

Storage capacity of correlated perceptrons

D. Malzahn, A. Engel, and I. Kanter*

Institut für Theoretische Physik, Otto-von-Guericke-Universität
Universitätsplatz 2, Postfach 4120, D-39106 Magdeburg, F. R. Germany

*Department of Physics, Bar Ilan University, Ramat Gan, 52100, Israel

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Abstract

We consider an ensemble of K single-layer perceptrons exposed to random inputs and investigate the conditions under which the couplings of these perceptrons can be chosen such that prescribed correlations between the outputs occur. A general formalism is introduced using a multi-perceptron costfunction that allows to determine the maximal number of random inputs as a function of the desired values of the correlations. Replica-symmetric results for $K = 2$ and $K = 3$ are compared with properties of two-layer networks of tree-structure and fixed Boolean function between hidden units and output. The results show which correlations in the hidden layer of multi-layer neural networks are crucial for the value of the storage capacity.

1 Introduction

One of the central tasks in the field of statistical mechanics of neural networks is a deeper understanding of the information processing abilities of multi-layer feed-forward networks (MLN). After a thorough analysis of the single-layer perceptron it soon became clear that the very properties that entail the larger computational power of MLN also make their theoretical description within the framework of statistical mechanics much harder. Even the simplest case with just one hidden layer containing much less units than the input layer and with a pre-wired Boolean function from the hidden layer to the output has proven to be rather complicated to analyze exactly [3, 4, 5, 6]. It is therefore important to develop useful and reliable approximate methods to study these practically important systems. For the characterization of the generalization ability *bounds* for the performance parameters have been shown to yield useful orientations [7, 8]. For the storage capacity, i.e. the typical maximal number of random input-output mappings that can be implemented by the network only rather crude bounds exist so far, and these are independent of the hidden-to-output mapping ([9]).

Let us start the discussion with a number of general open questions regarding the capacity of MLN. These questions, although only partially answered in the present work, may serve as a call for further investigation by the community of the statistical mechanics of neural networks.

Correlations among the hidden units: The increased computational power of MLN stems from the possibility that the different subperceptrons between input and hidden layer can all operate in the region beyond their storage capacity. The occurring errors typical of this regime can be compensated by other subperceptrons. However, this “division of labour” only works appropriately if the errors do not occur for all subperceptrons in *the same* patterns. Hence intricate correlations depending on the hidden to output

mapping develop in the hidden layer when the number of input-output pairs increases [14]. This qualitative picture has already been used to propose and analyze a learning algorithm for a special MLN, the parity-machine [15]. It has been observed for some time that the organization of internal representations described by these correlations is crucial for the understanding of the storage and generalization abilities of MLN [3, 10, 11, 12, 13].

The approximation suggested in this work is to replace “*division of labour*” by “*average division of labour*”. An approximate treatment of a MLN becomes possible if one does not require a definite mapping from the hidden layer to the output but instead prescribes the values for the correlations, i.e. the *average* relation between the hidden units and the output and also among the different hidden units themselves. The task is then to determine how many random inputs can be implemented by a set of K perceptrons, such that the outputs show definite correlations.

Interplay between correlations and the capacity: This approach will highlight which type of correlations is easy to implement and which is difficult, i.e. reduce the storage capacity significantly. It is already known that increasing the average correlation between each one of the hidden units and the desired output decreases the capacity. This result can be exemplified by the following well known limits. The lowest capacity is achieved for hidden units which are fully correlated with the desired outputs. In this case there is no division of labour and the MLN shrinks to a simple perceptron. The other limit is the parity machine, in which the correlation between each hidden unit and the output is zero. In this case the upper bound for the capacity of MLN with one hidden layer is achieved. Nevertheless, the general framework of how the capacity depends on the correlations between the output and a *partial set* of the hidden units is still unknown. The main problem is that with increasing K there is a trade-off between a more flexible division of labour and an increasing complexity of possible correlations.

