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Storage capacities of committee machines with overlapping and non-overlapping receptive fields

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Abstract. We present theoretical investigations via the replica theory of the storage capacities of committee machines with a large number M of hidden units and spherical weights. Difficulties arise in the solution of this problem in the limit of large M. In the case of overlapping receptive fields, as the number of patterns increases, both permutation symmetry and replica symmetry are broken, which leads to the appearance of many order parameters and causes additional difficulty. We observe that the relations among these order parameters yield a set of quantities which are small in the limit of large M, making the asymptotic calculation tractable. Using the one-step replica symmetry breaking scheme, we compute the asymptotic value α_c of the storage capacity per input unit in the limit of large M. We find that $\alpha_c \simeq (8\sqrt{2}/(\pi-2))M\sqrt{\ln M}$. The shift to the case of non-overlapping receptive fields can be made easily; we then find $\alpha_c \simeq (8\sqrt{2}/\pi)\sqrt{\ln M}$. Both values satisfy the bound of Mitchison and Durbin.

1. Introduction

Statistical mechanics has been a useful tool for the study of neural networks since it was successfully applied to the Hopfield model [1]. From the perspective of statistical mechanics, a neural network can be regarded as a thermodynamic system of quenched disorder. Many ideas and methods developed in studies of random systems, particularly spin glasses, have been used extensively to study neural networks. The replica theory [2, 3] is a useful method which has proven to be invaluable in theoretical approaches. Gardner developed the statistical mechanics formalism via replica theory for the storage capacities of feedforward neural networks, *perceptrons* [4]. She reproduced the storage capacity of a single-layer perceptron with continuous weights which Cover had obtained using geometrical arguments [5]. Later, Krauth and Mézard calculated the storage capacity of a single-layer perceptron with binary weights [6]. Exploiting Gardner's idea, Sompolinsky, Tishby and Seung studied generalization in learning from examples, and obtained interesting results for a single-layer perceptron [7].

There have also been theoretical studies on the storage capacities of more complicated networks, in particular, the committee machine and the parity machine. Barkai, Hansel and Kanter obtained the storage capacity of a parity machine with non-overlapping receptive fields (NRF) in the case of spherical weights [8]. Their value is exact within the one-step replica symmetry breaking (1RSB) scheme, and satisfies the mathematical bound obtained by Mitchison and Durbin [9]. This bound is derived using a method similar to that of Cover and is generally applicable to both machines. Later Barkai *et al* [10] and Engel *et al* [11] made extensive progress on committee machines. They first pointed out that the

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breaking of the symmetry in permuting hidden units, called permutation symmetry breaking (PSB), plays an important role for the machine with overlapping receptive fields (ORF). Their results seemed reasonable for a finite number of hidden units. For a large number of hidden units, however, their replica symmetric (RS) calculation, obtained only for the NRF case, violated the Mitchison–Durbin bound. They supposed that the 1RSB calculation would give a more accurate estimate of the storage capacity.

Our group [12, 13] and Schwarze *et al* [14] have devoted much effort to the study of generalization in learning from examples in the ORF committee machine. We found a novel first-order phase transition, driven by PSB, from the poor-learning phase to the good-learning phase. Overlaps between different hidden units were found to make non-negligible and important contributions. By deriving relations among order parameters, including the overlaps between different hidden units, we were able to calculate the generalization curve for a large number of hidden units. Unlike the case of storage capacity, the RS calculation was satisfactory for the generalization, as confirmed by the Monte Carlo simulation in the case of binary weights.

In this paper we extend our method, used in the studies of the generalization of the ORF committee machine, to the study of the storage capacity of the same machine. It is easy to shift to the NRF case, so that we can obtain storage capacities in both cases. We resolve the difficulty of the large M limit, a major reason why this problem has not been solved previously.

In this paper, most of the equations and discussions are given with regards to the ORF machine, and we simply shift to the NRF case at the end of the calculations. Our calculations are carried out within the 1RSB scheme, which seems to be, so far, the best tool available from the replica theory. In section 2 the statistical mechanics formalism, based on the Gardner method, is developed, and various order parameters are introduced. Section 3 is based on analysis in the regime where the number of patterns per input unit is of order M, far below the storage capacity. We discuss the physical implication of the breaking of permutation symmetry and replica symmetry. We derive relations among many order parameters that greatly reduce the technical difficulty. From these relations we can infer the asymptotic behaviour of many order parameters near the storage capacity. In section 4 we investigate the asymptotic behaviour of the order parameters near the storage capacity in the large M limit. We find the value α_c of the storage capacity per input unit. The result is found to satisfy the Mitchison–Durbin bound. In section 5 we discuss our results and related works in progress. In the appendix we present more technical details of the asymptotic calculation in section 4.

2. Statistical mechanics formalism

Consider a double layer committee machine with N input units, M hidden units and one output unit. The committee machine has the weight between every hidden unit and the output unit equal to one. Let W_{ji} be the weight between input unit i and hidden unit j, and let ξ_i^μ for $\mu = 1, \ldots, P$ be input variables on input units i. We choose the Boolean transfer function on the hidden units. Then the network produces an output value

$$o^\mu = \mathrm{sgn}\left(M^{-1/2}\sum_{j=1}^{M}\mathrm{sgn}(h_j)\right). \tag{1}$$

In this equation the local receptive fields h_j on hidden units j is given by $N'^{-1/2}\sum_{i=1} W_{ji}\xi_i^\mu$. Here the summation over i depends on the architecture of the machine. In a fully connected machine, all the i are swept and $N' = N$. In this case the h_j are called overlapping. In a tree-structure machine, input units are equally divided into M subgroups each of which is connected to one of hidden units, so $N' = N/M$. In this machine the i do not overlap for different js and the h_j are called non overlapping.

