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Invariant recognition in Potts glass neural networks

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Abstract. We show that a Potts glass neural network can be used for invariant recognition. Each neuron is modelled as a q state Potts variable and p Potts configurations are stored in the network. The learning rule is a generalized Hebb rule, so that all pq! permutations of the patterns are stabilized simultaneously. We analyse the model for an extensive number of patterns and present results of numerical simulations to confirm the analytical results and to illustrate the relaxation to equilibrium. The model is applied to the recognition of isomorphic graphs. Finally we show how to generalize the model, such that its stable states are patterns, where the permutational symmetry is broken in a hierarchical manner.

1. Introduction

Invariant pattern recognition has long been recognized as one of the most impressive computational abilities of biological neural networks. Various symmetries are important in many different contexts: for example, rotational, translational and scaling invariance in visual processing, time warping in speech recognition, topological invariance, if *relations* between features or objects are of interest—to quote just a few.

Two basic approaches have been followed in most attempts to achieve invariant recognition in artificial neural networks:

(i) The object to be recognized is coded in invariant form. For example, translational invariance can be achieved by coding Fourier transform magnitudes [1-3].

(ii) A preprocessing unit—in some cases another neural network—is used to transform the input, until the identification with the prototype is achieved [4-6].

In this paper we shall focus on topological invariance and discuss a neural network of type (i), which can store and retrieve relations between objects, for example nodes of a graph. The network consists of N neurons s_i , i = 1, ..., N, and each neuron is modelled by a q state Potts variable, $s_i \in \{e_i\}$, l = 1, ..., q. The vectors e_i point to the corners of a simplex in q-1 dimensions. Prescribed configurations $\{\xi_i^\nu\}$, $\nu = 1, ..., p$, of the network are stored in the synaptic matrix according to a generalized Hebb rule

$$J_{ij} = \frac{1}{N} \sum_{\nu=1}^{P} \boldsymbol{\xi}_{i}^{\nu} \cdot \boldsymbol{\xi}_{j}^{\nu}.$$
 (1)

Hence we suggest storing a *relation* between the state at site *i* and the state at site *j*, namely the angle between the two vectors ξ_i and ξ_j . For Potts vectors this angle takes only two values, depending on whether $\xi_i = \xi_j$ or $\xi_i \neq \xi_j$. Hence the synaptic matrix contains the information, whether or not any two sites are in the same state.

As shown below, the spin configuration $s_i = \xi_i^{\nu}$ is a global minimum of the network, as well as all spin configurations which are generated from one of the ξ_i^{ν} by a global permutation of the Potts states. This implies that if the network has learnt one pattern according to equation (1), it has simultaneously learnt q! patterns, corresponding to q! permutations of the Potts states. In general these degenerate minima of the energy are separated by barriers.

It may be possible to use this increase of capacity by a clever coding. Here we have in mind recognition processes, which require this invariance. For example:

(i) Recognition of structures in complicated chemical compounds. We represent a linear molecule by a string of letters, which characterize the constituents. If for a certain reaction two constituents are equivalent, then the two configurations with permuted states should be identified. For example, consider the molecules ATTGCACG and TAACGTGC which consist of the four functional groups A, C, G and T. Then, in a network that is invariant under the permutation

$$\pi = \begin{pmatrix} ACGT \\ TGCA \end{pmatrix}$$

the molecules would be identified.

(ii) Recognition of topological features of graphs. For simplicity we restrict ourselves to walks on a lattice with a fixed number of steps. The nodes are numbered $l=1, \ldots, q$ and the graph is represented by a string of numbers, indicating the order of the nodes visited. A few examples are shown in figures 4-6.

A related model—a clock model—has been discussed by Cook [7] in the context of neural networks. She models a neuron by a discrete set of planar vectors, so that the interaction (1) can take on many different values, depending on the number of states. Kanter [8] has discussed an 'anisotropic' Potts model, where the Hamiltonian can be written as

$$H = -\frac{1}{N} \sum_{\nu=1}^{p} \sum_{i \neq j}^{N} (\boldsymbol{\xi}_{i}^{\nu} \cdot s_{i}) (\boldsymbol{\xi}_{j}^{\nu} \cdot s_{j}).$$
(2)

In this case, precisely one Potts state is favoured at each lattice site. Bollé *et al* [9, 10] have discussed the generalization of Kanter's network to biased patterns.

Many intermediate variants in between the isotropic (1) and the anisotropic (2) model are possible and potentially useful. One can group the states into clusters and define couplings, such that the energy is invariant with respect to permutations of states within one cluster but not invariant with respect to permutations of states out of different clusters.

The paper is organized as follows. In section 2 the model is defined and a signal-to-noise analysis performed. Subsequently we discuss the stationary states for low loading (section 3) and calculate the capacity for a macroscopic number of patterns (section 4). In section 5 we present some numerical results to confirm the analytical calculations and to illustrate with a few examples the relaxation of an initial state. In section 6 we present a general Potts network which is invariant under permutations of Potts states within given subsets but not invariant under general permutations of states. Finally, in section 7 we discuss and demonstrate by examples how the networks can be used to recognize graphs.

2. The model

We consider a model of N neurons. Each neuron can be in one out of q possible

states denoted by $\sigma_i \in \{1, \ldots, q\}$, $i = 1, \ldots, N$. We define a local 'field' (energy) h_i as

$$h_i(\sigma, t) \coloneqq -\sum_{j(\neq i)}^N J_{ij} m_{\sigma, \sigma_j(t)}$$
(3)

where $m_{\alpha,\beta} \coloneqq q\delta_{\alpha,\beta} - 1 = e^{\alpha} \cdot e^{\beta}$ is the scalar product between Potts vectors and J_{ij} is the synaptic matrix, coupling different neurons. (For the calculation it is convenient to use σ_i and $m_{\sigma,\sigma_i} = s_i \cdot e^{\sigma}$ instead of s_i defined in the introduction.)

The dynamics of the neural network at finite temperature is defined as in [8]: the probability of neuron *i* to be in state $\sigma \in \{1, ..., q\}$ at time t+1 is given by

$$p(\sigma_i(t+1) = \sigma) = \frac{\exp(-\beta h_i(\sigma, t))}{\sum_{k=1}^{q} \exp(-\beta h_i(k, t))}.$$
(4)

In the limit $\beta \rightarrow \infty$ the dynamics becomes deterministic: the state of neuron *i* at time t+1 is determined by the requirement that $h_i(\sigma, t)$ must be minimized by $\sigma_i(t+1)$.

