1 Hopfield Networks (Contd.)

1.1 Recap

Last time, we started discussing *Hopfield networks*, where we consider n binary "neurons" $S_i \in \{-1, +1\}$ with dynamics for the system given by

$$S_i(t+1) \;=\; \mathrm{sgn}\Big(S_i \sum_j w_{ij}\, S_j(t)\Big),$$

with the [symmetric] weights are given by

$$w_{ij} \;=\; \sum_{\mu=1}^{p} V_i^{(\mu)}\, V_j^{(\mu)},$$

where each pattern $\mathbf{V}^{(\mu)} \in \{-1, +1\}^n$ is one desired attractor.

A useful construct in this context, often referred to as the system's *energy* is

$$E\,(\mathbf{S}) = -\sum_{i \neq j} w_{ij} S_i S_j = -\sum_i S_i \overbrace{\sum_{j \neq i} w_{ij} S_j}^{h_i}$$

Given the update rule, E is (non-strictly) decreasing with time, and so the dynamics converge to a local minimum of E (hopefully one of $\mathbf{V}^{(\mu)}$).

1.2 Stochastic Dynamics in the Hopfield Network

The description above considers *deterministic* dynamics. A useful extension, both for modeling purposes as well as practical design reasons, is to add noise, i.e. move to a stochastic dynamic system.

While there are many heuristic ways of doing this, a more structured approach is to treat the energy function as analogous to physical energy. If we assume/demand that the system converges to a unique stationary distribution, and that this stationary distribution is characterized by the fact that the [average] energy of the system reaches some typical value and stops changing

$$\langle E(t)\rangle = \langle E(\mathbf{S}(t))\rangle \xrightarrow[t\to\infty]{} C$$

Of all the distributions over system states with this property we want (drum roll...) the one with maximal entropy. A standard derivation (via Lagrange multipliers) will give us that the shape of the resulting steady state distribution must be of the following form

$$\pi(\mathbf{S}) \propto e^{-\beta E(\mathbf{S})}$$

known as a *Boltzmann distribution*.

So, given a desired stationary distribution, we need to construct a stochastic dynamical system which is guaranteed to converge to this distribution. We have already (in recitation 2) solved this

problem. We need to find transition probabilities between states which will obey detailed balance w.r.t. π.

There are many ways of constructing such a system, one which is very useful for systems such as ours, namely systems that naturally decompose into many interacting parts, is *Gibbs sampling*, where we sample at each time point one component (neuron, in our case) S_i uniformly and then sample its state at the next time according to

$$p(S_i) = \pi(S_i \mid S_{-i})$$

where S_{-i} denotes the $n-1$ components of $\mathbf{S}$ besides i. This means that our transition probabilities between states look like

$$p(\mathbf{S} \to \mathbf{S}') = \frac{1}{n} \pi(S_i' \mid S_{-i}) \text{ if } S_{-i} = S_{-i}' \text{ else } 0$$

Before showing that this gives us the desired result (converging to π), let's see why it is convenient in our setting. Given a state $\mathbf{S}$, fixing all neurons except i, we have

$$\pi\big(S_i \mid S_{-i}\big) = \frac{\pi\big(S_i, S_{-i}\big)}{\pi\big(S_{-i}\big)} \tag{1}$$

$$= \frac{1}{Z} \frac{e^{-\beta E\big(S_i, S_{-i}\big)}}{\pi\big(S_{-i}\big)} \tag{2}$$

$$= \frac{1}{Z} \frac{e^{-\beta \sum_{j \neq i} S_j h_j}}{\pi\big(S_{-i}\big)} e^{-\beta S_i h_i}. \tag{3}$$

and note that all but the final factor are the same between the different options for S_i, i.e. we have

$$\pi(S_i \mid S_{-i}) \propto e^{-\beta S_i h(S_i)}$$

so computing the probabilities for the different options for S_i require estimating only n interactions instead of the full n^2

To show detailed balance, and consequently that Gibbs sampling leads us to the desired stationary distribution, note that for all states $\mathbf{S}$ and $\mathbf{S}'$ which differ at only a single neuron i we have

$$\frac{p(\vec{S} \to \vec{S}')}{p(\vec{S}' \to \vec{S})} = \frac{\pi(S_i' \mid S_{-i})}{\pi(S_i \mid S_{-i}')} = \frac{\pi(S_i' \mid S_{-i})}{\pi(S_i \mid S_{-i})} = \frac{\pi(S')}{\pi(S)}$$

2 Evolution

2.1 Survival of The Fittest

> *Nothing in Biology Makes Sense Except in the Light of Evolution*
> –Theodosius Dobzhansky

Consider a replicator.

Specifically, let's say we start with an entity X which, given sufficient resources (which for now we'll say are present in infinite quantities), can create a perfect copy of itself in some typical time τ. Denoting by $N(t)$ the number of copies of our entity at time t. We can write

$$\dot{N} = \mu N$$

where $\mu = \frac{1}{\tau}$ is the growth rate, with the solution

$$N(t) = e^{\mu t}$$

We can also consider death. That is, assuming a constant probability $\delta \Delta t$ for death in an interval Δt, we can write

$$\dot{N} = \mu N - \delta N$$

and as long as $\mu > \delta$, this will still lead to exponential growth at rate $f = \mu - \delta$, which we will call Xs *fitness*.