A pattern μ is encoded by a number $\sigma^\mu \in \{-1, 1\}$ at the output via an input–output mapping $\{\xi_i^\mu\} \to \sigma^\mu$. A pattern μ is stored in the machine when weights can yield the correct output, that is, $o^\mu = \sigma^\mu$. The storage capacity is then defined as the maximum number P_c of input–output mappings that can be stored reliably in the machine. The volume V in the weight space in which weights correctly produce P input–output mappings, originally considered by Gardner, can be found from the partition function

$$Z = \mathrm{Tr}_{\{W_{ji}\}} \exp\left(-\beta \sum_{\mu=1}^{P} \Theta(-\sigma^\mu o^\mu) \right) \tag{2}$$

where $\Theta(x)$ is the Heaviside step function. As the inverse temperature $\beta \equiv 1/T$ goes to ∞, Z recovers the Gardner volume V. The trace is taken over continuous weights with a spherical constraint: $\sum_i W_{ji}^2 = N'$ and $\sum_j W_{ji}^2 = M$. When P reaches the storage capacity, $\ln V$ goes to $-\infty$. One can observe that the ORF machine and also the NRF machine, can store patterns safely for $P \propto N$ in the limit of large N. Let us write $P = \alpha N$ and $P_\mathrm{c} = \alpha_\mathrm{c} N$. Then we expect $\alpha_\mathrm{c} \gg \mathcal{O}(1)$.

The ξ_i^μ are drawn at random over a distribution with variance one, that is, $\langle\langle \xi_i^\mu \xi_j^\nu \rangle\rangle = \delta_{\mu\nu}\delta_{ij}$, where the double-bracket denotes the average over the ξ_i^μ. The σ^μ are also drawn at random from $\{-1, 1\}$. The network is now regarded as a thermodynamic system with the energy $\sum_{\mu=1}^{P} \Theta(-\sigma^\mu o^\mu)$ and the quenched disorder given by a random selection of the ξ_i^μ and the σ^μ. The average of $\ln Z$ over the quenched disorder can be performed using the replica theory. In the disorder average, we can put $\sigma^\mu = 1$ without loss of generality by changing $\sigma^\mu \xi_i^\mu \to \xi_i^\mu$. Then, the replica theory yields the disorder average $\langle\langle \ln Z \rangle\rangle = n^{-1} \ln\langle\langle Z^n \rangle\rangle$ in the $n \to 0$ limit.

We can now write the replicated partition function

$$\langle\langle Z^n \rangle\rangle = \mathrm{Tr}_{\{W_{ji}\}} \exp[P\mathcal{G}_r]. \tag{3}$$

Here $\mathcal{G}_r$ is given by

$$\mathrm{e}^{\mathcal{G}_r} = \int \prod_\sigma \frac{\mathrm{d}u^\sigma\, \mathrm{d}\hat{u}^\sigma}{2\pi} \int \prod_{j,\sigma} \frac{\mathrm{d}x_j^\sigma\, \mathrm{d}\hat{x}_j^\sigma}{2\pi} \exp\bigg[-\beta \sum_\sigma \Theta(-u^\sigma) + \mathrm{i} \sum_\sigma \hat{u}^\sigma u^\sigma + \mathrm{i} \sum_{j,\sigma} \hat{x}_j^\sigma x_j^\sigma - \frac{1}{2} \sum_{j,j',\sigma,\rho} \hat{x}_j^\sigma \hat{x}_{j'}^\rho Q_{j\sigma,j'\rho} - \frac{\mathrm{i}}{\sqrt{M}} \sum_{\sigma,j} \hat{u}^\sigma \mathrm{sgn}(x_j^\sigma) \bigg] \tag{4}$$

where σ, ρ are replica indices. The matrix $Q_{j\sigma,j'\rho}$ is defined by

$$Q_{j\sigma,j'\rho} = \frac{1}{N} \sum_{i=1}^{N} W_{ji}^\sigma W_{j'i}^\rho. \tag{5}$$

One can carry out the integrations over the x_j^σ by using the cumulant expansion in the limit of large M. Up to the zeroth order in $1/M$, (4) leads to

$$\mathrm{e}^{\mathcal{G}_r} = \int \prod_\sigma \frac{\mathrm{d}u^\sigma\, \mathrm{d}\hat{u}^\sigma}{2\pi} \exp\bigg[-\beta \sum_\sigma \Theta(-u^\sigma) + \mathrm{i} \sum_\sigma \hat{u}^\sigma u^\sigma - \frac{1}{2} \sum_{\sigma,\rho} \hat{u}^\sigma \hat{u}^\rho \frac{1}{M} \times \sum_{j,j'} \frac{2}{\pi} \sin^{-1}(Q_{j\sigma,j'\rho}) \bigg]. \tag{6}$$

This equation turns out to be valid as α goes up to $\mathcal{O}(M)$. This will be examined in the next section and some useful information will be given. However, near the storage capacity where $\alpha/M \gg \mathcal{O}(1)$, this cumulant expansion does not work. A more accurate method is required to estimate α_c.

The thermal average of the matrix $Q_{j\sigma,j'\rho}$ gives rise to the order parameters, which are averaged overlaps among hidden units and replicas. One can write $\langle\langle Z^n\rangle\rangle$ as a multiple integral where integration variables are $Q_{j\sigma,j'\rho}$ and their conjugate variables $\hat{Q}_{j\sigma,j'\rho}$, which are introduced in inserting delta functions associated with (5), that is, $\delta(Q_{j\sigma,j'\rho} - N^{-1}\sum_i W_{ji}^{\sigma} W_{j'i}^{\rho})$. The integral can be computed by the saddle-point method in the limit of large N. The values of $Q_{j\sigma,j'\rho}$ at the saddle point are identical with the corresponding order parameters. There are three classes of order parameters given by

$$Q^{\sigma} = \frac{1}{N}\sum_i \langle\langle\langle W_{ji}^{\sigma} W_{j'i}^{\sigma}\rangle_{\mathrm{T}}\rangle\rangle \qquad \text{for } j \neq j' \tag{7}$$

$$p^{\sigma\rho} = \frac{1}{N}\sum_i \langle\langle\langle W_{ji}^{\sigma} W_{j'i}^{\rho}\rangle_{\mathrm{T}}\rangle\rangle \qquad \text{for } j \neq j' \quad \sigma \neq \rho \tag{8}$$

$$q^{\sigma\rho} = \frac{1}{N}\sum_i \sum_j \langle\langle\langle W_{ji}^{\sigma} W_{ji}^{\rho}\rangle_{\mathrm{T}}\rangle\rangle \qquad \text{for } \sigma \neq \rho \tag{9}$$

where $\langle\cdots\rangle_{\mathrm{T}}$ denotes the thermal average. We assume that the order parameters are independent of indices of hidden units. Overlaps, Q^{σ} and $p^{\sigma\rho}$, between different hidden units are found to be of order $1/M$. Nevertheless, they make crucial contributions through rescaling

$$\bar{Q}^{\sigma} = (M-1)Q^{\sigma} \qquad \bar{p}^{\sigma\rho} = (M-1)p^{\sigma\rho}. \tag{10}$$