In the case of symmetric synaptic couplings $J_{ij} = J_{ji}$ fixed points of the deterministic dynamics are local minima of the following Potts Hamiltonian:

$$H = -\frac{1}{2} \sum_{i \neq j}^{N} J_{ij} m_{\sigma_n \sigma_j}.$$
 (5)

We want to achieve that the fixed points of the dynamics are strongly correlated with a given set of p patterns $\{\xi^{\mu}\}$ $(\mu = 1, ..., p)$. For simplicity we restrict ourselves to random independent variables with a uniform distribution over Potts states

$$P(\xi_i^{\mu} = k) = \frac{1}{q}$$
 for $k = 1, ..., q$

and choose a generalized Hebbian learning rule

$$J_{ij} = \frac{1}{N} \sum_{\mu=1}^{p} m_{\xi_{i}^{\mu}, \xi_{j}^{\mu}}.$$
 (6)

Because $m_{\alpha,\beta} = m_{\pi(\alpha),\pi(\beta)}$ holds for any permutation π of $\{1, \ldots, q\}$, the Hamiltonian is invariant under permutations π of the Potts states $\sigma_i \in \{1, \ldots, q\}$.

In the general form of a Potts Hamiltonian

$$H = -\frac{1}{2} \sum_{i \neq j}^{N} \sum_{k,l}^{q} J_{ij}^{kl} m_{\sigma_{j,k}} m_{\sigma_{j,l}}$$
(7)

our model corresponds to

$$J_{ij}^{kl} = \frac{1}{Nq^2} m_{k,l} \sum_{\mu=1}^{p} m_{\xi_{i}^{\mu},\xi_{j}^{\mu}}$$
(8)

whereas Kanter has chosen

$$J_{ij}^{kl} = \frac{1}{Nq^2} \sum_{\mu=1}^{p} m_{\xi_{i,k}^{\mu}} m_{\xi_{j,l}^{\mu}}.$$
(9)

The main difference is that we store the information whether or not two neurons are in the same state, whereas in Kanters model information about the specific Potts state at each site is stored. In order to check if the network stabilizes a finite number of patterns as well as the patterns which are obtained from the stored ones by arbitrary permutations π of the Potts states we perform a signal-to-noise analysis. First we consider the case of storing only one pattern:

$$h_i(\sigma) = -\frac{1}{N} \sum_{j(\neq i)}^N m_{\xi_i, \xi_j} m_{\sigma, \sigma_j}.$$

The aim is to test local stability, so assume that all neurons except neuron *i* are in the state $\sigma_j = \xi_j$ ($j \neq i$). It has to be shown that $h_i(\sigma)$ has a minimum for $\sigma = \xi_j$. Now $h_i(\sigma)$ can be written as \dagger

$$h_i(\xi_i) = -\sum_{\substack{\xi_i = \xi_j \\ \xi_i \neq \xi_j}} (q-1)^2 - \sum_{\substack{\xi_u \neq \xi_j \\ \xi_i \neq \xi_j = \sigma}} (q-1) - \sum_{\substack{\xi_i \neq \xi_j = \sigma}} (q-1) - \sum_{\substack{\xi_i \neq \xi_j \neq \sigma}} 1 \quad \text{for } i \neq j.$$

The condition $h_i(\sigma) \ge h_i(\xi_i)$ then reads

$$0 \le (q-1) \# \{ j(\ne i) \colon \xi_i = \xi_j \} + \# \{ j(\ne i) \colon \xi_i \ne \xi_j = \sigma \}$$
(10)

which is obviously true.

For stability to hold one still has to ensure that equality in (10) is impossible. So let us assume that (10) holds as an equality, i.e. $\xi_j \in \{1, \ldots, q\} \setminus \{\sigma, \xi_i\}$. In this case the state with ξ_i and σ exchanged can be obtained from pattern ξ by changing the corresponding Potts states of ξ_i and σ which means performing a special permutation under the Potts states.

So one stored pattern is dynamically stable at T = 0 unless there exists a permutation of Potts states which acts on the pattern as a one-spin flip. But this is a rather improbable situation for a large network for its probability vanishes for $N \rightarrow \infty$ as

$$p(\exists i, k, l: \xi_j \neq k, l \forall j \neq i) = \frac{1}{q^N} Nq^2 (q-1)^{N-2} = N \left(1 - \frac{1}{q}\right)^{N-2}$$

With the same arguments one can see that all 'Potts-permuted' versions of the patterns are stabilized. In this case h reads

$$h_{i}(\sigma) = -\frac{1}{N} \sum_{j(\neq i)}^{N} m_{\xi_{i},\xi_{j}} m_{\sigma,\pi(\xi_{j})} = \frac{1}{N} \sum_{j(\neq i)}^{N} m_{\xi_{i},\xi_{j}} m_{\sigma,\pi(\xi_{j})}$$

so with the same arguments as above one gets the minimal value of h for $\pi^{-1}(\sigma) = \xi_i$, i.e. $\sigma = \pi(\xi_i)$.

For the case of storing a finite number p of patterns one has to separate the local field into signal and noise terms. Assuming $\sigma_j = \xi_j^1$ for $j \neq i$ as before this reads

$$h_i(\sigma) = -\frac{1}{N} \sum_{j(\neq i)}^N m_{\varepsilon_i^1, \varepsilon_j^1} m_{\sigma, \varepsilon_j^1} - \underbrace{\frac{1}{N} \sum_{\mu=2}^p \sum_{j(\neq i)}^N m_{\varepsilon_i^\mu, \varepsilon_j^\mu} m_{\sigma, \varepsilon_j^1}}_{=\mathcal{N}}.$$
 (11)

For random unbiased patterns $\langle\!\langle \mathcal{N} \rangle\!\rangle = 0$ and

$$\langle\!\langle \mathcal{N}^2 \rangle\!\rangle = \frac{(p-1)(N-1)(q-1)^2}{N^2} \xrightarrow{N \to \infty} 0$$

so finitely many patterns will be stabilized in the limit $N \rightarrow \infty$ by the signal term.

$$\dagger \Sigma'_{\xi_i = \xi_i} = \Sigma_{j(\neq i), \xi_i = \xi_i} \text{ etc.}$$

will be confirmed in section 4 by a replica calculation.

The explicit formula for the \mathcal{N} -variance can be used to give an estimate of the q-dependence of the critical storage capacity. For a uniform distribution of the Potts states, the average value of $h_i(\xi_i)$ is (q-1). The critical storage capacity will be reached if the noise becomes of the same order as the signal. This gives $p_c/N = \alpha_c = \mathcal{O}(1)$ which

3. Mean-field theory for low loading

Starting from the Hamiltonian (5) with the learning rule (6) and applying the same techniques as in [11] one gets the following free energy density:

$$f = \frac{1}{2} \sum_{\mu=1}^{p} \sum_{k,l}^{q} (x_{\mu kl})^{2} - \frac{1}{\beta} \left\langle \left\langle \ln \sum_{\sigma=1}^{q} \exp\left[\frac{\beta}{q} \sum_{\mu=1}^{p} \sum_{k,l=1}^{q} x_{\mu kl} m_{\sigma,k} m_{\xi^{\mu},l}\right] \right\rangle \right\rangle$$
(12)

with the corresponding saddle-point equations

$$x_{\mu k l} = \frac{1}{q} \left\langle \left\langle \frac{\Sigma_{\sigma}^{q} m_{\sigma,k} m_{\xi^{\mu},l} \exp[(\beta/q) \Sigma_{\mu,k,l} x_{\mu k l} m_{\sigma,k} m_{\xi^{\mu},l}]}{\Sigma_{\sigma-1}^{q} \exp[(\beta/q) \Sigma_{\mu,k,l} x_{\mu k l} m_{\sigma,k} m_{\xi^{\mu},l}]} \right\rangle \right\rangle.$$
(13)