Possible scaling for the capacity: Of particular interest is the limit of an infinite number K of hidden units for which only few analytical results are known. For the AND machine the capacity is of $O(1)$ [10], whereas for the committee-machine and the parity machine the capacity is of order $(\log K)^\delta$, with $\delta = 1/2$ [13] and 1 [4], respectively. These results may suggest one of the following two possible scenarios: In the first scenario, the capacity varies continuously as a function of the hidden/output correlations. Any $0 \leq \delta \leq 1$ can be found, depending on the correlations. In the second possible scenario, $\delta = 1$ holds for the parity machine only, and all other hidden/output correlations result in a δ with a finite distance from 1.

Space of possible correlations: The simultaneous prescription of correlations involving several hidden units has to take into account that not all combinations of correlations are possible since they all derive from a common probability distribution. The question of whether there are forbidden combinations of correlations and what is their measure, will be partially answered in the following discussion.

The paper is organized as follows. Section 2 sets the task and fixes the notations. In section 3 the formalism is presented which is a generalization of the canonical phase space method developed by Gardner and Derrida [18] for the single-layer perceptron. Section 4 contains general results for an arbitrary number K of perceptrons with a special subset of fixed correlations. In sections 5 and 6 we study in detail the situations of $K = 2$ and $K = 3$ perceptrons respectively and compare the results with those known for tree-structured MLN with the same number of hidden units. Finally, section 7 comprises our conclusions.

2 The storage problem for correlated perceptrons

We consider K spherical perceptrons with N/K inputs, one output, and couplings $\mathbf{J}_k \in \mathbb{R}^{N/K}$, $\mathbf{J}_k \mathbf{J}_k = N/K$ with $k = 1, \dots, K$. Moreover we choose a set of $(\alpha N)K$ random inputs $\xi_k^\nu \in \mathbb{R}^{N/K}$ and one overall random output $\sigma^\nu = \pm 1$ with $\nu = 1, \dots, \alpha N$. The total number of random input and output bits is

hence $\alpha N(N + 1)$ and the number of adjustable weights is N as for the standard perceptron and for multilayer networks with tree-structure and fixed Boolean function between hidden units and output.

The outputs of the K perceptrons are given by

$$\tau_k^\nu = \text{sgn} \left(\sqrt{\frac{K}{N}} \mathbf{J}_k \boldsymbol{\xi}_k^\nu \right) \quad (1)$$

Our aim is to determine the critical number $\alpha_c N$ of patterns for which coupling vectors \mathbf{J}_k exist such that the averages

$$\begin{aligned} c_1 = \langle \tau_k \sigma \rangle &= \frac{1}{\alpha N} \sum_\nu \tau_k^\nu \sigma^\nu \\ c_2 = \langle \tau_k \tau_l \sigma \rangle &= \frac{1}{\alpha N} \sum_\nu \tau_k^\nu \tau_l^\nu \sigma^\nu \\ c_3 = \langle \tau_k \tau_l \tau_m \sigma \rangle &= \frac{1}{\alpha N} \sum_\nu \tau_k^\nu \tau_l^\nu \tau_m^\nu \sigma^\nu \\ &\vdots \\ c_K = \langle \tau_1 \cdots \tau_K \sigma \rangle &= \frac{1}{\alpha N} \sum_\nu \tau_1^\nu \cdots \tau_K^\nu \sigma^\nu \end{aligned} \quad (2)$$

$$(3)$$

have prescribed values c_1, c_2, \dots, c_K . This can be seen as a generalization of the program of Gardner and Derrida [18] who considered only one perceptron, i.e. $K = 1$, and determined α_c in dependence on the fraction of errors f_{GD} related to c_1 by $c_1 = 1 - 2f_{GD}$. The new aspect of the present investigation is that not only the correlation of each individual output τ_k with σ but also the correlation between different τ_k is taken into account.