Using the relation $\langle\langle Z^n\rangle\rangle = \exp(-n\beta F)$, we can write the free energy F as

$$-n\beta\frac{F}{N} = \mathcal{G}_0(\bar{Q}^{\sigma}, \bar{p}^{\sigma\rho}, q^{\sigma\rho}, \hat{Q}^{\sigma}, \hat{p}^{\sigma\rho}, \hat{q}^{\sigma\rho}) + \alpha\mathcal{G}_r(\bar{Q}^{\sigma}, \bar{p}^{\sigma\rho}, q^{\sigma\rho}). \tag{11}$$

The saddle-point condition is obtained from the stationary condition of the free energy F with respect to $\bar{Q}^{\sigma}$, $\bar{p}^{\sigma\rho}$, $q^{\sigma\rho}$ and their conjugate order parameters $\hat{Q}^{\sigma}$, $\hat{p}^{\sigma\rho}$, $\hat{q}^{\sigma\rho}$. The order parameters can be determined by solving the saddle-point equations. One can then find $\alpha = \alpha_c$ at which $q_1 = 1$, that is, weights composing the Gardner volume collapse to a single point in the weight space.

3. Symmetry breaking and order parameters

As the number of patterns increases, the volume of the *allowed* region in the weight space, where weights correctly produce the desired input–output mappings, decreases. The output, therefore the energy, of the ORF machine is invariant under the permutation of hidden units. This property is called permutation symmetry (PS). In the PS phase, specialization in hidden units does not occur, that is, the weights that can be transformed by the permutation of hidden units are sited in a single allowed region. As a result, the overlap $p^{\sigma\rho}$ between different hidden units and the self-overlap $q^{\sigma\rho}$ are not distinguishable. Therefore we expect $q^{\sigma\rho} = p^{\sigma\rho} = 0$ in the leading order. Note that $p^{\sigma\rho}$ is always $\mathcal{O}(1/M)$.

As α increases, PS becomes broken. In this situation, the allowed region of correct pattern in the weight space is decomposed into many islands. Weights that can be transformed by permutation of hidden units are not sited in the same islands. In this case, specialization in hidden units takes place, which leads to the increase of self-overlap, that is, $q^{\sigma\rho} > 0$. This characterizes the PSB phase. There should be a phase transition at a certain α from the PS phase to the PSB phase.

Another source of the decomposition of the weight space is replica symmetry breaking (RSB). PSB is unique to the ORF machine, but RSB is a more general phenomenon. If further segmentation within each of the islands separated by PSB is possible, RSB is diagnostic to it. For the generalization of the ORF machine, a similar phase transition driven by the PSB is observed, but the PSB phase is found to preserve RS, as confirmed by the Monte Carlo simulation [13]. This difference might be explained by the argument that for the generalization, the presence of a target network, as a particular attractor in the weight space, strongly drives the machine into a specific island. The situation is less clear for continuous weights, where no Monte Carlo simulation has been carried out.

The above scenario can be confirmed by investigating in detail the behaviour of order parameters. Interesting properties are observed for $\mathcal{O}(\alpha) \geqslant M$. Let α' be α/M. In this regime of α we can find the free energy up to the leading order

$$\begin{aligned}
-n\beta\frac{F}{NM} &= -\frac{1}{2}\sum_{\sigma}(1+\bar{Q}^{\sigma})\hat{Q}^{\sigma} - \frac{1}{2}\sum_{\sigma,\rho}{}'(q^{\sigma\rho}+\bar{p}^{\sigma\rho})\hat{p}^{\sigma\rho} - \frac{1}{2}\sum_{\sigma,\rho}{}' q^{\sigma\rho}\hat{q}^{\sigma\rho} \\
&\quad + \ln \mathrm{Tr}_{\{W^\sigma\}} \exp\left[\frac{1}{2}\sum_{\sigma,\rho}{}'\hat{q}^{\sigma\rho}W^{\sigma}W^{\rho}\right] \\
&\quad + \alpha' \ln \int \prod_{\sigma} \frac{\mathrm{d}x^{\sigma}\,\mathrm{d}\hat{x}^{\sigma}}{2\pi} \exp\left[-\beta\sum_{\sigma}\Theta(-x^{\sigma}) + \mathrm{i}\sum_{\sigma}\hat{x}^{\sigma}x^{\sigma}\right. \\
&\quad \left. -\frac{1}{2}\sum_{\sigma}(1+2\pi\bar{Q}^{\sigma})(\hat{x}^{\sigma})^{2} - \frac{1}{2}\sum_{\sigma,\rho}{}'\left(\frac{2}{\pi}\sin^{-1}q^{\sigma\rho} + \frac{2}{\pi}\bar{p}^{\sigma\rho}\right)\hat{x}^{\sigma}\hat{x}^{\rho}\right]
\end{aligned} \tag{12}$$

where $\sum'$ denotes the summation excluding the same indices. This equation holds for both binary and spherical weights. In fact, for spherical weights, we can eliminate the hatted order parameters and find $\mathcal{G}_0$ exactly, defined in equation (11), which is given in the next section. Some results in the following also hold independent of weights, and can be used in the study of binary weights, so we keep this rather general expression.

