Part II

Combinatorial Models

5 A Sketch of Basic Statistical Physics

$$\text{Statistical physics} = \text{Thermodynamics (macroscopic)}$$
$$+ \text{Statistical mechanics (microscopic)}$$

5.1 Thermodynamics

A *thermodynamic system* is characterised by (macroscopic, observable) variables T ("temperature") and $X_1, \ldots, X_n$. These variables determine "all interesting" properties of the system.

E.g. in the classical ideal gas model a sufficient set of variables is T, p, V and N. ($N \sim$ the number of molecules is here for simplicity thought of as a continuous quantity. This might be easier if N was replaced by $n = N/N_0$, the amount in moles of gas, where $N_0 = 6.02 \cdot 10^{23}$ is Avogadro's number.)

The system is in (*thermal*) *equilibrium* if it satisfies a characteristic *state equation*

$$g(T, X_1, \ldots, X_n) = 0$$

E.g. ideal gas: $pV - NkT = 0$, where $k = 1.38 \cdot 10^{-23} J/K$ is *Boltzmann's constant*, or $pV - nRT = 0$, where $R = 8.32 J/K$ is the *gas constant*.

A *potential* or *energy function* for the system is some sufficiently smooth function

$$F = F(T, X_1, \ldots, X_n).$$

In classical thermodynamics, a key role is given to the *total energy* function determined by the *First Law of Thermodynamics*:

$$dU = dQ + dW, \tag{1}$$

where dQ is the amount of "heat" added to a system and dW is the amount of "work" performed on it.

Integrating the potential given e.g. the state equation of the ideal gas yields

$$U(T,p,N) = U_0 + \left(\frac{1}{2}fN + N - S_0\right)(T - T_0) - NT\ln\left(\left(\frac{T}{T_0}\right)^{1+f/2}\frac{p_0}{p}\right),$$

where U_0, S_0, T_0 and p_0 are reference values and $f/2$ a constant ("specific heat").[1]

In classical thermodynamics, the system variables are divided into *extensive* and *intensive*, depending on whether their values depend on the "size" of the system or not. E.g. T and p are intensive, V and N extensive.

Two systems at the same temperature may be "combined", and if F is otherwise a function of extensive variables only, then it is linear, i.e.

$$F(T, X_1 + X_1', \ldots, X_n + X_n') = F(T, X_1, \ldots, X_n) + F(T, X_1', \ldots, X_n').$$

By the total derivative formula:

$$dF = \left(\frac{\partial F}{\partial T}\right)dT + \sum_{i=1}^{n}\left(\frac{\partial F}{\partial X_i}\right)dX_i. \tag{2}$$

State variables are *conjugate* (with respect to F), if

$$X = \frac{\partial F}{\partial Y} \qquad \text{or} \qquad Y = \frac{\partial F}{\partial X}.$$

In classical thermodynamics conjugates of extensive variables are intensive, and vice versa. The conjugate of T w.r.t. U,

$$S = \frac{\partial U}{\partial T}$$

is called the *entropy* of the system.

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[1]To be precise, since T and p are not "natural" variables of the energy function U arising from its differential definition (1), this equation refers to a variant of U expressed in terms of T, p and N, so called "Gibbs free energy".

Conjugate variables may be interchanged via the *Legendre transform*, yielding new forms of a given potential function. E.g. in the case of the ideal gas with fixed N, $U = U(S, V)$ and

$$dU = dQ + dW = T dS - p dV.$$

Here we may interchange S for T by considering instead of U the *Helmholz free energy* $F = U - ST$. This satisfies:[2]

$$dF = dU - S dT - T dS = T dS - p dV - S dT - T dS = -S dT - p dV.$$

In the classical setting, it is a law of nature (the *Second Law of Thermodynamics*) that in equilibrium processes (evolutions) entropy never decreases:

$$dS \geq 0.$$

Processes for which entropy stays constant ($dS = 0$) are called *adiabatic*.