As usual we assume that the components of the input patterns $\boldsymbol{\xi}_k^\nu$ as well as the overall outputs σ^ν are independent random variables with zero mean and unit variance. The transformation $\boldsymbol{\xi}_k^\nu \rightarrow \sigma^\nu \boldsymbol{\xi}_k^\nu$ then preserves the statistical properties of the inputs. In the following we therefore take $\sigma^\nu = 1$ for all $\nu = 1, \dots, \alpha N$ without loss of generality.

Note that due to the independence of the inputs at different perceptrons all outputs τ_k have identical statistical properties. Therefore the correlations c_m as defined in (2) do not depend on the particular subset of hidden units for which they are calculated. This corresponds to the permutation symmetry between hidden units in MLN with appropriate decoder functions ([4, 5, 6]).

It is in particular interesting to enforce correlations c_m that are identical to those which develop spontaneously in MLN with special Boolean functions between hidden layer and output. It has recently been shown how these correlations can be calculated from the joint probability distribution of the stabilities at the hidden units [14]. For the parity machine with K hidden units one finds $c_m = 0$ for $m < K$ and $c_K = 1$. For the committee machine the expressions are more complicated, for $K = 3$ one finds $c_1 = 5/12, c_2 = -1/6, c_3 = -3/4$.

3 Formalism

To analyze the storage abilities of correlated perceptrons we use a generalization of the formalism introduced by Gardner and Derrida [18]. A well suited form for our purposes is the one proposed by Griniasty

and Gutfreund [19]. We are hence led to introduce a *multiperceptron cost function* [20]

$$E(\mathbf{J}_1, \dots, \mathbf{J}_K) = \sum_{\nu} V(\tau_1^{\nu}, \dots, \tau_K^{\nu}) \quad (4)$$

$$= \sum_{\nu} \left[-\sum_k \tau_k^{\nu} + \mu_2 \sum_{(k,l)} \tau_k^{\nu} \tau_l^{\nu} + \mu_3 \sum_{(k,l,m)} \tau_k^{\nu} \tau_l^{\nu} \tau_m^{\nu} + \dots + \mu_K \tau_1^{\nu} \dots \tau_K^{\nu} \right]. \quad (5)$$

The parameters μ_m play the role of chemical potentials determining the costs for a violation of the constraints on the correlations c_m . Our aim is to characterize the coupling vectors \mathbf{J}_k that minimize $E(\mathbf{J}_1, \dots, \mathbf{J}_K)$ and to find the critical threshold α_c for the number of inputs for which no couplings $(\mathbf{J}_1, \dots, \mathbf{J}_k)$ exist that realize the desired correlations. This can be done by calculating the free energy

$$f(\alpha, \beta, \mu_2, \dots, \mu_K) = - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \langle \log \int \prod_{k=1}^K d\mu(\mathbf{J}_k) \exp(-\beta E(\mathbf{J}_1, \dots, \mathbf{J}_K)) \rangle \quad (6)$$

where $\langle \dots \rangle$ denotes the quenched average over the inputs and $d\mu(\mathbf{J}) = (2\pi e)^{-N/2K} \prod_{i=1}^{N/K} dJ_i \delta(\sum_{i=1}^{N/K} J_i^2 - N/K)$ is the usual integration measure for spherical perceptrons. Then

$$g(\alpha_c, \mu_2, \dots, \mu_K) = \lim_{\beta \rightarrow \infty} f(\alpha, \beta, \mu_2, \dots, \mu_K) \quad (7)$$

gives the typical minimum of $E(\mathbf{J}_1, \dots, \mathbf{J}_K)$. The limit $\beta \rightarrow \infty$ corresponds to the saturation limit $\alpha \rightarrow \alpha_c$. The values $c_m^{(s)}$ of the correlations c_m defined in eq.(2) in this saturation limit are from (4, 6) given by

$$\frac{1}{\alpha_c} g(\alpha_c, \mu_2, \dots, \mu_K) = -K c_1^{(s)} + \mu_2 \binom{K}{2} c_2^{(s)} + \dots + \mu_K c_K^{(s)} \quad (8)$$

$$\frac{1}{\alpha_c} \frac{\partial g(\alpha_c, \mu_2, \dots, \mu_K)}{\partial \mu_k} = \binom{K}{k} c_k^{(s)} \quad k = 2, \dots, K \quad (9)$$

Inverting these equations we find the saturation values α_c and $\mu_m^{(s)}$ as functions of c_1, \dots, c_K which is what we were looking for.