The hatted order parameters appear only in $\mathcal{G}_0$. Then two saddle-point equations can be obtained from vanishing derivatives of $\mathcal{G}_0$ with respect to $\hat{Q}^{\sigma}$ and $\hat{p}^{\sigma\rho}$

$$1+\bar{Q}^{\sigma} = 0 \tag{13}$$

$$q^{\sigma\rho}+\bar{p}^{\sigma\rho} = 0. \tag{14}$$

Strictly speaking, these are correct up to the zeroth order in $1/M$ and corrections could be obtained by examining the neglected term of $\mathcal{O}(M^{-1}\ln M)$. This result is interesting in that it is independent of the RSB scheme and the nature of the weights.

We now apply the 1RSB scheme for the order parameters. We write the corresponding relations to (13) and (14)

$$1+\bar{Q} = 0 \tag{15}$$

$$q_1+\bar{p}_1 = 0 \tag{16}$$

$$q_0+\bar{p}_0 = 0 \tag{17}$$

where q_1, $\bar{p}_1$ are elements in diagonal blocks and q_0, $\bar{p}_0$ are elements in off-diagonal blocks of the 1RSB order parameter matrices, $q^{\sigma\rho}$ and $\bar{p}^{\sigma\rho}$. Also, $\bar{Q}^{\sigma}$ is assumed to be independent of the replica, equal to $\bar{Q}$.

Let G_0 be $\mathcal{G}_0/n$ and G_r be $\mathcal{G}_r/n$. G_0 depends on the nature of weights. For spherical weights we find

$$\frac{G_0}{M} = \frac{1}{2} - \frac{1-m}{2m}\ln(1-q_1) + \frac{1}{2m}\ln(1-q_1+m(q_1-q_0)) + \frac{q_0}{2(1-q_1+m(q_1-q_0))}. \tag{18}$$

As well as the hatted order parameters, the overlaps between different hidden units are eliminated using (15)–(17).

We can find G_r, which is common to binary and spherical weights, as

$$\begin{aligned} G_r &= \ln(1-\mathrm{e}^{-\beta}) + \frac{1}{m}\int Dt_0 \ln \int Dt_1 [H(a_0t_0+a_1t_1) + (\mathrm{e}^{\beta}-1)^{-1}]^m \\ a_0 &= \left[\frac{(2/\pi)(\sin^{-1}q_0 - q_0)}{1-(2/\pi)-(2/\pi)(\sin^{-1}q_1-q_1)}\right]^{-\frac{1}{2}} \\ a_1 &= \left[\frac{(2/\pi)(\sin^{-1}q_1 - q_1 - \sin^{-1}q_0 + q_0)}{1-(2/\pi)-(2/\pi)(\sin^{-1}q_1-q_1)}\right]^{-\frac{1}{2}} \end{aligned} \tag{19}$$

where we use $Dt = (\mathrm{d}t/\sqrt{2\pi})\,\mathrm{e}^{-t^2/2}$ and $H(t) = \int_t^\infty Dx$. m is the size of diagonal blocks of the $n \times n$ 1RSB order parameter matrices. It goes to a value in $[0, 1]$ in the limit $n \to 0$ and gains the physical meaning of the probability of having overlap equal to q_0. The order parameters of overlaps between different hidden units are also eliminated. Now the free energy becomes a function of q_1 and q_0.

There is a simple solution, $q_1 = q_0 = 0$. One can see that both PS and RS hold, so that it is the solution for the PS phase. The PSB solution is supposed to have non-zero q_1. Note that q_0 appears in the form of $\sin^{-1}q_0 - q_0$. Then we find that $q_0 = 0$ is always possible, so a PSB solution has $q_1 > 0$ and $q_0 = 0$. RS is broken in this solution. There is another PSB solution where $q_1 > q_0 > 0$. This solution is only possible for relatively large α', compared to the former PSB solution.

A phase transition takes place at $\alpha' = \alpha'_1$ from the PS phase with $q_1 = q_0 = 0$ to the PSB phase with $q_1 > 0$ and $q_0 = 0$. We can see that PSB and RSB occur simultaneously. The second phase transition from this PSB phase to another PSB phase with $q_1 > q_0 > 0$ occurs at $\alpha' = \alpha'_2$. Recently Urbanczik found $\alpha'_1 \simeq 4.91$ and $\alpha'_2 \simeq 15.4$ [15]. The machine reaches its maximal storage capability in the last PSB phase. In this phase both q_1 and q_0 go to one for large α'. One might think that the solution recovers RS; however, we find

$$1-q_1 \sim \frac{m^2}{\alpha'^8} \qquad 1-q_0 \sim \frac{1}{\alpha'^2} \qquad -\ln m \sim \frac{1}{\alpha'^2} \tag{20}$$

as $\alpha' \to \infty$. We can observe $1-q_0 \gg 1-q_1$, showing the difference from the RS solution. However, this only implies $\alpha'_\mathrm{c} \to \infty$. We need a more accurate method to find the dependence of α'_c on M in the limit of large M.

4. Asymptotic calculation of storage capacities

As α' gets close to α'_c, $1-q_1$ and $1-q_0$ become very small. As seen in (15)–(17), other small quantities include $1+\bar{Q}$, $q_1+\bar{p}_1$, and $q_0+\bar{p}_0$, but they are found to vanish only in the leading order. Fortunately, we only need to deal with small quantities, which makes the following asymptotic calculation tractable. It is possible to estimate α_c in the limit of large