Now assume that there are actually M different *types* of replicators, $\{X_i\}_{i=1}^M$, each with its own fitness f_i. The quantity which will interest us is not the absolute number of each replicator type, or species, but rather their relative abundance $x_i = \frac{N_i}{\sum N_j}$, we can write

$$\dot{x}_i = x_i \left(f_i - \phi \right)$$

where $\phi = \sum x_i f_i$ is there to ensure the x_i sum to unity. We thus see that the frequency of x_i will increase iff it is larger than the current average population fitness.

This defines a dynamical system over the simplex S_M, where each point represents a specific population structure, and will asymptotically converge to to one of its corners, representing the survival of a single species (the one with the maximal fitness) and the exclusion of all others.

> **Exercise**
>
> Prove this. Namely, if forall i, j we have $f_i \neq f_j$, then regardless of the initial population composition, it will converge to have all of the population in the fittest type.

2.2 An example - Selection of Regulatory Mechanisms

Consider an organism in an environment which shifts between two states, E_1 and E_2 whose long term occurrence frequencies are p and $1 - p$ respectively. The organism can produce some resource Z which is beneficial in E_1 with benefit b, but useless in E_2. Further assume that the resource has some cost associated with its production which we'll call c (and of course $b > c$). Now, it would seem that the best strategy would be for the organism to only generate Z when in E_1, thus maximizing fitness. However, such regulation does not come free, as the machinery required to sense the environment and process the information has a cost associated with it, call it r.

The organism is now faced with three strategies, it can either always produce Z (call this strategy X_{on}), not bother and never produce Z (X_{off}) or invest in regulation and only produce Z when it is required (X_{reg}).

The corresponding fitness values are

$$f_{\text{on}} = pb - c$$

$$f_{\text{reg}} = pb - pc - r$$

and finally

$$f_{\text{off}} = 0$$

> **Exercise**
>
> What are the units of b and c? Can you formulate this scenario in terms of the formalism from the first section?
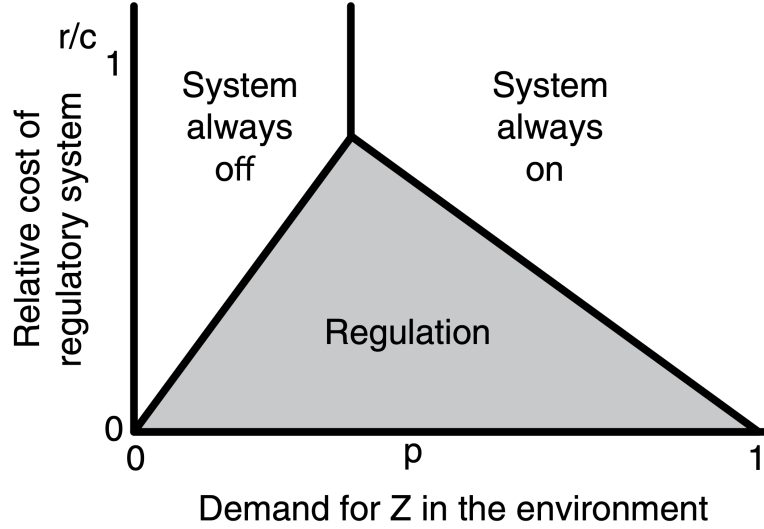
Regulation (X_{reg}) will be selected when

$$f_{\text{reg}} = \max \{ f_{\text{on}}, f_{\text{reg}}, f_{\text{off}} \}$$

which happens when

$$\left(p < 1 - \frac{r}{c} \right) \wedge \left(p > \frac{r}{b - c} \right)$$

A similar calculation leads to the conclusion that X_{on} will be selected over X_{off} when

$$p > \frac{c}{b}$$

Relative cost of regulatory system — r/c

Demand for Z in the environment

2.3 Mutations

The model we have described for evolution is arguably the simplest description of the concept of "Survival of the fittest". Namely, in any model where we have replicators with variability in their propensity to reproduce, and where at least to some degree this propensity is heritable, we will observe evolution of the population towards over representation of the fitter variants and increased overall fitness. However, as we've just seen, this simple model permits evolution up to a point (takeover of the fittest variant), and no more. The next ingredient we need is a constant new supply of variation.

To that end, let us now consider the possibility of *mutation*. That is, replication of an X_i can result in an additional copy of X_j instead of X_i and this happens with probability $q_{i,j}$.

We therefore write

$$\dot{x}_i = \sum_j x_j f_j q_{j,i} - \phi x_i$$

This is known as the *quasi-species equation*, one of the most fundamental equations in population genetics. Note that the probability of mutating from X_i to X_j, $q_{i,j}$ is independent of f_i and f_j. That is, in this model (and in most of modern biological thinking) mutation is random with respect to fitness.