The physical meaning of the order parameters $x_{\mu kl}$ is given by

$$x_{\mu k l} = \frac{1}{q} \left\langle\!\left\langle m_{\langle \sigma \rangle, k} m_{\xi^{\mu}, l} \right\rangle\!\right\rangle \tag{14}$$

Here $\langle \cdot \rangle$ denotes the thermal average and $\langle \cdot \rangle$ an average over patterns. So the $x_{\mu kl}$ are generalized overlaps which have the following special values: $x_{\mu kl} = (1/q)\delta_{\mu\nu}m_{k,l}$ for $\sigma_i = \xi_i^{\mu}$; $x_{\mu kl} = (1/q)\delta_{\mu\nu}m_{k,\pi(l)}$ for $\sigma_i = \pi(\xi_i^{\nu})$ and $x_{\mu kl} = 0$ for completely uncorrelated σ_i and ξ_i^{μ} . Moreover the $x_{\mu kl}$ have the following property:

$$\sum_{l=1}^{q} x_{\mu kl} = \sum_{k=1}^{q} x_{\mu kl}.$$
(15)

Because of the symmetry between different Potts states in our model we make the following general ansatz for the $x_{\mu kl}$:

$$x_{\mu k l} = a_{\mu} \delta_{k, \pi(l)} + b_{\mu} (1 - \delta_{k, \pi(l)})$$
(16)

where π again denotes a permutation of $\{1, \ldots, q\}$. Applying (15) one can see that a_{μ} and b_{μ} are not independent, so the general ansatz reads

$$x_{\mu kl} = \frac{c_{\mu}}{q(q-1)} m_{k,\pi(l)}.$$
 (17)

Inserting (17) into the saddle-point equation (13) one finally arrives at the following effective fixed-point equations for the c_{μ} :

$$c_{\mu} = \left\langle \left\langle \frac{\sum_{\sigma=1}^{q} m_{\sigma,\xi^{\mu}} \exp[(\beta/q) \sum_{\mu=1}^{p} c_{\mu} m_{\sigma,\xi^{\mu}}]}{\sum_{\sigma=1}^{q} \exp[(\beta/q) \sum_{\mu=1}^{p} c_{\mu} m_{\sigma,\xi^{\mu}}]} \right\rangle \right\rangle.$$
(18)

Rescaling the inverse temperatures as $\beta \rightarrow (q-1)\beta$ gives exactly the same saddle-point equations as in Kanter's network model [8]. In what follows we briefly discuss solutions of (18) at finite β . In [8] the solutions of the saddle-point equations were only discussed for $\beta \rightarrow \infty$. We furthermore analyse the stability of the fixed points for $\beta \rightarrow \infty$. This is considerably more complicated than in [8], because we have to check stability with respect to nq^2 fluctuations $\delta x_{\mu kl}$.

3.1. Mattis states

First we assume $c_{\mu} = c\delta_{\mu 1}$, i.e. we look for solutions which correspond to retrieval of one pattern or its permutations. It is then possible to perform the average over the patterns to get the free energy

$$f(c) = \frac{c^2}{2(q-1)} - \frac{1}{\beta} \ln(e^{\beta c} + (q-1)e^{-\beta c(q-1)}).$$
(19)

The minima of f are plotted in figure 1 for the case q = 4. There is a first-order transition at a critical value β_c where a positive solution appears. Above $\beta = 1$ the solution c = 0becomes unstable and a negative solution appears. Special values of β_c are $\beta_c = 0.916$ for q = 3, $\beta_c = 0.804$ for q = 4, $\beta_c = 0.712$ for q = 5 and $\beta_c = 0.490$ for q = 9. However, a minimum of f(c) is not necessarily stable with respect to arbitrary fluctuations in $x_{\mu kl}$ -space. We can merely prove that for $\beta \to \infty$ the positive solution $c \to (q-1)$ is stable. In order to show this note that the matrix of second derivatives in case of Mattis states $x_{\mu kl} = [c\delta_{\mu 1}/q(q-1)]m_{k,\pi(l)}$ reads

$$\frac{\partial^2 f}{\partial x_{\nu rs} \partial x_{\mu kl}} = \delta_{\mu\nu} \delta_{rk} \delta_{ls} - \frac{\beta}{q^2} \langle\!\langle \langle m_{\sigma,k} m_{\xi^{\mu},l} m_{\sigma,r} m_{\xi^{\nu},s} \rangle \rangle - \langle m_{\sigma,k} m_{\xi^{\mu},l} \rangle \langle \langle m_{\sigma,r} m_{\xi^{\nu},s} \rangle \rangle \rangle \rightleftharpoons A_{\mu k l \nu rs}$$
(20)

where $\langle \cdot \rangle$ denotes

$$\langle f(\sigma) \rangle = \frac{\sum_{\sigma=1}^{q} f(\sigma) \exp[(\beta/q) \sum_{\mu,k,l} x_{\mu,k,l} m_{\sigma,k} m_{\xi^{\mu},l}]}{\sum_{\sigma=1}^{q} \exp[(\beta/q) \sum_{\mu,k,l} x_{\mu,k,l} m_{\sigma,k} m_{\xi^{\mu},l}]}.$$
(21)

Inserting (21) into (20) one arrives at

$$A_{\mu k l \nu r s} = \delta_{\mu \nu} \delta_{r k} \delta_{l s} - \frac{\beta}{q^2} \langle \langle m_{\xi^{\mu}, l} m_{\xi^{\nu}, s} \{ \langle m_{\sigma, k} m_{\sigma, r} \rangle - \langle m_{\sigma, k} \rangle \langle m_{\sigma, r} \rangle \} \rangle$$

with

$$E = \frac{a_{kr} e^{\beta c(q-2)/(q-1)} + b_{kr} e^{-\beta c2(q-1)}}{(e^{\beta c} + (q-1) e^{-\beta c/(q-1)})^2}$$



Figure 1. Extrema of the effective free energy density f(19) as a function of β for q = 4. Broken lines denote maxima, full lines denote minima. However, for stability to hold one has to investigate the full matrix of second derivatives of f.

where a_{kr} , b_{kr} do not depend on β . So for $\beta \rightarrow \infty$ and positive c, A tends to the unit matrix which means that the Mattis states (including permutations) are locally stable with respect to deterministic dynamics. Bollé and Mallezie [9] have investigated Kanter's model and its generalization to biased patterns at finite temperature for the case of low q and p by studing the dynamics of the overlaps. For Kanter's model they find a first-order transition to the Mattis states for q = 3, 4 at $T_3 = 2.185$, $T_4 = 3.728$, respectively. These values are in accordance with our values for β_c if one rescales the temperatures as indicated above. However, their results about stability cannot be applied to our model.