M by investigating the asymptotic behaviour of these small quantities. For convenience we use the following notations:

$$w = 1 + \bar{Q} - q_1 - \bar{p}_1 \tag{21}$$

$$v_1 = q_1 + \bar{p}_1 \tag{22}$$

$$v_0 = q_0 + \bar{p}_0 \tag{23}$$

with $w' = w/M$, $v_1' = v_1/M$, and $v_0' = v_0/M$. Avoiding the cumulant expansion, we integrate over u^σ and $\hat{u}^\sigma$ in (4) and obtain

$$\begin{aligned}
mG_r &= \int Dz_0 \int \prod_j Dt_{0j} \ln\left[\sum_{\{\eta_j=\pm1\}} \int Dz_1 \int_0^\infty \prod_j Dt_{1j} A^m\right] \\
A &= \sum_{\{\tau_j=\pm1\}} \Theta\left(\sum_j \tau_j\right) \int Du \prod_j H\left[\left[\frac{q_1 - q_0 - (v_1' - v_0')}{1 - q_1 - w'}\right]^{\frac{1}{2}} \tau_j \eta_j (t_{1j} + s_j)\right. \\
&\quad \left. + \left[\frac{1 - q_1 - w}{1 - q_1 - w'}\right]^{\frac{1}{2}} \frac{\mathrm{i}}{\sqrt{M}} u \tau_j\right] \\
s_j &= \left[\frac{q_1 - q_0 - (v_1 - v_0)}{q_1 - q_0 - (v_1' - v_0')}\right]^{\frac{1}{2}} \frac{\mathrm{i}}{\sqrt{M}} \eta_j z_1 + \left[\frac{q_0 - v_0'}{q_1 - q_0 - (v_1' - v_0')}\right]^{\frac{1}{2}} \eta_j t_{0j} \\
&\quad + \left[\frac{q_0 - v_0}{q_1 - q_0 - (v_1' - v_0')}\right]^{\frac{1}{2}} \frac{\mathrm{i}}{\sqrt{M}} \eta_j z_0.
\end{aligned} \tag{24}$$

As α goes to α_c, we assume the following scaling

$$1 - q_1 - w' = \frac{m}{c} \qquad w = \frac{m}{d} \tag{25}$$

with $m \to 0$, $1/c \to 0$, $1/d \to 0$. A similar scaling for q_1, $1 - q_1 = m/c$, was used in the previous study of the storage capacity of the NRF parity machine [8]. We can shift to the case of the NRF machine by simply setting $v_1 = v_0 = 0$, erasing the integrations over z_1 and z_0, and replacing α' by α. We also assume the form $1 - q_1 = m/c$ in the NRF case.

G_0 can be found exactly in the case of spherical weights, and is given by

$$\begin{aligned}
2m\frac{G_0}{M} &= \ln(1 + c(1 - q_0 - (v_1' - v_0'))) + \frac{1}{M}\ln(1 + d(v_1 - v_0)) \\
&\quad + \frac{c(q_0 - v_0')}{1 + c(1 - q_0 - (v_1' - v_0'))} + \frac{dv_0}{M(1 + d(v_1 - v_0))}.
\end{aligned} \tag{26}$$

In the limit of large c we expand G_r as

$$mG_r = f^{(0)} + f^{(1)} \tag{27}$$

where $f^{(0)}$ and $f^{(1)}$ are of the zeroth and the first order, respectively, in $1/\sqrt{c}$. Technical steps for the computation of $f^{(0)}$ and $f^{(1)}$ are presented in detail in the appendix, and the resultant forms are given in (A17) and (A24).

Then we keep only terms relevant for saddle-point equations in $f^{(0)}$ and $f^{(1)}$. We use $H(x) \to (\sqrt{2\pi}x)^{-1}\,\mathrm{e}^{-x^2/2}$ for large x. From (A17), we find

$$f^{(0)} \simeq -\frac{1}{4}\frac{(2/\pi)\sin^{-1}(Q_0'/(1 + Q_0')) - (2/\pi)(Q_0/(1 + Q_0'))}{1 - (2/\pi)\sin^{-1}(Q_0'/(1 + Q_0')) - (2/\pi)(W^2/(1 + Q_0'))} \tag{28}$$

where Q_0', Q_0 and W are given in equations (A2)–(A4). In $f^{(1)}$, we can keep only terms relevant for saddle-point equations for c and d. From equation (A24), we find

$$f^{(1)} \simeq \sqrt{\frac{M(1-(2/\pi))}{2\pi}}\sqrt{\frac{1+(c/Md)}{c}}\frac{1}{1-(2/\pi)\sin^{-1}(Q_0'/(1+Q_0'))}. \tag{29}$$

Now the free energy is given by

$$-\frac{\beta F}{MN} = \frac{G_0}{M} + \frac{\alpha'}{m}(f^{(0)} + f^{(1)}). \tag{30}$$

The five saddle-point equations are obtained from the stationary condition of F with respect to c, d, $1 - q_0 - (v_1' - v_0')$, $v_1 - v_0$ and v_0.

Solving the saddle-point equations, we find the following result:

$$c \simeq \frac{(\pi-2)^3}{2048}M\alpha'^4 \tag{31}$$

$$d \simeq c \tag{32}$$

$$v_1 - v_0 = q_1 + \bar{p}_1 - q_0 - \bar{p}_0 \simeq \frac{32}{\pi-2}\frac{1}{M\alpha'^2} \tag{33}$$

$$v_0 = q_0 + \bar{p}_0 \simeq \frac{\pi-2}{M\alpha'} \tag{34}$$

$$1 - q_0 - (v_1' - v_0') = \frac{128}{(\pi-2)^2}\frac{1}{\alpha'^2}. \tag{35}$$

An additional equation comes from the condition that $\partial F/\partial m = 0$ as $m \to 0$. This yields $-m\beta F/MN \to 0$, then we have

$$0 \simeq \ln(1 + c(1 - q_0 - (v_1' - v_0'))) + \frac{1}{1 - q_0 - (v_1' - v_0')} - \alpha'\frac{\pi-2}{4\sqrt{2}}\frac{1}{\sqrt{1 - q_0 - (v_1' - v_0')}}. \tag{36}$$

This gives the asymptotic value α_c of the storage capacity per input unit

$$\alpha_c \simeq \frac{8\sqrt{2}}{\pi-2}M\sqrt{\ln M}. \tag{37}$$

The shift to the NRF case can be made easily by replacing $\pi - 2$ by π and α' by α in the above result. Therefore we have:

$$c \simeq \frac{\pi^3}{2048}M\alpha^4 \tag{38}$$

$$1 - q_0 \simeq \frac{128}{\pi^2}\frac{1}{\alpha^2} \tag{39}$$

$$\alpha_c \simeq \frac{8\sqrt{2}}{\pi}\sqrt{\ln M}. \tag{40}$$

The storage capacities per weight are given by α_c/M from (37) for the ORF machine, and by α_c in (40) for the NRF machine. These values are smaller than the mathematical bound $\sim \ln M$ obtained by Mitchison and Durbin.