The calculation of $g(\alpha_c, \mu_2, \dots, \mu_K)$ proceeds along similar lines as for the single perceptron case studied in [19]. Within replica symmetry one has to introduce an order parameter q characterizing the typical overlap between two coupling vectors that contribute significantly to the free energy (6). In the limit $\beta \rightarrow \infty$ it is convenient to replace this order parameter by $x = \beta(1 - q)$. If the minimum of the costfunction is not degenerated we will find $q \rightarrow 1$ for $\beta \rightarrow \infty$ with x remaining of order 1. Qualitatively x describes the steepness of the minimum of the costfunction. The smaller x the fewer couplings contribute significantly to the free energy for large β , i.e. the steeper the minimum of the costfunction. Accordingly $x = \infty$ correspondes to a degenerated minimum since $q \neq 1$ even for $\beta \rightarrow \infty$.

For all choices of the parameters μ_m there is a minimum $V_{min} = \min_{\{\tau_k\}} V(\tau_1, \dots, \tau_K)$ of $V(\tau_1, \dots, \tau_K)$ and hence $\alpha N V_{min}$ is a lower bound for the costfunction $E(\mathbf{J}_1, \dots, \mathbf{J}_K)$. Now consider the subset of $\{\tau_k\}$ -configurations that realize V_{min} and calculate the correlations c_m for this subset. The resulting values for the c_m are special in two respects. First the value of α_c corresponding to them will occur for $x = \infty$ since the minimum of E is degenerated for $\alpha < \alpha_c$. Second exactly these values of c_m will occur in a MLN with that Boolean function between hidden layer and output that maps all the $\{\tau_k\}$ -configurations that realize V_{min} on the output +1. Consequently MLN with K hidden units and fixed Boolean function between

hidden layer and output will show up as “pure cases” defined by $x = \infty$ at α_c in our analysis and all situations with $x < \infty$ can be interpreted as these pure cases above saturation. Changing the parameters μ_m or equivalently the prescribed values of the c_m will hence induce continuous transformations between the different possible MLN.

The main steps of the formal analysis are sketched in appendix A. The final result reads (cf. (30)(31))

$$g(\alpha_c, \mu_2, \dots, \mu_k) = -\min_x \left[\frac{1}{2x} - \alpha_c \int \prod_k Dt_k F(x, t_k) \right] \quad (10)$$

where

$$F(x, t_k) = \min_{\lambda_1, \dots, \lambda_K} \left[\frac{1}{2x} \sum_k (\lambda_k - t_k)^2 + V(\text{sgn}(\lambda_1), \dots, \text{sgn}(\lambda_K)) \right] \quad (11)$$

and $Dt = \exp(-t^2/2)dt/\sqrt{2\pi}$.

The minimization in (11) is non-trivial. The quadratic terms in (11) are smallest for $\lambda_k^0 = t_k$. They compete with the step functions in $V(\text{sgn}(\lambda_1), \dots, \text{sgn}(\lambda_K))$ giving rise to discontinuous jumps in F whenever one λ_k crosses zero. Closer inspection shows that for the global minimum one has

$$\lambda_k^0 = t_k \text{ or } \lambda_k^0 = \begin{cases} 0^+ & \text{if } t_k < 0 \\ 0^- & \text{if } t_k > 0 \end{cases} \quad (12)$$

The saddlepoint equation which determines x can be written in the form

$$\frac{1}{\alpha_c} = \int \prod_k Dt_k \sum_k (\lambda_k^0 - t_k)^2 \quad (13)$$

Note that in this equation only those regions in the gaussian integrals contribute for which $\lambda_k^0 \neq t_k$.

