = \epsilon$ for $\epsilon > 0$. In this (*transcritical*) scenario, a stable and an unstable fixed point collide and exchange stability.



The quadratic term in Eq. (4.35) is generically present, unless forbidden by a symmetry. In particular, the symmetry $y \to -y$ is consistent only with odd powers of y in the equation for $\dot{y}$, in which case Eq. (4.35) has to be replaced with

$$\dot{y} = \epsilon y - y^3 \,. \tag{4.34}$$

In such a *(supercritical) pitchfork bifurcation* a pair of stable fixed points appears at $\pm\sqrt{\epsilon}$ for $\epsilon > 0$, and the choice of one or the other is by *spontaneous symmetry breaking*.

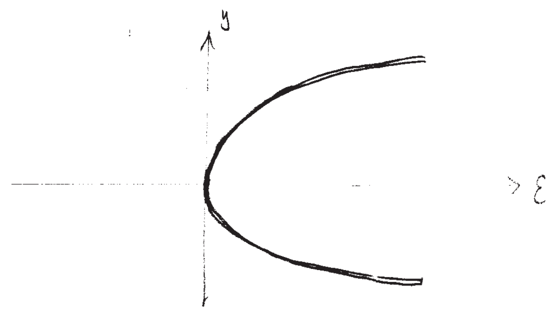


An inverted *(subrcritical) pitchfork bifurcation* occurs if the sign of the cubic term in Eq. (4.35) is changed to positive, i.e. $\dot{y} = \epsilon y + y^3$. The stable fixed point for $\epsilon < 0$ is now bounded by two unstable fixed points, which merge at $\epsilon = 0$, and the original (now lone) fixed point becomes unstable for $\epsilon > 0$.

The above examples indicate that change of stability occurs only when two or more fixed points collide or merge. This is required to ensure the continuity of flows in the phase space of parameters. Indeed, the same continuity requires the alternation of stable and unstable fixed points observed in the above examples. For the same reason a fixed point cannot appear or disappear in isolation, but must do so by merging with another fixed point. This is illustrated by the equation

$$\dot{y} = \epsilon - y^2 \,, \tag{4.35}$$

where a pair of fixed points (one stable and one unstable), absent for $\epsilon < 0$, is created (at $\pm\sqrt{\epsilon}$) for $\epsilon > 0$.

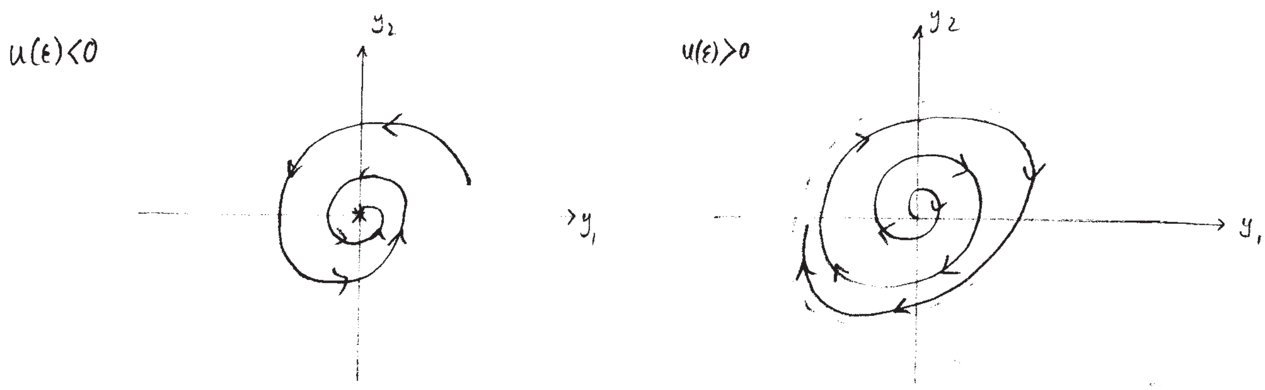


Conversely for

$$\dot{y} = \epsilon + y^2 - y^3 \,, \tag{4.36}$$

the pair of stable/unstable fixed points (with eigenvalues $\pm\sqrt{\epsilon}$) collide and disappear for $\epsilon > 0$ in a *fold bifurcation.* Note that to prevent divergence to infinity a stabilizing term $-y^3$ is added to the equation. For small ϵ, this leads to an additional stable fixed point at $y^* \approx 1$. Outcomes attracted to the stable fixed point at $-\sqrt{-\epsilon}$ for $\epsilon < 0$ now jumps discontinuously to $y^* \approx 1$ for $\epsilon > 0$.