5. Discussion

Despite their almost identical values of storage capacity per weight, the weight space structures are quite different in the two machines. For the ORF machine there are three phases with two transitions. For $\alpha' < \alpha'_1$, there is the PS phase with the RS solution. For $\alpha'_1 < \alpha' < \alpha'_2$, there is the PSB phase with RSB solution where $q_1 > q_0 = 0$. For $\alpha' > \alpha'_2$ there is another PSB phase, with a different RSB solution where $q_1 > q_0 > 0$. In this last phase the number of patterns reaches its maximal value, that is, the storage capacity. On the other hand, for the NRF machine there is only one phase transition, from the RS phase to the RSB phase.

In a usual spin-glass phase, q_0 becomes smaller as q_1 gets closer to one; this means that the distance between islands or valleys becomes greater as the volume of each island shrinks. In this study we find that both q_1 and q_0 go to one, although q_1 approaches one much faster, and this property is common to both machines. We might give a partial explanation for this rather unusual phenomenon by supposing the following landscape picture in the weight space. Let us imagine a group of islands in the weight space. As each island shrinks, the distances between islands also decrease. This is possible when the overall boundary surrounding the islands is contracting.

Monasson and Zecchina (MZ) proposed an interesting formalism [16] different from the conventional Gardner method, which can analyse the weight space structure and the internal representations. From the RS calculation, they reproduced the known result for the NRF parity machine [8] and obtained a new result for the NRF committee machine. For the parity machine, they showed that the RS solution is marginally stable in the limit of infinite M [17], while it is unstable for a finite M where the 1RSB solution appears. They expected that the RS solution in their approach becomes exact asymptotically as M grows. This new approach is fascinating in that it only relies on the relatively simple RS calculation, compared to the complicated RSB calculation in the conventional approach as carried out in this paper. It also seems to take into account the disconnected structure of the weight space in the RS ansatz, which was seen in the numerical simulations on binary parity machine [18]. An interesting variant from the weight space to the coupling (output) space was made for the combined theory of the Vapnik–Chervonenkis dimension and the storage capacity [19].

However, we find a little discrepancy of our results with what they found. Their value of α_c is larger by a factor $\sqrt{2}$, i.e. $\alpha_c \simeq (16/\pi)\sqrt{\ln M}$, than that in (40). Recently, we have applied the MZ approach to the ORF committee machine [20]. We have recently been informed that an equivalent work was also done independently by Urbanczik [21]. The result, $\alpha_c \simeq (16/(\pi - 2))M\sqrt{\ln M}$, also shows the same difference of the factor $\sqrt{2}$ with that in (37). At the present stage, the reason for this discrepancy is not clear since the two approaches have different formalisms. From the point of view of the Gardner approach, though the 1RSB solution is found where the RS solution is incorrect, it may not be exact. The stability test of the 1RSB solution or the pursuit of a higher-step RSB solution would be a very complicated task and has not been accomplished in our cases. The 1RSB calculation itself has been incomplete until our results. On the other hand, the RS solution in the MZ approach was found to be marginally stable for infinite M, though only shown explicitly for the NRF parity machine. It would be interesting to check whether the RSB solution that appears for finite M still exists as M increases.

We expect that the ORF committee machine with binary weights can also be studied. It can be observed $\alpha_c \sim \mathcal{O}(M)$. The result for the regime $\alpha \sim \mathcal{O}(M)$ in section 3 will be helpful, where many equations and properties also hold for binary weights. The reduction to the NRF case can also be made easily. The 1RSB solution also exists in this case. This study is now in progress.

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Appendix. Asymptotic expansion in the limit of large M

We use the following expressions to write equations in simpler forms

$$Q_0^* = 1 - q_0 - (v_1' - v_0') \tag{A1}$$

$$Q_0' = \frac{q_0 - v_0'}{1 - q_0 - (v_1' - v_0')} \tag{A2}$$

$$Q_0 = \frac{q_0 - v_0}{1 - q_0 - (v_1' - v_0')} \tag{A3}$$

$$W = \left[\frac{1 - q_0 - (v_1 - v_0)}{1 - q_0 - (v_1' - v_0')}\right]^{\frac{1}{2}} \tag{A4}$$

$$\tilde{c} = c\,\frac{1 - q_0 - (v_1' - v_0')}{1 + (c/Md)} \tag{A5}$$

$$\bar{t}_{0j} = t_{0j} + \frac{\mathrm{i}}{\sqrt{M}}\sqrt{\frac{Q_0}{Q_0'}}\,z_0. \tag{A6}$$

Note that $Q_0^* \to 0$, $Q_0' \to \infty$, $Q_0 \to \infty$, $W \to 1$ and $\tilde{c} \to \infty$. In the following calculations we assume $cQ_0^* \to \infty$, which can be justified self-consistently from the final result, given in (31) and (35). Then A in (24) is given by

$$A = \sum_{\{\tau_j = \pm 1\}} \Theta\left(\sum_j \tau_j\right) \int Du \prod_j H\left[\sqrt{\frac{cQ_0^*}{m}}\tau_j\eta_j\left(t_{1j} + \frac{1}{\sqrt{M}} W z_1 \eta_j + \sqrt{Q_0'}\,\bar{t}_{0j}\eta_j\right) + \frac{\mathrm{i}}{\sqrt{M}}\sqrt{1 - \frac{c}{d}}\,\tau_j u\right]. \tag{A7}$$