4 General results for prescribed highest and lowest correlation

Of particular interest is the case in which only the values of c_1 and c_K are prescribed, i.e. $\mu_2 = \mu_3 = \dots \mu_{K-1} = 0$ in the costfunction (4). It describes the interpolation between individual perceptrons ($\mu_K = 0$) and the parity machine ($\mu_K \rightarrow \pm\infty$) which is known to saturate the asymptotic upper bound $\alpha_c = \log K / \log 2$ for the storage capacity for large K [4]. This special case is also sufficient to discuss the relation with the most important tree-structured MLN for $K = 2$ and $K = 3$. Moreover the necessary algebra simplifies somewhat.

Let us first note that the correlation coefficients c_1 and c_K are not independent of each other. It is hence not possible to prescribe arbitrary values for them. According to their definition (2,3) we have always $c_1, c_K \in (-1, +1)$. Moreover it is sufficient to consider positive values of c_1 only which is guaranteed by the structure of the costfunction (4). Finally the relation

$$c_K \geq Kc_1 - (K - 1) \quad (14)$$

must hold. It is a consequence of the obvious observation that the difference between c_1 and c_K is maximal if for every pattern at most one perceptron has negative output which corresponds to the equality sign in (14).

To perform the detailed analysis we denote μ_K simply by μ to get

$$E(\mathbf{J}_1, \dots, \mathbf{J}_K) = \sum_{\nu} \left[-\sum_k \tau_k^{\nu} + \mu \prod_k \tau_k^{\nu} \right]. \quad (15)$$

Accordingly eq.(11) simplifies to

$$F(x, t_k) = \min_{\lambda_1, \dots, \lambda_K} \left[\frac{1}{2x} \sum_k (\lambda_k - t_k)^2 - \sum_k \text{sgn}(\lambda_k) + \mu \text{sgn}(\lambda_1 \lambda_2 \dots \lambda_K) \right]. \quad (16)$$

In appendix B the following expressions for the correlation coefficients c_1 and c_K are derived:

$$c_1 = 1 - 2H(2\sqrt{x}) - \left[f_1(|\mu|, x, 0) - f_2(|\mu|, x, 0) \right] \quad (17)$$

$$c_K = 2^K [1/2 - H(2\sqrt{x})]^K - K \text{sgn}(\mu) \left[f_1(|\mu|, x, 0) + f_2(|\mu|, x, 0) \right] \quad (18)$$

Moreover the saddlepoint equation fixing x can be transformed into

$$\frac{1}{K \alpha_c} = \frac{1}{2} - H(2\sqrt{x}) - 2\sqrt{x} \frac{e^{-2x}}{\sqrt{2\pi}} + \frac{1}{2} \left[f_1(|\mu|, x, 1) + f_2(|\mu|, x, 1) \right]. \quad (19)$$

As usual we have used the abbreviation $H(x) = \int_x^{\infty} Dt$. $f_1(|\mu|, x, L)$ and $f_2(|\mu|, x, L)$ (with $L = 0, 1$) are integrals over sums of products of error functions explicitly given in appendix B. The final analysis of these equations has to be done numerically.

As discussed in the last section it is of particular interest to find the correlations c_1 and c_K for which $x = \infty$ at α_c . From eqs.(17)-(19) and (39)-(42) we find the following results

	μ	$c_1(x = \infty)$	$c_K(x = \infty)$	$1/\alpha_c(x = \infty)$
I	$\mu < 1$	1	1	$K/2$
II	$\mu = 1$	$1 - 2/K + 1/2^{(K-1)}K$	$-1 + 1/2^{(K-1)}$	$K/2 - K \int_{-\infty}^0 Dt t^2 [H(t)]^{K-1}$
III	$\mu > 1$	$1 - 2/K$	-1	$K/2 - K \int_0^{\infty} Dt t^2 ([H(-t)]^{K-1} - [H(t)]^{K-1})$

Table 1: *Correlation coefficients and storage capacity for an ensemble of K perceptrons in the pure cases characterized by $x = \infty$ (see text).*

Note that all three pairs $(c_1, c_K)|_{(x=\infty)}$ lie on the line given by (14), in fact (I) and (III) are the endpoints of this line.