5.2   Statistical Mechanics

Let us consider a thermodynamic energy function framed in terms of extensive variables:

$$U = U(S, X_1, \dots, X_n),$$

and assume that the value of U expresses in fact only the *average* of a large number of microscopic potentials:

$$U = \langle H \rangle = \sum_\omega p_\omega H(\omega).$$

The micropotential function $H(\omega)$ is also called the *Hamiltonian* of the system. We shall furthermore assume, motivated by the additivity of U, that the Hamiltonian of a system consisting of two independent subsystems at thermal equilibrium can be decomposed as:

$$H(\langle \omega_1, \omega_2 \rangle) = H(\omega_1) + H(\omega_2).$$

What is now the distribution of the microstates p_ω, given the constraint that $\langle H \rangle = U$? We assume that all microstates with the same value of the Hamiltonian are equally probable, so that p_ω has the form $p_\omega = g(H(\omega))$.

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[2]There is an unfortunate sign difference here as compared to formula (2). We could have fixed this by defining $F = ST - U$, but this would have been against convention.
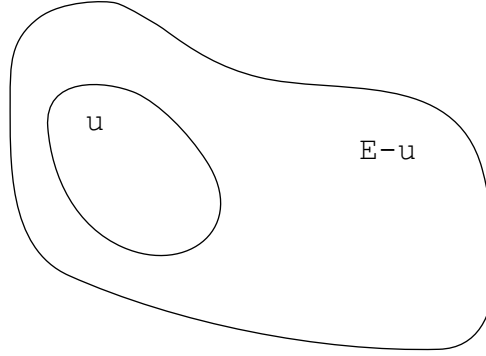
Figure 1: A heat bath.

To further specify the functional form of the distribution, think of our system $\mathcal{S}$ as being in thermal equilibrium with, but otherwise independent of, a much larger system or "reservoir" $\mathcal{R}$. Denote the total system consisting of $\mathcal{S}$ and $\mathcal{R}$ by $\mathcal{T}$ (This is called a "heat bath" arrangement; cf. Figure 1.)

For any given system, denote by $\Omega(u) = |H^{-1}(u)|$ the number of its microstates at potential u. (Whether we are referring to $\mathcal{S}$, $\mathcal{R}$ or $\mathcal{T}$ should always be clear from the context.) Fix some reference potential level $E \gg U$ for the total system $\mathcal{T}$, and observe that by our assumption, all microstates of $\mathcal{T}$ with potential E have the same probability.

Now for every microstate ω of $\mathcal{S}$, there are exactly $\Omega(E - H(\omega))$ microstates ω^r of $\mathcal{R}$ such that the combined state $\langle \omega, \omega^r \rangle$ of $\mathcal{T}$ has potential E. Since all of these are equally probable, it follows that $p_\omega \propto \Omega(E - H(\omega))$. Taking logarithms and applying Taylor's formula yields:

$$\begin{aligned} \ln p_\omega &= \ln \Omega\left(E - H(\omega)\right) + \text{const.} \\ &= \ln \Omega(E) - \left(\frac{\partial \ln \Omega(E')}{\partial E'}\right)_{E'=E} H(\omega) + \cdots \\ &= \ln \Omega(E) - \beta H(\omega) + \cdots, \end{aligned}$$

where $\beta = \partial \ln \Omega / \partial E$ is a parameter whose value is to be determined later.

Taking exponentials again, we obtain the so called *Gibbs* (or *Boltzmann*) *distribution*

$$p_\omega \propto e^{-\beta H(\omega)} \tag{3}$$

with normalisation constant (actually, function)

$$Z = Z_\beta = \sum_\omega e^{-\beta H(\omega)}, \tag{4}$$

known as the *partition function*. (In fact, $Z = Z(\beta, X_1, \ldots, X_n)$.) Now the value of β is in principle determined implicitly by the condition

$$\langle H \rangle = \frac{1}{Z} \sum_\omega e^{-\beta H(\omega)} H(\omega) = U,$$

but we shall obtain a more transparent representation for it below.