Expanding up to the order $1/\sqrt{c}$, G_r can be written as

$$mG_r = \int Dz_0 \int \prod_j Dt_{0j} \ln(I_m^{(0)} + I_m^{(1)}). \tag{A8}$$

$I_m^{(0)}$ is the dominant term, which is obtained from a partial sum in (24) over the η_j and the τ_j where $\sum_j \eta_j < 0$ and $\eta_j = -\tau_j$ for all j. Then $A^m \to 1$ as $m \to 0$ and $c \to \infty$. $I_m^{(1)}$ is of the first order in $1/\sqrt{c}$. It can be obtained from another partial sum where each term is given by the condition that $\eta_j = \tau_j = 1$ for one j and $\sum_{j'(\neq j)} \eta_{j'} = 0$, $\eta_{j'} = -\tau_{j'}$ for $j' \neq j$. In this case, $A^m \to \exp(-\tilde{c}t_{1j}^2/2)$, where the change of variables $t_{1j} + (\mathrm{i}/\sqrt{M})Wz_1\eta_j + \sqrt{Q_0'}\,\bar{t}_{0j}\eta_j \to t_{1j}$ is made. Then $f^{(0)}$ and $f^{(1)}$ in (27) are given by

$$f^{(0)} = \int Dz_0 \int \prod_j Dt_{0j} \ln(I_m^{(0)}) \tag{A9}$$

$$f^{(1)} = \int Dz_0 \int \prod_j Dt_{0j} \frac{I_m^{(1)}}{I_m^{(0)}}. \tag{A10}$$

Using the integral representation used in [10] for $\Theta(-\sum_j \eta_j)$, $I_m^{(0)}$ can be given by

$$I_m^{(0)} = \int_0^\infty \frac{d\lambda}{2\pi} \int dx\, e^{i\lambda x} \int Dz_1\, e^{\frac{1}{2}W^2 z_1^2} \left(\prod_j \sum_{\eta_j} e^{ix\eta_j} \int_{-\sqrt{Q_0'}\bar{t}_{0j}\eta_j}^\infty Dt_{1j}\, e^{(i/\sqrt{M})Wz_1\eta_j t_{1j}} \right). \tag{A11}$$

Following [10], the integrand is observed to be dominant near $x = 0$, so that we expand it up to the second order in x, assuming $x \sim \mathcal{O}(1/\sqrt{M})$. The integrations over the t_{1j} can also be carried out by the cumulant expansion up to the order $1/M$

$$\int_x^\infty Dt\, e^{-(i/\sqrt{M})Wz_1 t} = H(x) \exp\left[-\frac{i}{\sqrt{M}} Wz_1 \frac{\int_x^\infty Dt\, t}{H(x)} - \frac{W^2 z_1^2}{2M} \left(\frac{\int_x^\infty Dt\, t^2}{H(x)} - \left(\frac{\int_x^\infty Dt\, t}{H(x)} \right)^2 \right) \right]. \tag{A12}$$

As a result, we obtain

$$I_m^{(0)} = H\left[\frac{T}{\sqrt{1 - G - 4W^2 L^2}} \right]. \tag{A13}$$

In this equation

$$T = \frac{1}{\sqrt{M}} \sum_j (1 - 2H(\sqrt{Q_0'}\bar{t}_{0j}))$$
$$G = \frac{1}{M} \sum_j (1 - 2H(\sqrt{Q_0'}\bar{t}_{0j}))^2$$
$$L = \frac{1}{M} \sum_j H'(\sqrt{Q_0'}\bar{t}_{0j}) \tag{A14}$$

where $H'(t) = -e^{-t^2/2}/\sqrt{2\pi}$. Then $f^{(0)}$ can be obtained by the cumulant expansion for the integrations over the t_{0j}, equivalent to the central limit theorem. Integrating z_0 out, we have

$$f^{(0)} = \int \frac{dT\, d\hat{T}}{2\pi} e^{iT\hat{T} - (\hat{T}^2/2)(G - (2/\pi)(Q_0/(1+Q_0')))} \ln H\left[\frac{T}{\sqrt{1 - G - 4W^2 L^2}} \right]. \tag{A15}$$

Here G and L are replaced by averaged quantities

$$G = \langle (1 - 2H(\sqrt{Q_0'}t))^2 \rangle = \frac{2}{\pi} \sin^{-1}\left(\frac{Q_0'}{1 + Q_0'} \right)$$
$$L = \langle H'(\sqrt{Q_0'}t) \rangle = -\frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{1 + Q_0'}} \tag{A16}$$

where $\langle \cdots \rangle = \int Dt \ldots$. Integrating over $\hat{T}$ and changing the integral variable, we obtain

$$f^{(0)} = \int Dt \ln H\left[\left[\frac{(2/\pi)\sin^{-1}(Q_0'/(1 + Q_0')) - (2/\pi)(Q_0/(1 + Q_0'))}{1 - (2/\pi)\sin^{-1}(Q_0'/(1 + Q_0')) - (2/\pi)(W^2/(1 + Q_0'))} \right]^{\frac{1}{2}} t \right]. \tag{A17}$$

On the other hand, $I_m^{(1)}$ can be written by

$$I_m^{(1)} = \sum_j \sum_{\{\eta_{j'}, j' \neq j\}} \delta\left(\sum_{j'} \eta_{j'}, 0\right) \int Dz_1 \int_0^\infty \prod_{j''} \frac{\mathrm{d}t_{1j''}}{\sqrt{2\pi}} \times \exp\left[-\frac{1}{2}\tilde{c}t_{1j}^2 - \frac{1}{2}\sum_{j''(\neq j)}\left(t_{1j''} - \frac{\mathrm{i}}{\sqrt{M}} W z_1 \eta_{j''} - \sqrt{Q_0'}\bar{t}_{0j''}\eta_{j''}\right)^2\right] \tag{A18}$$

where $\delta(a, b)$ denotes the usual Kronecker delta function, δ_{ab}. Using (A13), $f^{(1)}$ can be given by