It is at first sight surprising that the parity machine does not occur in table (1). However from the structure of the cost-function (15) it is clear that the internal representations of the parity function realize V_{min} only in the limit $\mu \rightarrow \pm\infty$. For finite $|\mu|$ the first term in (15) suppresses configurations with more than one negative output and gives rise to case (I) or (III).

5 $K = 2$

The simplest case to apply the above concepts is provided by two perceptrons with $N/2$ inputs each corresponding to $K = 2$. The only relevant correlations are c_1 and c_2 (see eqs.(2,3)). The relative importance of these in the cost-function (15) is regulated by μ .

Solving (19) numerically for the case $K = 2$ we find $c_1(\alpha_c, \mu)$ and $c_2(\alpha_c, \mu)$ from eqs.(17,18) and inverting these dependencies we arrive at $\alpha_c(c_1, c_2)$.

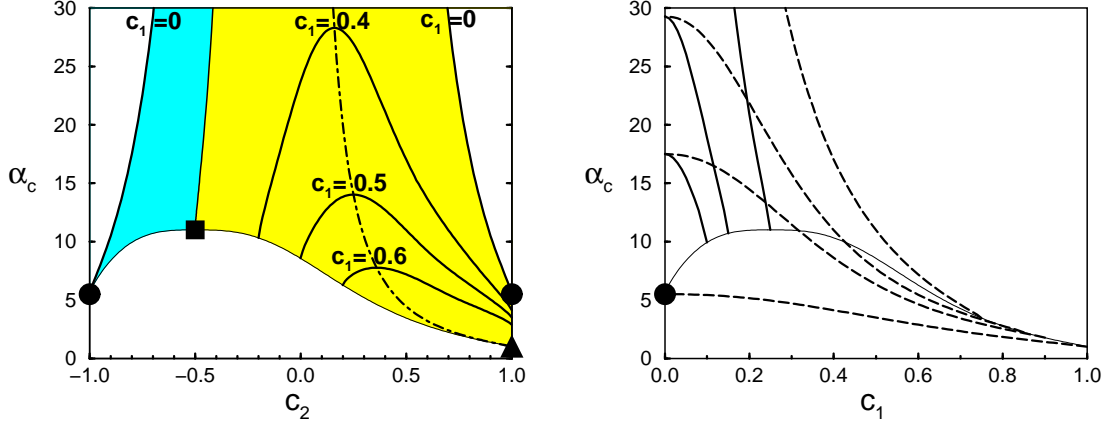


Figure 1: **Storage capacity $\alpha_c(c_1, c_2)$ for $K = 2$ correlated perceptrons.**

Left: $\alpha_c(c_2)$ for $c_1 = 0, 0.4, 0.5$ and 0.6 . Outside the shaded areas no solutions exist, dark shade corresponds to $\mu > 1$ light shade to $\mu < 1$. The dashed-dotted line ($\mu = 0$) gives the location of the maxima. The symbols denote the pure cases corresponding to the MLN summarized in table 2.

Right: $\alpha_c(c_1)$ for (from bottom to top): $c_2 = 1, 0.8, 0.7$, and 0.5 (dashed) and $c_2 = -0.8, -0.7$ and -0.5 (full). The lines end at the thin line given by $c_2 = 2c_1 - 1$. The symbol corresponds to the parity machine.