The (logarithm of the) partition function (4) can be used to compute several macroscopic quantities:

First:

$$\begin{aligned}
\frac{\partial \ln Z}{\partial \beta} &= \frac{1}{Z} \frac{\partial Z}{\partial \beta} \\
&= \frac{1}{Z} \frac{\partial}{\partial \beta} \sum_\omega e^{-\beta H(\omega)} \\
&= \frac{1}{Z} \sum_\omega e^{-\beta H(\omega)} (-H(\omega)) \\
&= -\sum_\omega p_\omega H(\omega) \\
&= -U.
\end{aligned}$$

Second: Consider an extensive variable X_i and its conjugate $\mu_i = \partial U / \partial X_i$.

$$\begin{aligned}
\frac{\partial \ln Z}{\partial X_i} &= \frac{1}{Z} \sum_\omega \frac{\partial}{\partial X_i} e^{-\beta H(\omega; X_i)} \\
&= \frac{1}{Z} \sum_\omega e^{-\beta H(\omega; X_i)} \left(-\beta \frac{\partial H(\omega; X_i)}{\partial X_i} \right) \\
&= -\beta \sum_\omega p_\omega \frac{\partial H(\omega; X_i)}{\partial X_i} \\
&= -\beta \left\langle \frac{\partial H(\omega; X_i)}{\partial X_i} \right\rangle \\
&= -\beta \mu_i.
\end{aligned}$$

Third:

$$d \ln Z = \frac{\partial \ln Z}{\partial \beta} d\beta + \sum_{i=1}^{n} \frac{\partial \ln Z}{\partial X_i} dX_i$$

$$= -U d\beta - \beta \sum_{i=1}^{n} \mu_i dX_i$$

$$= -d(\beta U) + \underbrace{\beta dU - \beta \sum_{i=1}^{n} \mu_i dX_i}_{\beta T dS}.$$

$$\therefore T dS = \frac{1}{\beta} d\left(\ln Z + \beta U\right)$$

$$\therefore \frac{1}{\beta} = kT, \quad dS = kd\left(\ln Z + \beta U\right), \quad k = \frac{1}{\beta T} \text{ constant}$$

$$\therefore \frac{1}{\beta} = kT, \quad S = k \ln Z + \frac{U}{T} + \text{const.}$$

$$\therefore \beta = \frac{1}{kT}, \quad -kT \ln Z = U - TS = F \quad \text{(Helmholz free energy)}$$

Conversely, let us expand the entropy variable as a microscopic average:

$$S = k \ln Z + k\beta U$$
$$= k \ln Z + \sum_{\omega} p_\omega \beta H(\omega) \qquad \left| \begin{array}{l} p_\omega = \frac{1}{Z} e^{-\beta H(\omega)} \\ \Rightarrow \beta H(\omega) = -\ln(Z p_\omega) \end{array} \right.$$
$$= k\left(\ln Z - \sum_{\omega} p_\omega (\ln Z + \ln p_\omega)\right)$$
$$= -k \sum_{\omega} p_\omega \ln p_\omega. \qquad \left| \sum_{\omega} p_\omega = 1 \right.$$

One more, simplified expression for entropy: partition the range of possible potential values into narrow bands (of width ΔU, say), and denote the number of microstates falling in band r as

$$\Omega(U_r) = \left| \{\omega : U_r \leq H(\omega) < U_r + \Delta U\} \right|$$

Then the partition function is approximately

$$Z \approx \sum_{r} \Omega(U_r) e^{-\beta U_r}$$

In fact, since the number of microstates in a typical system is huge, the microstate potentials are highly concentrated around the average $U = \langle H \rangle$, and so in fact

$$Z \approx \Omega(U)e^{-\beta U},$$

whence

$$S = \frac{1}{T}(-F + U) = k \ln Z + \frac{U}{T} \approx k \ln U \underbrace{-\beta k U + \frac{U}{T}}_{=0} \approx k \ln \Omega(U).$$

6 The Ising Model, Spin Glasses and Neural Networks

6.1 The Ising Model

The following model was introduced by Ernst Ising in 1925 to explain magnetism in materials.