3.2. Symmetric states

As a second kind of solutions to the saddle-point equations we consider symmetric states, i.e. we assume $c_{\mu} = c_l$ for $\mu = 1, ..., l$ and $c_{\mu} = 0$ for $\mu > l$. These states are equally correlated to the first l patterns.

We consider two special cases: symmetric states with l=2 equal overlaps at finite temperatures and general symmetric states for $\beta \rightarrow \infty$.

Performing the average in the case l=2 leads to the following form of the free energy density:

$$f(c_2) = c_2^2 - \frac{q-1}{\beta} \left\{ \frac{1}{q} \ln((q-1) e^{-2\beta c_2/(q-1)} + e^{2\beta c_2}) + \frac{q-1}{q} \ln((q-2) e^{-2\beta c_2(q-1)} + 2 e^{\beta c_2(q-2)/(q-1)}) \right\}.$$
(22)

The structure of the minima of f is exactly the same as for Mattis states. The corresponding critical values β_c for q = 3, 4, 5 and 9 are $\beta_c = 0.969$, 0.909, 0.852 and 0.677, respectively. These values are higher and the corresponding temperatures lower than for Mattis states with l = 1. This is different from the Ising case where symmetric solutions for arbitrary l all appear beyond the critical inverse temperature $\beta_c = 1$ [11].

In order to perform a stability analysis for $\beta \rightarrow \infty$ and general *l* one again has to consider the matrix A which for general *l* has the following block structure in the pattern indices μ and ν :

$$A = \begin{pmatrix} B & D & \dots & D & & \\ D & B & \vdots & 0 & \\ \vdots & \ddots & D & & \\ D & \dots & D & B & & \\ D & \dots & D & B & & \\ & & & C & & \\ 0 & & & \ddots & & \\ & & & & & C \end{pmatrix}$$

with B, D and C, $q^2 \times q^2$ matrices. In appendix 1 it is shown that in the case of $p > l \ge 2$ one of the eigenvalues of C becomes negative for $c_l > 0$ and $\beta \to \infty$ which implies instability of the symmetric states in this limit. However, the derivation given in appendix 1 does not work for l=1. This is clear because, as shown above, Mattis states are stable for $\beta \to \infty$. Moreover, we cannot exclude stability of the symmetric states with l=p, because in this case, the matrix C does not exist.

4. The storage capacity of the network

In the following we calculate the storage capacity within the replica-symmetric approximation. Using standard techniques [8, 12, 13] we find the following free energy density in the limit $N \rightarrow \infty$ for finite $\alpha = p/N$ and one condensed pattern ξ^1 :

$$f = \frac{\alpha}{2} (q-1)^{2} + \lim_{n \to 0} \left\{ -\frac{\alpha(q-1)}{2\beta} \frac{1}{n} \operatorname{Tr} \ln \left(1 - \frac{\beta}{q} \mathbf{q} \right) + \alpha \beta \frac{1}{n} \sum_{\rho \sigma k l} r_{k l}^{\rho \sigma} q_{k l}^{\rho \sigma} + \frac{1}{2n} \sum_{\rho k l} (m_{k l}^{\rho})^{2} - \frac{1}{n \beta} \left\langle \left\langle \ln \operatorname{Tr}_{\sigma^{\rho}} \exp \left[\frac{\beta}{q} \sum_{\rho k l} m_{k l}^{\rho} m_{\sigma^{\rho}, k} m_{\xi^{1}, l} + \alpha \beta^{2} \sum_{\rho \sigma k l} r_{k l}^{\rho \sigma} m_{\sigma^{\rho}, k} m_{\sigma^{\sigma}, l} \right] \right\rangle \right\rangle_{\xi^{1}} \right\}.$$
(23)

with

$$\sum_{\rho \sigma k l}' \coloneqq \sum_{\rho < \sigma}^{n} \sum_{k,l}^{q} + \sum_{\rho = \sigma}^{n} \sum_{k \leq l}^{q} .$$
(24)

The order parameters m_{kl}^{ρ} , $q_{kl}^{\rho\sigma}$ and $r_{kl}^{\rho\sigma}$ have the following interpretation:

$$m_{kl}^{\rho} = \frac{1}{Nq} \sum_{i=1}^{N} \left\langle \! \left\langle m_{\langle \sigma_i^{\rho} \rangle, k} m_{\xi_{i}^{l}, l} \right\rangle \! \right\rangle$$
(25)

$$q_{kl}^{\rho\sigma} = \frac{1}{N} \sum_{i=1}^{N} \left\langle \left\langle m_{\langle \sigma_i^{\rho} \rangle, k} m_{\langle \sigma_i^{\sigma} \rangle, l} \right\rangle \right\rangle$$
(26)

$$r_{kl}^{\rho\sigma} = \frac{1}{\alpha q^2} \sum_{\mu=s+1}^{p} \sum_{k',l'}^{q} m_{k',l'} \langle\!\langle m_{\mu kk'}^{\rho} m_{\mu ll'}^{\sigma} \rangle\!\rangle \qquad \text{for } k \neq l$$
(27)

$$r_{kk}^{\rho\sigma} = \frac{1}{\alpha q^2 2} \sum_{\mu=s+1}^{p} \sum_{k',l'}^{q} m_{k',l'} \langle\!\langle m_{\mu kk'}^{\rho} m_{\mu ll'}^{\sigma} \rangle\!\rangle.$$
(28)

So the m_{kl}^{ρ} are the overlaps with the condensed patterns and the $q_{kl}^{\rho\sigma}$ are generalized Edwards-Anderson parameters. The $r_{kl}^{\rho\sigma}$ describe the accumulated overlap with the non-condensed patterns. We now assume replica symmetry, i.e.