Another route to instability is when the real part of a complex eigenvalue pair, $\lambda_\pm = u(\epsilon) \pm iv$, changes sign. In this case, we can focus on the two dimensional plane spanned by the corresponding two eigenvectors. The trajectories on this plane now transition from stable inward spirals (for $u < 0$) to unstable outward spirals (when $u > 0$).



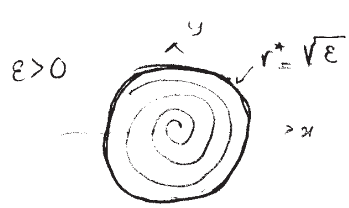
Of course bounded variables cannot spiral out forever, and the *Poincáre–Bendixon* theorem states that the bounded spiral must approach a closed curve around which it cycles. As an example, let us consider the pair of equations

$$\begin{aligned}\dot{x} &= \epsilon x - \omega y - (x^2 + y^2)x \\ \dot{y} &= \omega x + \epsilon y - (x^2 + y^2)y\,. \end{aligned} \tag{4.37}$$

The linear terms are chosen, such that the fixed point at the origin has complex eigenvalues $\lambda_\pm = \epsilon \pm i\omega$, turning unstable for $\epsilon > 0$. The nonlinear terms are added so that the flows at large x and y are always pointed towards the origin, preventing flows to infinity. In fact, the above equations were constructed to have a simple form in polar coordinates (r, θ) in terms of which $x = r\cos\theta$ and $y = r\sin\theta$. It is then easily verified that Eqs. (4.37) are equivalent to

$$\begin{aligned}\dot{\theta} &= \omega \\ \dot{r} &= \epsilon r - r^3\,. \end{aligned} \tag{4.38}$$

The trajectory thus rotates at a uniform angular velocity ω, converging to the center for $\epsilon \le 0$, and to a circle of radius $r^* = \sqrt{\epsilon}$ for $\epsilon > 0$.



Note that a symmetric matrix $M_{ij} = M_{ji}$ only has real eigenvalues. Complex eigenvalues, and hence periodic cycles can only occur for antisymmetric matrices. In the above example, the asymmetry is parametrized by ω which sets the angular velocity, but does not enter in the equation for r. It is easily verified that for a two by two matrix, complex eigenvalues are only obtained if the off-diagonal elements have opposite signs (as is the case in Eq. (4.37)). Indeed, in the biological context, a simple scheme for generating oscillations is to use an excitatory element (represented by positive interactions) in concert with an inhibitory component (corresponding to negative couplings). Other schemes, with three elements each inhibiting the next in a cycle, as in the reprisselator[2], also lead to oscillations by this mechanism.

A well known example of oscillations is provided by the **Lotka–Volterra** equations modeling predator–prey interactions. The populations x (prey) and y (predator) obey the differential equations

$$\begin{aligned} \dot{x} &= ax - bxy \\ \dot{y} &= dxy - cy\,. \end{aligned} \tag{4.39}$$

If by itself the prey population grows exponentially at rate a, but is culled by the predator y which needs the population of prey to grow, as it would otherwise decay. This system of equations has a fixed point $x^* = y^* = 0$, and anothe at $x^* = c/d$ and $y^* = a/b$. The first fixed point has one stable and one unstable direction (eigenvalues $-c$ and $+a$), corresponding to isolated decay of predator and growth of prey. For $y = 0$ (and in the absence of stabilizing terms), x grows to infinity, but any finite value of y moves trajectories away from this axis, moving them towards finite values of x and y. There is indeed an interesting fixed point at $x^* = c/d$ and $y^* = a/b$ with linear stability matrix

$$M = \begin{pmatrix} a - by^* & -bx^* \\ dy^* & dy^* - c \end{pmatrix} = \begin{pmatrix} 0 & -bc/d \\ ad/b & 0 \end{pmatrix}\,. \tag{4.40}$$

This matrix has a pair of complex eigenvalues $\lambda = \pm i\sqrt{ac}$, and resembles that of a harmonic oscillator. While the detailed description of resulting trajectories is complex. the model predicts oscillations in the populations.

[2]M. B. Elowitz and S. Leibler; Nature. **403**, 335 (2000).