At a microscopic level, Ising's model system consists of N *sites* arranged in a lattice, either 1-D, 2-D ($N = L^2$), or maybe even 3-D. At each site $i = 1,\dots,N$ is located a magnetic ion or *spin* pointing either *up* or *down* ($S_i = \pm 1$). Neighbouring sites $\langle ij \rangle$ are related by an *interaction coefficient* J_{ij}, which in Ising's model is uniformly either a positive $J > 0$ ("ferromagnetic case") or a nonpositive $J \le 0$ ("antiferromagnetic case"). A system whose internal interactions are all weak ($J_{ij} \approx 0$) is "paramagnetic". In addition, there may be an *external field h* influencing the orientation of each of the spins. (More generally, one could have separate fields h_i for each spin S_i.)

The Hamiltonian of spin state $\sigma = \langle S_1, \dots, S_N \rangle$ is

$$H(\sigma) = -J \sum_{\langle ij \rangle} S_i S_j - h \sum S_i,$$

where the sum is taken over *nearest neighbour pairs* $\langle ij \rangle$ and periodic boundary conditions are assumed for simplicity.

States σ yielding the global minimum value of $H(\sigma)$ are called *ground states* of the system. For a ferromagnetic system, the ground state has either all $S_i = +1$ if $h > 0$, or all $S_i = -1$ if $h < 0$. If $h = 0$, these two states are both equally good.

As a very simple example, let us compute the partition function for a trivial Ising paramagnet with N spins and $J = 0$. Denote $\Omega = \{+1, -1\}^N$. Then:

$$
\begin{aligned}
Z_\beta &= \sum_{\sigma \in \Omega} e^{-\beta H(\sigma)} \\
&= \sum_{\sigma \in \Omega} \exp(\beta h \sum_i S_i) \\
&= \sum_{S_1 = \pm 1} \sum_{S_2 = \pm 1} \cdots \sum_{S_N = \pm 1} e^{\beta h S_1} e^{\beta h S_2} \cdots e^{\beta h S_N} \\
&= \left(\sum_{S_1 = \pm 1} e^{\beta h S} \right)^N \\
&= \left(2\cosh(\beta h) \right)^N
\end{aligned}
\qquad\qquad \cosh x = \frac{e^x + e^{-x}}{2}
$$

Define the *(total) magnetisation* of state σ as

$$
M(\sigma) = \sum_{i=1}^{N} S_i.
$$

The corresponding thermodynamic average at given β is

$$
\begin{aligned}
\langle M \rangle &= \frac{1}{Z} \sum_{\sigma \in \Omega} M(\sigma) \exp(-\beta H(\sigma)) \\
&= \frac{1}{Z} \underbrace{\sum_{\sigma \in \Omega} \left(\sum_i S_i \right) \exp(-\beta H(\sigma))}_{(\star)}.
\end{aligned}
$$

However now in fact $(\star) = \frac{\partial Z}{\partial(\beta h)}$, so fortuitously:

$$
\begin{aligned}
\langle M \rangle &= \frac{1}{Z} \frac{\partial Z}{\partial(\beta h)} = \frac{\partial \ln Z}{\partial(\beta h)} \\
&= N \frac{\partial \ln(2\cosh(\beta h))}{\partial(\beta h)} \\
&= N \frac{2(\partial \cosh(\beta h)/\partial(\beta h))}{2\cosh(\beta h)} \\
&= N \frac{2\sinh(\beta h)}{2\cosh(\beta h)} \\
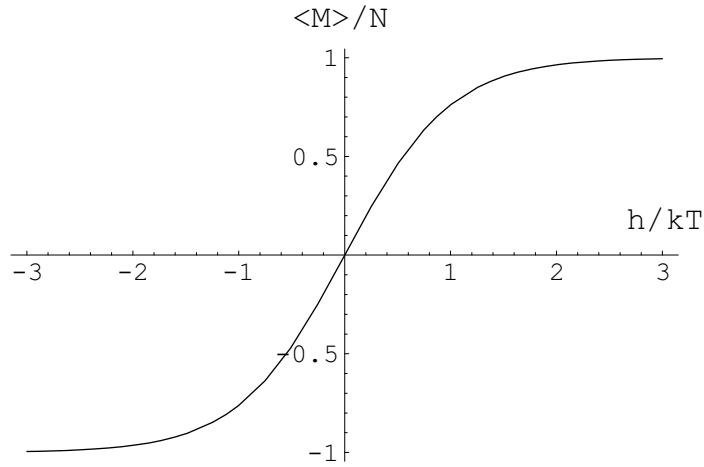&= N \tanh(\beta h).
\end{aligned}
$$

Figure 2: Magnetisation of an Ising paramagnet.