$$q_{kl}^{\rho\sigma} = \begin{cases} Q_{kl} & \rho \neq \sigma \\ \hat{Q}_{kl} & \rho = \sigma \end{cases}$$
(29)

$$r_{kl}^{\rho\sigma} = \begin{cases} \bar{r}_{kl} & \rho \neq \sigma \\ \hat{r}_{kl} & \rho = \sigma \end{cases}$$
(30)

$$m_{kl}^{\rho} = m_{kl}.$$

In order to perform the limit $n \to 0$ in (23) one has to make further assumptions about the k- and l-dependence of the order parameters. Let us assume $\sigma_i = \pi(\xi_i^1)$ for all *i*. Then the order parameters are given by $m_{kl} = (1/q)m_{k,\pi(l)}$ and $Q_{kl} = m_{k,l}$. This has led us to make the following Potts symmetric ansatz for Mattis states:

$$Q_{kl} = Qm_{k,l} \qquad r_{kl} = rm_{k,l} \qquad (32)$$

$$\hat{Q}_{kl} = \hat{Q}m_{k,l} \qquad \hat{r}_{kl} = \hat{r}m_{k,l} \qquad (32)$$

$$m_{kl} = mm_{k,\pi(l)}$$

After equations (29)-(32) have been substituted in (23) and the limit $n \rightarrow 0$ has been taken, we obtain for the free energy:

$$f = \frac{\alpha}{2} (q-1)^{2} + \frac{q^{2}(q-1)}{2} m^{2} + \frac{\alpha\beta}{2} q(q-1)(2q-1)\hat{r}(\hat{Q}-1) - \frac{\alpha\beta}{2} q^{2}(q-1)r(Q-1) + \frac{\alpha}{2} (q-1)^{2} \left\{ \frac{1}{\beta} \ln(1-\beta(\hat{Q}-Q)) - \frac{Q}{1-\beta(\hat{Q}-Q)} \right\} - \frac{1}{\beta} \left\langle \! \left\langle \ln \operatorname{Tr}_{\sigma} \exp \beta \left[qmm_{\sigma,\xi^{1}} + \sqrt{\alpha rq} \sum_{k} m_{\sigma,k} z_{k} \right] \right\rangle \! \right\rangle_{\xi^{1},z}.$$
(33)

In this formula $\langle \rangle_{\xi^1,z}$ denotes averaging over the condensed pattern ξ^1 and q Gaussian random variables z_k . We want to calculate the storage capacity in the limit $\beta \to \infty$. This is done by performing the limit $\beta \to \infty$ in the saddle-point equations which then are given by

$$q(q-1)m' = -1 + q \int_{-\infty}^{\infty} \frac{dz}{\sqrt{\pi}} e^{-z^2} \left[\frac{1}{2} \left(1 + \operatorname{erf}\left(z + m'\sqrt{\frac{q}{2\alpha r'}}\right) \right) \right]^{q-1}$$
(34)

$$r' = \frac{q-1}{q^2(1-c)^2}$$
(35)

$$q(q-1)c = \sqrt{\frac{2q}{\pi\alpha r'}} \int_{-\infty}^{\infty} dz \, z \, e^{-z^2} \left[\left(\frac{1}{2} \left(1 + \operatorname{erf}\left(z + \sqrt{\frac{q}{2\alpha r'}} \right) \right) \right)^{q-1} + (q-1) \left(\frac{1 + \operatorname{erf}(z)}{2} \right)^{q-2} \left(\frac{1}{2} \left(1 + \operatorname{erf}\left(z - \sqrt{\frac{q}{2\alpha r'}} \right) \right) \right) \right]$$
(36)

$$\hat{r} = \frac{(q-1)(2Q-1+1/\beta)}{q(2q-1)(1-\beta(1-Q))^2}$$
(37)

$$\hat{Q} = 1 \tag{38}$$

where m' = mq and $r' = rq^2$ have been substituted and c is defined by $c = \beta(1-Q)$. Now the equations for m', r' and Q can be transformed into a single equation for $y = m'\sqrt{q/2\alpha r'}$:

$$y = \left(q \int_{-\infty}^{\infty} dz \, e^{-z^2} \left(\frac{1 + \operatorname{erf}(z+y)}{2}\right)^{q-1} - \sqrt{\pi}\right) \\ \times \left(2 \int_{-\infty}^{\infty} dz \, e^{-z^2} z \left[\left(\frac{1 + \operatorname{erf}(z+y)}{2}\right)^{q-1} + (q-1)\left(\frac{1 + \operatorname{erf}(z)}{2}\right)^{q-2} \left(\frac{1 + \operatorname{erf}(z-y)}{2}\right)\right] \\ + (q-1)\sqrt{\frac{2\alpha\pi(q-1)}{q}}\right)^{-1}.$$
(39)

 \hat{Q} and \hat{r} can be obtained from the other three variables, once a solution has been found. The storage capacity α_c is given by the value of α above which no solutions of (39) exist with y > 0. Inspection of the equation shows that it is identical with the corresponding equation of Kanter's model [8] if we rescale $\alpha \rightarrow \alpha/(q-1)^2$. So the storage capacity of the isotropic model can be mapped onto that of Kanter's network by $\alpha = \alpha_{\text{Kanter}}/(q-1)^2$. This reduction by a factor of $\mathcal{O}(q^2)$ is plausible, because in our model we store the information whether or not the states at two different sites are the same. The coupling constant is a scalar quantity, independent of q. In Kanter's model every coupling is a $q \times q$ matrix, so that $\mathcal{O}(q^2N^2)$ couplings can be adapted to ppatterns. Solving (39) gives the values $\alpha_c = 0.104$, 0.092, 0.086 and $\alpha_c = 0.076$ for q = 3, 4, 5 and q = 9, respectively. Kanter pointed out that his storage capacity was close to the approximate formula $\alpha_c(q) = (q(q-1)/2)\alpha_c(2)$ ($\alpha_c(2) = 0.138$). In our case this gives the formula $\alpha_c(q) = (q/2(q-1))0.138$. So the storage capacity decreases from its Hopfield value 0.138 for q = 2 to 0.138/2 for $q \to \infty$ which means it is $\mathcal{O}(1)$ for $q \to \infty$. Kanter's approximate formula contradicts the results of Nadal and Rau [14], who calculated the capacity of a Potts network without specifying the couplings. They found $\alpha = \mathcal{O}(q)$ and not $\mathcal{O}(q^2)$ as suggested by Kanter. Note, however, that Nadal and Rau require stability at every site, whereas the Hebb rule gives rise to stationary states, which are not perfectly correlated with the patterns.

5. Simulations

In this section we present results of numerical simulations to confirm the analytical calculations and to illustrate with a few examples the relaxation to equilibrium. In addition to the dynamical updating rule (4) we also consider another process defined by the prescription:

- (i) Choose a random direction $k \in \{1, ..., q\}$ with equal probability.
- (ii) Decide if a flip into direction k will be performed according to the probability

$$P(\sigma_i(t+1) = \sigma | \sigma_i(t)) = \frac{\exp(-\beta h_i(\sigma))}{\exp(-\beta h_i(\sigma)) + \exp(-\beta h_i(\sigma_i(t)))}.$$
(40)

In the limit $\beta \to \infty$ the updating rule is to choose a random direction σ and to flip into this direction, if the local field $h_i(\sigma)$ is decreased, i.e. if $h_i(\sigma) < h_i(\sigma_i(t))$. Otherwise the spin at site *i* will be left unchanged. The dynamics so defined is the application of a general process proposed by Binder [15]. It obeys the principle of detailed balance, so for $t \to \infty$ the possible states will be visited according to the canonical distribution. Therefore both (4) and (40) should give the same results concerning stability of the equilibrium states.