In fig.1(left) the dependence of α_c on c_2 for several values of c_1 is shown. Solutions exist only inside the shaded areas the boundaries of which correspond to $c_1 = 0$ and $c_2 = 2c_1 - 1$ respectively (cf.(14)). The maxima of $\alpha_c(c_2)$ at constant c_1 occur for the uncorrelated system $\mu = 0$ implying $c_2 = c_1^2$ as expected since an additional constraint on c_2 can only reduce α_c . The values of $\alpha_c(c_1, c_1^2)$ at these maxima are consistent with the results of Gardner and Derrida for the minimal fraction of errors $f_{GD} = (1 - c_1)/2$ [18].

Complementary the dependence $\alpha_c(c_1)$ for fixed c_2 is shown in the right part of fig.1. Lines for c_2 and $-c_2$ start at the same point for $c_1 = 0$. It corresponds to $\mu = \pm\infty$ where the value of c_1 has negligible influence in the cost-function (15). With increasing c_1 the value of α_c always decreases because additional constraints are to be satisfied. These new constraints give rise to $c_1 > 0$ and are hence harder to satisfy for negative values of c_2 . Finally all lines end at the thin line given by $c_2 = 2c_1 - 1$.

The pure cases for $K = 2$ defined by $x = \infty$ at α_c are indicated by symbols in fig.1. They correspond to two-layer networks with two hidden units and fixed Boolean functions between hidden layer and output and are summarized in table 2.

In our analysis the AND-machine denotes the situation in which the two perceptrons have to give *simultaneously* the correct output $\sigma^\nu = +1$ for all patterns. The storage capacity is hence given by the Gardner result, i.e. $\alpha_c = 1$ since each perceptron has $N/2$ couplings only. Note that the AND-machine investigated in [10] has random outputs $\sigma^\nu = \pm 1$ and therefore the value for α_c is different. The XOR function defines the $K = 2$ parity machine for which the replica symmetric α_c was first obtained in [3, 4]. The result for the OR-machine is new, again it refers to the situation where random inputs have all to be mapped on $\sigma^\nu = +1$. Finally let us note that there is another rather trivial pure case given by $c_1 = c_2 = 0$

symbol in fig.1	c_1	c_2	$\alpha_c(x = \infty)$	μ	Boolean function
triangle	1	1	1	< 1	AND
square	1/4	-1/2	11.01	$= 1$	OR
circle	0	-1	5.50	> 1	XOR

Table 2: *Patterns of correlations for $K = 2$ perceptrons equivalent to two-layer networks with fixed Boolean function between hidden units and output.*

with $\alpha_c = \infty$ corresponding to the Boolean function that gives output +1 on any input.

The results obtained for $K = 2$ are summarized in fig.2 showing the region of allowed values in the c_1 - c_2 -plane together with lines of constant α_c and constant μ . The arrows at the lines of constant μ point to smaller values of α_c . The above discussed hidden unit machines are again marked by the symbols of table2. All other points can be interpreted as these machines above their storage capacity. Note that the same point could be associated with different machines beyond saturation since by prescribing the correlations appropriately we can induce continuous transitions between different machines.

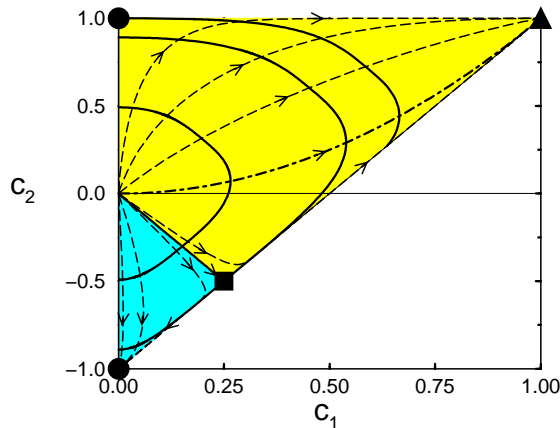


Figure 2: **Contour map of $\alpha_c(c_1, c_2)$ and $\mu(c_1, c_2)$ for $K = 2$ correlated perceptrons.** Full lines correspond to $\alpha_c = 100, 11.01 = \alpha_c^{OR}, 5.50 = \alpha_c^{XOR}$ (from left to right), dashed lines to $\mu = -10, -2, -1, 0, 0.99, 1.01, 2, \text{and } 10$ (from bottom to top). Symbols denote the same MLN as in table 2.