Thus the average magnetisation per site or "magnetisation density" of a totally decoupled Ising paramagnet at external field h and temperature $T = 1/k\beta$ equals

$$\langle M \rangle = \tanh\left(\frac{h}{kT}\right).$$

A plot of this function is presented in Figure 2.

The ferromagnetic 1-D Ising model is also explicitly solvable with somewhat more work. The 2-D ferromagnetic case with $h = 0$ was solved by L. Onsager in 1944, and in a simpler way by Kasteleyn & Fisher in 1961. The 2-D case with $h \neq 0$ and higher dimensions are still open.

6.2   Spin Glasses

Spin glasses generalise the Ising model with more general interactions. Also the spins may be nonbinary, in which case such models are called *Potts glasses*.

The general form of the (binary-state) spin glass Hamiltonian is

$$H(\sigma) = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - \sum_i h_i S_i,$$

where $J_{ij}, h_i \in \mathbb{R}$. Also the neighbourhood relation may correspond to an arbitrary *graph*, not necessary a lattice.

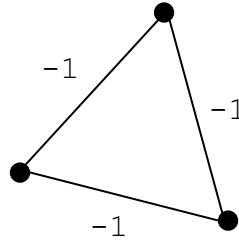Several varieties of spin glass models have been introduced, e.g.:

Figure 3: Frustrated spin glass configuration.

- The Sherrington-Kirkpatrick model: Hamiltonian as above, complete interconnection graph, coefficients J_{ij} according to a specific probability distribution.

- The Edwards-Anderson model: Hamiltonian

$$H(\sigma) = -\sum_{\langle ij \rangle} J_{ij} S_i S_j,$$

regular lattice topology (e.g. cubic), J_{ij} independent Gaussian variables.

A phenomenon that makes spin glass models even less tractable than the Ising model is *frustration*. E.g. in the spin glass neighbourhood in Figure 3 there is no completely "consistent" choice of spin values.

Frustration means that the "landscape" determined by the Hamiltonian can have a very complicated structure, with large numbers of local minima, and no obvious location for the globally minimal ground state.

In fact, the problem of determining the ground state of a given SK-spin glass instance $\langle \bar{J}, \bar{h} \rangle$ is *NP-complete*, even with $\bar{h} = 0$.

This can be seen by reduction from the well-known NP-complete MAX CUT problem: Given a graph $G = (V, E)$, determine the partition $V = V_1 \cup V_2$ that maximizes $w(V_1, V_2) = \left| \{(i, j) \in E : i \in V_1 \wedge j \in V_2 \} \right|$.

The reduction is as follows:

Given a graph $G = (V, E)$, let $\bar{J}$ be an SK system with sites corresponding to V, and J_{ij} determined by

$$J_{ij} = \begin{cases} -1, & \text{if } \langle i, j \rangle \in E, \\ 0, & \text{otherwise.} \end{cases}$$

Let then $C = (V_1, V_2)$ be a cut in G, and divide the edges in G corresponding as

$$
\begin{aligned}
E_1 &= \{\langle i,j \rangle \in E : i,j \in V_1\}, \\
E_2 &= \{\langle i,j \rangle \in E : i,j \in V_2\}, \\
E_C &= \{\langle i,j \rangle \in E : i \in V_1 \wedge j \in V_2\}.
\end{aligned}
$$

Consider the spin glass state σ determined as

$$
S_i = \begin{cases} +1, & \text{if } i \in V_1, \\ -1, & \text{if } i \in V_2. \end{cases}
$$

For this,

$$
\begin{aligned}
H(\sigma) &= -\sum_{\langle ij \rangle} J_{ij} S_i S_j = \sum_{\langle ij \rangle \in E} S_i S_j \\
&= \sum_{\langle ij \rangle \in E_1} S_i S_j + \sum_{\langle ij \rangle \in E_2} S_i S_j + \sum_{\langle ij \rangle \in E_C} S_i S_j \\
&= |E_1| + |E_2| - |E_C| \\
&= |E| - 2|E_C| \\
&= |E| - 2w(C).
\end{aligned}
$$

Conversely, given any spin glass state σ, one obtains a cut C satisfying $w(C) = \frac{1}{2}|E| - \frac{1}{2}H(\sigma)$.