We first discuss the question of what is an appropriate choice of the order parameter, given the permutational symmetry of our model. One possibility is to take the complete order parameter matrices $x_{\mu kl}$. We have simulated the network to get these order parameters and a typical result can be seen in table 1 where the $x_{\mu kl}$ have been rescaled to $x_{\mu kl} = (1/N(q-1))\sum_{i=1}^{N} m_{\sigma_{i}k}m_{\xi_{i}^{n},i}$. The results show that the order parameters $x_{\mu kl}$ behave as was expected, indicating retrieval by the structure $x_{\mu kl} = \delta_{\mu 4}m_{k,l}/(q-1)$ after relaxation. As expected, presenting a permuted version of a stored pattern as initial condition leads to the structure $x_{\mu kl} = \delta_{\mu\nu}(1/(q-1))m_{k,\pi(l)}$. This also indicates that permuted patterns are stabilized by the network.

However, the $x_{\mu kl}$ give a redundant description of the network state. So a better choice for an order parameter could be

$$\tilde{m}_{\mu} \coloneqq \max_{k} x_{\mu k 1} \tag{41}$$

the maximal element of the first x_{μ} -column. These quantities are permutation invariant

Table 1. Temporal development of the full order parameter matrices $x_{\mu kl}$ for a network with N = 400 neurons, q = 3 Potts states, p = 4 stored patterns and the dynamics (4). Only the overlaps with patterns 3 and 4 are shown. It was checked independently that the network state at time 3 was identical to pattern 4.

	Pattern 3	3		Pattern 4	ļ (
t	x_{3kl}			x_{4kl}		
0	0.001	-0.033	0.031	0.193	-0.039	-0.134
	0.046	-0.021	-0.025	-0.134	0.200	-0.066
	-0.048	0.054	-0.006	-0.059	-0.141	0.200
1	-0.029	~0.006	0.035	0.995	-0.539	-0.456
	-0.003	0.009	-0.006	-0.543	1.040	-0.498
	0.032	-0.003	0.029	-0.453	-0.501	0.954
2	-0.025	-0.003	0.028	0.999	-0.546	-0.453
	-0.006	0.005	0.001	-0.546	1.048	-0.501
	0.031	-0.003	-0.029	-0.453	-0.501	0.954



Figure 2. Dynamical evolution of the overlaps for N = 400, q = 3, p = 5 and the updating rule (4) (full line) and Binder's dynamics (40) (broken curve).



Figure 3. Instability of the symmetric mixture states. Parameters are the same as in figure 2 but the initial configuration has been chosen as a symmetric mixture of three states.

and give $\tilde{m}_{\mu} = \delta_{\mu\nu}$ for $\sigma_i = \xi_i^{\nu}$ or $\sigma_i = \pi(\xi_i^{\nu})$ and $\tilde{m}_{\mu} = 0$ for uncorrelated states as $N \to \infty$. For finite N the $x_{\mu k i}$ are expected to fluctuate around these values.

Figures 2 and 3 present the results of some typical network simulations, always plotting the \tilde{m}_{μ} -overlaps with the different stored patterns as a function of time. In figure 2 we show ordinary retrieval at T=0, realizing both different dynamics. One can see that retrieval is faithfully performed; presenting a permuted version of one of the stored patterns gives the same results. The two dynamical updating rules are different with respect to their time-scales. For Kanter's dynamics the network relaxes in two steps, for Binder's dynamics it takes approximately 15 steps. This is due to the fact that the Kanter-rule always chooses the flip with maximal decrease of energy, whereas the rule (40) possibly chooses Potts directions which only slightly decrease the energy. However, one should keep in mind that the single time step in Kanter's dynamics takes roughly q times longer than in Binder's dynamics.

Retrieval dynamics at finite β has also been investigated numerically. The results look very similar to those of figure 2 as long as $\beta > \beta_c$.

The instability of symmetric mixture states for deterministic dynamics is demonstrated in figure 3. Starting with three equal overlaps always gives a flow towards a single Mattis state. In section 2 we showed that the symmetric mixture states are unstable to fluctuations in the space of patterns with initial overlap zero. In the simulations we observe that one of the patterns with initial overlap 1/l always wins. Presumably there are other unstable modes, which grow faster.

6. Generalized Potts networks

In this section we shall discuss a network of Potts neurons, which is invariant under permutations of Potts states within given subsets, but not invariant under permutations of states out of different subsets. Kanter's model and our permutation-invariant model are two special cases of this more general Potts network.

Consider a network of N neurons where each neuron can take on q different states as before. The states are grouped into r subsets, each containing m = q/r states. For a given state k define functions g and u such that g(k) gives the index of the group and u(k) the index within the group:

$$g(k) = (k-1) \operatorname{div} m + 1$$
$$u(k) = (k-1) \operatorname{mod} m + 1$$

where $q \operatorname{div} p$ denotes integer division. A simple example are nine states which are grouped into three subsets:

k	1	2	3	4	5	6	7	8	9
g(k) u(k)	1	1 2	1 3	2	2	23	3	3 2	3

In our model the local energy is given by

$$h_i(\sigma) = -\sum_{j(\neq i)}^N \sum_{k,l}^q J_{ij}^{kl} m_{\sigma,k} m_{\sigma_j,l}$$

with the learning rule

$$J_{ij}^{kl} = \frac{1}{Nq^2} \sum_{\mu=1}^{p} \{ m_{g(\xi_i^{\mu}), g(k)} m_{g(\xi_j^{\mu}), g(l)} + \delta_{g(\xi_i^{\mu}), g(\xi_j^{\mu})} \delta_{g(k), g(l)} m_{u(\xi_i^{\mu}), u(\xi_j^{\mu})} m_{u(k), u(l)} \}.$$
(42)

Here the $m_{\alpha,\beta}$ -operators are defined with respect to the group index, $m_{g(k),g(l)} = r\delta_{g(k),g(l)} - 1$, or with respect to the index of the members of a group, $m_{u(k),u(l)} = m\delta_{u(k),u(l)} - 1$ for $k, l \in \{1, ..., q\}$.

Kanter's model and the isotropic model are reproduced by choosing m = 1, r = q (Kanter) and m = q, r = 1 (isotropic), respectively. To obtain new results we always assume $m, r \ge 2$ in what follows. The dynamical updating rule shall be the same as for the models considered so far ((4) or (40)).

Making use of the fact that $\sum_{k=1}^{q} J_{ij}^{kl} = \sum_{l=1}^{q} J_{ij}^{kl} = 0$ one can calculate the local energy

$$h_{i}(\sigma) = -\frac{1}{N} \sum_{\mu=1}^{p} \left\{ \sum_{j(\neq i)}^{N} m_{g(\xi_{i}^{\mu}),g(\sigma)} m_{g(\xi_{j}^{\mu}),g(\sigma_{j})} + \sum_{\substack{j(\neq i): \\ g(\xi_{i}^{\mu}) = g(\xi_{j}^{\mu}) \\ g(\sigma) = g(\sigma_{j})}} m_{u(\xi_{i}^{\mu}),u(\xi_{j}^{\mu})} m_{u(\sigma),u(\sigma_{j})} \right\} - c$$
(43)

where $c = \sum_{k,l} J_{ij}^{kl}$ does not depend on the dynamical variables σ , σ_j and hence can be neglected in the following.