$$f^{(1)} = M \begin{pmatrix} M-1 \\ ((M-1)/2) \end{pmatrix} \int Dz_0 \int \prod_j Dt_{0j} H^{-1}\left[\frac{T}{\sqrt{1 - G - 4W^2L^2}}\right] \tilde{I}_m^{(1)} \tag{A19}$$

where

$$\tilde{I}_m^{(1)} \simeq \frac{1}{2\sqrt{\tilde{c}}} \int Dz_1\, \mathrm{e}^{(W^2/2)z_1^2 - \frac{1}{2}Q_0'\bar{t}_{0M}^2 - (\mathrm{i}/\sqrt{M})Wz_1\sqrt{Q_0'}\bar{t}_{0M}} \prod_{j=1}^{((M-1)/2)} \left(\int_{\sqrt{Q_0'}\bar{t}_{0j}}^\infty Dt\, \mathrm{e}^{-(\mathrm{i}/\sqrt{M})Wz_1 t}\right) \times \prod_{j=((M+1)/2)}^{M-1} \left(\int_{-\sqrt{Q_0'}\bar{t}_{0j}}^\infty Dt\, \mathrm{e}^{(\mathrm{i}/\sqrt{M})Wz_1 t}\right). \tag{A20}$$

Using (A12), $f^{(1)}$ can be written by

$$f^{(1)} = \frac{M}{2} \begin{pmatrix} M-1 \\ ((M-1)/2) \end{pmatrix} \frac{1}{\sqrt{\tilde{c}}} \frac{1}{\sqrt{1 + Q_0'}} \int Dz_0\, \mathrm{e}^{(Q_0/2Q_0')z_0^2} \int Dz_1 \int \frac{\mathrm{d}T\,\mathrm{d}\hat{T}}{2\pi} \int \frac{\mathrm{d}G\,\mathrm{d}\hat{G}}{2\pi} \times \int \frac{\mathrm{d}L\,\mathrm{d}\hat{L}}{2\pi} \int \frac{\mathrm{d}D\,\mathrm{d}\hat{D}}{2\pi} \int \frac{\mathrm{d}E\,\mathrm{d}\hat{E}}{2\pi}\, \mathrm{e}^{\mathrm{i}\tilde{T}T + \mathrm{i}\tilde{G}G + \mathrm{i}\tilde{L}L + \mathrm{i}\tilde{D}D + \mathrm{i}\tilde{E}E - \mathrm{i}Wz_1D - (W^2/2)Ez_1^2} \times H^{-1}\left[\frac{T}{\sqrt{1 - G - 4W^2L^2}}\right] \prod_{j=1}^{((M-1)/2)} \left(\int Dt\, H(\sqrt{Q_0'}t)\, \mathrm{e}^{S_+}\right) \times \prod_{j=((M+1)/2)}^{M-1} \left(\int Dt\, H(-\sqrt{Q_0'}t)\mathrm{e}^{S_-}\right) \tag{A21}$$

where

$$S_\pm = -\mathrm{i}\frac{\hat{T}}{\sqrt{M}}(1 - 2H(\sqrt{Q_0'}t)) - \mathrm{i}\frac{\hat{G}}{M}(1 - 2H(\sqrt{Q_0'}t))^2 - \mathrm{i}\frac{\hat{L}}{M}H'(\sqrt{Q_0'}t) \pm \mathrm{i}\frac{z_0}{\sqrt{M}}\sqrt{\frac{Q_0}{Q_0'}}t \mp \mathrm{i}\frac{\hat{D}}{\sqrt{M}} \frac{(1/\sqrt{2\pi})\,\mathrm{e}^{-(Q_0'/2)t^2}}{H(\pm\sqrt{Q_0'}t)} \mp \frac{\hat{E}}{M}\left(\frac{(1/\sqrt{2\pi})\sqrt{Q_0'}t\,\mathrm{e}^{-(Q_0'/2)t^2}}{H(\pm\sqrt{Q_0'}t)} \mp \left(\frac{(1/\sqrt{2\pi})\,\mathrm{e}^{-(Q_0'/2)t^2}}{H(\pm\sqrt{Q_0'}t)}\right)^2\right). \tag{A22}$$

We use the following cumulant expansion:

$$\int Dt\, H(\sqrt{Q_0'}t)\,\mathrm{e}^S \simeq \frac{1}{2}\exp\left(2\int Dt\, HS + \frac{1}{2}\left(2\int Dt\, HS^2 - \left(2\int Dt\, HS\right)^2\right)\right) \tag{A23}$$

where $\int Dt\, H(\sqrt{Q_0'}t) = 1/2$ is used. The remaining calculation of $f^{(1)}$ is involved, but can be done by the successive Gaussian integrations. Some important integrals involving $H(\sqrt{Q_0'}t)$ are as follows: $2\int Dt\, H(1-2H)^2 = \int Dt(1-2H)^2 = G$, $2\int Dt\, H(1-2H) =$

$-G$, $\int Dt\, HH' = L$, $2\int Dt\, Ht^2 = 1$, $2\int Dt\, Ht = -2\int Dt\, H(1-2H)t = 2\sqrt{Q_0'}L$, where G and L are given in (A16). Using the Stirling formula to find

$$\binom{M-1}{((M-1)/2)} \simeq 2^M/\sqrt{2\pi M}$$

we finally obtain

$$f^{(1)} = \left[\frac{M}{2\pi\tilde{c}(1+Q_0')}\right]^{\frac{1}{2}} [(1+2W^2E)(1-G)-4W^2L]^{-\frac{1}{2}} \int \frac{\mathrm{d}t}{\sqrt{2\pi}}$$
$$\times H^{-1}\left[\left[\frac{G-4L^2Q_0}{1-G-4W^2L^2}\right]^{\frac{1}{2}} t\right]$$
$$\times \exp\left[-\frac{1}{2}\frac{(1-4L^2B)(1+2W^2E)-4W^2L^2}{(1+2W^2E)(1-G)-4W^2L^2}t^2\right] \qquad \text{(A24)}$$

where $E = \pi^{-1}\int Dt\, \mathrm{e}^{-Q_0't^2} H^{-1}(\sqrt{Q_0'}t)$.

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