Thus, graph cuts and spin glass states correspond one-to-one, with $w(C) \propto -H(\sigma)$, and minimizing one is equivalent to maximising the other.

The result means that the SK spin glass ground state problem is in a sense "universal" difficult problem, i.e. it contains as special cases all the $\sim$2000 other known NP-complete problems.

For $J_{ij} > 0$ and arbitrary $\bar{h}$ the problem reduces to network flow, and can be solved in polynomial time. For planar G and $\bar{h} = 0$ the problem also has a polynomial time algorithm (Fisher 1966 (2-D lattices), Barahona 1982). However, for planar G with $\bar{h} \neq 0$, and for 3-D lattices the problem is NP-complete (Barahona 1982). It is also NP-complete for every other nonplanar crystal lattice graph (Istrail 2000). Thus, the dimensionality of the system is not crucial to the complexity of the ground state problem; the key is rather the planarity of the interconnection graph.

6.3 Neural Networks

John Hopfield proposed, in an influential paper in 1982, to use the SK model as a basis for "neural associative memories". The idea is to create an N-site SK

system whose local potential minima correspond to a set of N-bit vectors to be stored. These local minima are also stable states of the system's deterministic (0-temperature) "Glauber dynamics". When such a system is initialised at a state which is "close" to one of the stored stable states, the dynamics (presumably) tends to return it to the nearby local minimum. Thus small perturbations in the stable states tend to get corrected, and the system has "error-correcting" or "associative" capabilities.

More precisely, the deterministic dynamics of such a system is as follows: at a given discrete time instant, a randomly (or in a round-robin manner) chosen site k is updated according to the local rule:

$$S'_k = \text{sgn}\underbrace{\left(\sum_{\langle kj \rangle} J_{kj}S_j + h_k\right)}_{(\bigstar)}$$

$$= \begin{cases} +1, & \text{if } (\bigstar) > 0, \\ -1, & \text{if } (\bigstar) < 0, \\ S_k, & \text{if } (\bigstar) = 0, \end{cases}$$

It can be seen that each time a site changes state, the value of $H(\sigma)$ decreases: Assume $S'_k \neq S_k$. Consider

$$\begin{aligned} H(\sigma') - H(\sigma) &= -\sum_{\langle ij \rangle} J_{ij}S'_iS'_j - \sum_i h_iS'_i \\ &\quad + \sum_{\langle ij \rangle} J_{ij}S_iS_j + \sum_i h_iS_i \\ &= -\sum_{\langle kj \rangle} J_{kj}S'_kS_j + \sum_{\langle kj \rangle} J_{kj}S_kS_j - h_k(S'_k - S_k) \\ &= -\underbrace{(S'_k - S_k)}_{\blacktriangle}\underbrace{\left(\sum_{\langle kj \rangle} J_{kj}S_j + h_k\right)}_{\blacktriangledown} \\ &< 0, \end{aligned}$$

where $\blacktriangledown$ and $\blacktriangle$ have the same sign.

Thus, since the value of $H(\sigma)$ is lower bounded by

$$H(\sigma) \geq -\sum_{\langle ij \rangle} |J_{ij}| - \sum_i |h_i|,$$

the system converges eventually to a local minimum of its Hamiltonian.

How should one then craft the interaction coefficients so that a given set of patterns become stable states of the system's dynamics? This can in principle be done in various ways, of which Hopfield proposed the following adaptation of "Hebb's rule":[3]

Consider first a single pattern $\sigma = (S_1, \ldots, S_N) \in \{+1, -1\}^N$ and choose $J = \sigma\sigma^T - I = [S_i S_j]_{ij} - I, h = 0$. Then the dynamics operates as follows:

$$\text{sgn}(J\sigma) = \text{sgn}\left((\sigma\sigma^T - I)\sigma\right) = \text{sgn}\left((||\sigma^2|| - 1)\sigma\right) = \sigma,$$

i.e. σ is a stable state of the dynamics.