We shall now discuss the signal-to-noise analysis of this model and show that it stabilizes the patterns as well as their permuted versions. If we consider first, the case of one single stored pattern and assume $\sigma_j = \xi_j$ for all $j \neq i$ (*i* fixed) we have to show that $h_i(\sigma)$,

$$Nh_{i}(\sigma) = -\sum_{j(\neq i)}^{N} m_{g(\xi_{i}),g(\sigma)}(r-1) - \sum_{\substack{j(\neq i):\\g(\xi_{i})=g(\xi_{j})=g(0)}} m_{u(\xi_{i}),u(\xi_{j})}m_{u(\sigma),u(\xi_{j})}$$
(44)

becomes minimal for $\sigma = \xi_i$. The expression for $h_i(\sigma)$ can be rewritten as

$$Nh_{i}(\sigma) = -(N-1)(r-1)m_{g(\xi_{i}),g(\sigma)} - \delta_{g(\sigma),g(\xi_{i})} \left\{ (m-1)|A_{1}|m_{u(\sigma),u(\xi_{i})} - \sum_{j \in A_{2}} m_{u(\sigma),u(\xi_{j})} \right\}$$

where the sets A_1, A_2 are defined by

$$A_{1} = \{ j(\neq i) : \xi_{i} = \xi_{j} \}$$
$$A_{2} = \{ j(\neq i) : g(\xi_{i}) = g(\xi_{j}) \land u(\xi_{i}) \neq u(\xi_{j}) \}.$$

Now, in general, $Nh_i(\sigma)$ can take on three different values:

$$Nh_{i}(\xi_{i}) = -(N-1)(r-1)^{2} - (m-1)^{2}|A_{1}| - |A_{2}|$$

$$Nh_{i}(g(\xi_{i}), u(\sigma))$$

$$= -(N-1)(r-1)^{2} + |A_{1}|(m-1) + (m-1)|B_{1}| - |B_{2}|$$
for $u(\sigma) \neq u(\xi_{i})$
(46)

$$Nh_i(g(\sigma), u(\sigma)) = (N-1)(r-1)$$
 for $g(\sigma) \neq g(\xi_i)$ and $u(\sigma) \neq u(\xi_i)$. (47)

Here B_1 and B_2 are given by

$$B_1 = \{ j(\neq i) \colon g(\xi_i) = g(\xi_j) \land u(\xi_i) \neq u(\xi_j) \land u(\sigma) = u(\xi_j) \}$$
$$B_2 = \{ j(\neq i) \colon g(\xi_i) = g(\xi_j) \land u(\xi_i) \neq u(\xi_j) \land u(\sigma) \neq u(\xi_j) \}.$$

So the stability condition $h_i(\xi_i) < h_i(\sigma) \forall \sigma \neq \xi_i$ reduces to the two inequalities $h_i(\xi_i) < h_i(g(\xi_i), u(\sigma))$ and $h_i(\xi_i) < h_i(g(\sigma), u(\sigma))$. This can be rewritten as follows:

$$|A_1|(m-1)m + |A_2| + (m-1)|B_1| - |B_2| = |A_1|(m-1) + m|B_1| > 0$$
(48)

and

$$(N-1)(r-1)r + (m-1)^2 |A_1| + |A_2| > 0.$$
(49)

Now inequality (49) is always true. The left-hand side of equation (48) is positive semidefinite. Equation (48) holds as an equality if $A_1 = \emptyset$ and $B_1 = \emptyset$ because $B_1 \cup B_2 = A_2$. $A_1 = \emptyset$ implies that the Potts state at site *i* does not occur anywhere else in the network. $B_1 = \emptyset$ implies that $u(\sigma)$ does not occur anywhere among those states, which belong to the same group as ξ_i (and hence σ). Both events are very unlikely as $N \to \infty$, as discussed after equation (10). Hence we have shown that $\sigma_i = \xi_i$ is a locally stable state, except for global permutations which leave the groups unchanged and which can be achieved as single spin flips.

The stability of the permuted pattern $\pi(\xi)$ can be easily seen: π will leave the groups invariant, i.e. $g(\pi(k)) = g(k)$ and $u(\pi(k)) = \pi(u(k))$. Now assume $\sigma_j = \pi(\xi_j)$ for such a permutation. Then $h_j(\sigma)$ reads

$$Nh_{i}(\sigma) = -\sum_{j(\neq i)}^{N} m_{g(\xi_{i}),g(\sigma)} m_{g(\xi_{j}),g(\xi_{j})} - \sum_{\substack{j(\neq i):\\g(\xi_{i})=g(\xi_{j})\\g(\sigma)=g(\xi_{i})}} m_{u(\xi_{i}),u(\xi_{j})} \underbrace{m_{u(\sigma),\pi(u(\xi_{j}),u(\xi_{j}),u(\xi_{j})}}_{m_{\pi^{-1}(u(\sigma)),u(\xi_{j})}} \cdot \underbrace{m_{u(\sigma),\pi(u(\xi_{j}),u(\xi_{j}),u(\xi_{j}),u(\xi_{j}),u(\xi_{j}),u(\xi_{j})}}_{m_{\pi^{-1}(u(\sigma)),u(\xi_{j})}}$$

So the stability of the unpermuted pattern means that $h_i(\sigma)$ becomes minimal for $\pi^{-1}(u(\sigma)) = u(\xi_i)$ and $g(\sigma) = g(\xi_i)$ which is equivalent to $\sigma = \pi(\xi_i)$.

An exception is the case of two groups (r=2). Then one has Ising symmetry in the couplings among the groups, so that patterns which have undergone an exchange of their group indices g(k) are also stabilized.

The case of storing p patterns is now straightforward: a separation of signal- and noise-terms gives the results

$$\langle\!\langle \mathcal{N} \rangle\!\rangle = 0$$
$$\langle\!\langle \mathcal{N}^2 \rangle\!\rangle = \frac{(p-1)(N-1)}{N^2} \left((r-1)^2 + \left(\frac{m-1}{r}\right)^2 \right).$$

So, for finite m and r_1 and for $N \rightarrow \infty$ the signal-term will stabilize the patterns and their permuted versions.

Again, the explicit formula for the variance of \mathcal{N} gives a rough estimate for the *m*and *r*-dependence of the critical storage capacity α_c . If one takes into account that the average value for the signal-term (for equally probable Potts states) is of order

$$(r-1)^2 + (m-1)/r$$
 for $N \to \infty$ one gets

$$\alpha_{\rm c} \sim \frac{((r-1)^2 + (m-1)/r)^2}{(r-1)^2 + ((m-1)/r)^2}$$
(50)

as the value of p/N where signal and noise $\sqrt{\langle\!\langle N^2 \rangle\!\rangle}$ become of the same magnitude.