Given then a (smallish) set of patterns $\sigma_1, \ldots, \sigma_m$, choose

$$J = \sum_{p=1}^{m} \sigma_p \sigma_p^T - mI \qquad \left(\text{or normalised } J = \frac{1}{m}\sum_p \sigma_p \sigma_p^T - I\right).$$

If the patterns are random, independent identically distributed bit vectors, and there are only $m \ll N$ of them, they are "almost orthogonal", and we may approximate:

$$\text{sgn}(J\sigma_k) = \text{sgn}\left(\left(\sum_{p=1}^{m} \sigma_p \sigma_p^T - mI\right)\sigma_k\right)$$

$$= \text{sgn}\left(\underbrace{(||\sigma_k||^2 - m)\sigma_k}_{\text{'signal'}} + \underbrace{\sum_{p \neq k} \overbrace{\left(\sigma_p^T \sigma_k\right)}^{\approx 0} \sigma_p}_{\text{'noise'}}\right)$$

$$= \sigma_k,$$

"with high probability".

This analysis has been performed rigorously many times under different assumptions, and the number of patterns m that can be reliably stored has been estimated under different criteria. Typically, the "reliable" storage capacity comes out as $m \approx 0.14N \ldots 0.18N$.

The deterministic Glauber dynamics of SK spin glasses has also other computationally interesting features. One can e.g. show that convergence to a stable state

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[3]In a 1949 book, D. O. Hebb suggested as a basic mechanism of neuronal memory that simultaneous activity reinforces the interconnections between neurons. Physiologically this suggestion is still controversial, but mathematically the idea has been used as a basis of several learning mechanisms in artifi cial neural networks.

can require a number of spin flips that is exponential in N (A. Haken et al. ca. 1989), and that one can in fact embed arbitrary computations in the dynamics (Orponen 1995). (More precisely, determining whether a given "output spin" is $+1$ or -1 in the local minimum reached from a given initial state is a "PSPACE-complete" problem.)

6.4   The NK Model

Introduced by Stuart Kauffman (ca. 1986) as a "tunable family of fitness landscapes".

A *fitness landscape* is a triple $\langle X, R, f \rangle$, where X is the *configuration* (or *state*) *space*, $R \subseteq X \times X$ is a *neighbourhood relation* on X, and $f : X \to \mathbb{R}$ is a *fitness* (or *objective*) *function*.

A point $x \in X$ is a *local optimum* (of f on X) if

$$f(y) \le f(x) \quad \forall \, yRx$$

and a *global optimum* (*maximum*) if

$$f(y) \le f(x) \quad \forall \, y \in X$$

Questions of the "ruggedness" of landscapes (correlation structure), number and height of local optima, sizes of "attraction basins" of local optima with respect to "hill-climbing" algorithms etc. are of great interest for natural landscapes.

In Kauffman's NK models, $X = A^N$ (usually just $X = \{0,1\}^N$) and K is a tunable neighbourhood size parameter that influences the landscape characteristics, especially its ruggedness (cf. Figure 4).

The model can be seen as a toy model of "epigenetic interactions in chromosomes" — or also a generalisation of the spin glass model.

In Kauffman's model, a *chromosome* is a N-vector of *loci* (*genes*, "positions"), each of which has a value from a set of *allelles* A (usually just $A = \{0,1\}$). A "filled-in" chromosome $\alpha \in A^N$ is called a *genotype*.

The fitness of each gene $i \in \{1, \dots, N\}$ in a genotype $\alpha = (a_1, \dots, a_N) \in A^N$ depends on the allele a_i and K other alleles $a_1^i, \dots, a_K^i$ via some local fitness function $f^i(\alpha) = f^i(a_i; a_1^i, \dots, a_K^i)$, usually normalised so that $f^i(\alpha) \in [0,1]$. The total fitness of a genotype $\alpha \in A^N$ is the normalised sum of its genes' local fitnesses:

$$f(\alpha) = \frac{1}{N} \sum_{i=1}^{N} f^i(a_i; a_1^i, \dots, a_k^i) \quad \in [0,1].$$