7. Application to the recognition of graphs

In this section we discuss an application of our multistate network models to the recognition of graphs. In the context of graph theory, one can identify a special network state $\sigma = (\sigma_1, \ldots, \sigma_N)$ with $\sigma_i \in \{1, \ldots, q\}$ as a walk on a graph of q vertices, defined by the sequence of directed edges $(\sigma_1, \sigma_2), \ldots, (\sigma_{N-1}, \sigma_N)$. So, recognition of a certain pattern can be interpreted as recognition of the corresponding walk. The main property of our first network model, namely the automatic stabilization of permuted versions of every stored pattern, can be interpreted in this context as the identification of walks which are generated by permutations of the vertices. Note that the underlying graphs are topologically equivalent (homeomorphic). So, the isotropic network can be used to classify classes of topologically equivalent graphs. The application of our model is straightforward if we restrict ourselves to graphs with a fixed number of vertices (q) and a fixed number of steps (N), such that q/N is small (see stability analysis above). In other words, the graphs under consideration have in general repeated edges (graphs with this property are called *multigraphs* [16]).

An illustration of graph recognition by a Potts network is shown in figures 4-6. In the simplest case a network of six neurons with q = 4 states each, is used to store one graph with six edges and four vertices. The network can recognize all isomorphisms of the stored graph. Successful recognition is achieved in two time steps. In figure 5 we show results for a network of 10 neurons with two stored graphs. Relaxation of a noisy input to the correct isomorphism is seen to take place in a few time steps.



Figure 4. Storage of one walk in the isotropic model with q = 4 and N = 5. Stored pattern ξ (top) and dynamical evolution of a noisy walk into the permutted pattern $\pi(\xi)$ (bottom).

The general network of section 6 can also be used in the context of graph recognition. The grouping of Potts states corresponds to a grouping of vertices, for example by colouring. A simple example is shown in figure 6 for a network of eight neurons with six states each. The six states have been divided into three groups (1, 2), (3, 4), (5, 6). We again show the relaxation of a noisy input into a stationary state, which can be obtained from the stored pattern by permuting states within a group.



Figure 5. Storage of two walks in the isotropic model now with q = 4, N = 10. Stored patterns ξ_1, ξ_2 (top) and dynamical evolution of a noisy walk into the permuted pattern $\pi(\xi_1)$ (bottom).



Figure 6. Storage of one single walk in the generalized Potts model with r = 3 groups and m = 2 states per group. Stored pattern ξ (top) and dynamical evolution of an arbitrary initial state into a permuted version $\pi(\xi)$ of the pattern (bottom).

Appendix 1. Instability of symmetric mixture states for $\beta \rightarrow \infty$

As indicated in the main text, we have to show that one of the eigenvalues of C becomes negative for $\beta \rightarrow \infty$. C reads

$$C = \begin{pmatrix} E - (\beta/q^2)(q-1)\tilde{C} & (\beta/q^2)\tilde{C} \\ & \ddots & \\ (\beta/q^2)\tilde{C} & E - (\beta/q^2)(q-1)\tilde{C} \end{pmatrix}$$

where \tilde{C} denotes the symmetric matrix with elements

$$\bar{C}_{kr} = \langle\!\langle m_{\sigma,k} m_{\sigma,r} \rangle - \langle m_{\sigma,k} \rangle \langle m_{\sigma,r} \rangle\!\rangle_{\xi^1, \dots, \xi^l}$$
(51)

with E the $q \times q$ unity matrix. The eigenvalues of C are thus given by 1 and $1 - (\beta/q)c_i$ with c_i the eigenvalues of \tilde{C} . Now \tilde{C} itself has the form $\tilde{C}_{kr} = \delta_{kr}\hat{c} + (1 - \delta_{kr})c$ with eigenvalues $\hat{c} + (q-1)c$ and $\hat{c} - c$. Moreover one shows that $\hat{c} + (q-1)c = 0$ and so $\hat{c} - c = -qc$. Therefore $1 + \beta c$ is an eigenvalue of C, so of A. We now show that c becomes negative for $\beta \to \infty$.

c can be shown to give

$$c = -q^{2} \frac{1}{q^{l}} \sum_{\boldsymbol{\xi}} \frac{\exp[\beta m \sum_{\mu=1}^{l} (m_{1,\boldsymbol{\xi}^{\mu}} + m_{2,\boldsymbol{\xi}^{\mu}})]}{(\sum_{\sigma=1}^{q} \exp[\beta m \sum_{\mu=1}^{l} m_{\sigma,\boldsymbol{\xi}^{\mu}}])^{2}}$$
(52)

where Σ_{ξ} means $\Sigma_{\xi^{l}=1}^{1} \dots \Sigma_{\xi^{l}=1}^{q}$ and $m = c_{l}/q$. Let $\sigma_{1}^{*}(\xi), \dots, \sigma_{s}^{*}(\xi)$ be defined by

$$\max_{\sigma} \sum_{\mu=1}^{i} m_{\sigma,\xi^{\mu}} =: \sum_{\mu=1}^{i} m_{\sigma_{k}^{*},\xi^{\mu}} \qquad \dot{k} = 1, \ldots, s.$$

Now c can be written as

$$c \xrightarrow{\beta \to \infty} -q^{2-l} \sum_{\xi} \frac{\exp[\beta m \sum_{\mu=1}^{l} (m_{1,\xi^{\mu}} + m_{2,\xi^{\mu}})]}{s^{2} \exp[2\beta \sum_{\mu=1}^{l} m_{\sigma_{k}^{k},\xi^{\mu}}]} \qquad k \in \{1, \dots, s\}$$
(53)

in the limit $\beta \to \infty$. All summands of this expression are non-positive. Exactly those terms yield a negative contribution for $\beta \to \infty$ for which $s \ge 2$ and $1, 2 \in \{\sigma_1^*, \ldots, \sigma_s^*\}$ hold. But such terms can always be given explicitly:

(i) $l \leq q$: consider $\boldsymbol{\xi} = (\xi^l, \dots, \xi^l)$ with components different in pairs and $1, 2 \in \{\xi^1, \dots, \xi^l\}$. In this case $s = l, l \geq 2$ and any $\sigma^* \in \{\xi^1, \dots, \xi^l\}$ maximizes the sum $\sum_{\mu=1}^l m_{\sigma,\xi^{\mu}}$.

(ii) l > q: now consider l = 2k (or 2k+1). Then take the term $\boldsymbol{\xi} = (1, \ldots, 1, 2, \ldots, 2, (\xi^3))$. This yields a twofold degenerate maximum (s = 2) with the corresponding σ_k^* given by $\sigma_1^* = 1, \sigma_2^* = 2$.

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