6 $K = 3$

A similar analysis can be performed for $K = 3$. As discussed in section 4 we set $\mu_2 = 0$ and denote μ_3 simply by μ . Similar to the last section we can then determine $\alpha_c(c_1, c_3)$ from a numerical analysis of eqs.(17,18).

Fig.3(left) shows the dependence of the critical storage capacity α_c on c_3 for fixed values of c_1 . The dependencies are rather similar to the case $K = 2$ shown in the left part of fig.1. Again solutions $c_1(\alpha_c, c_3)$ exist only in shaded areas. The maxima of the $\alpha_c(c_3)$ -curves lie on the dashed-dotted line corresponding

to independent perceptrons ($\mu = 0$). They are hence characterized by $c_3 = c_1^3$ and are again consistent with the Gardner-Derrida results on the minimal fraction of errors for perceptrons above saturation [18].

Complementary the dependence $\alpha_c(c_1)$ for fixed values of c_3 is shown in the right part of Fig.3. Again similar to the case $K = 2$ we find that α_c decreases with increasing c_1 . In particular the lines for $c_3 = \pm 1$ show how the storage capacity decreases from the value of the $K = 3$ -parity machine at $c_1 = 0$ if additional constraints showing up in $c_1 > 0$ are included. All lines end at the thin line given by $c_3 = 3c_1 - 2$.

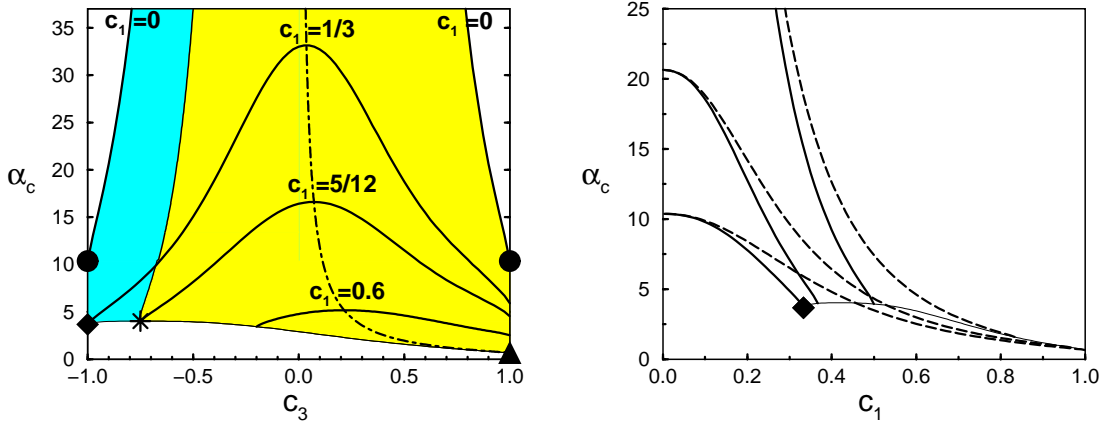


Figure 3: **Storage capacity $\alpha(c_1, c_3)$ for $K = 3$ correlated perceptrons.**

Left: $\alpha_c(c_3)$ for $c_1 = 0, 1/3, 5/12$ and $3/5$. Outside the shaded areas no solutions exist, dark shade corresponds to $\mu > 1$ light shade to $\mu < 1$. The dashed-dotted line ($\mu = 0$) gives the location of the maxima. The symbols denote the pure cases corresponding to the MLN summarized in table 3.

Right: $\alpha_c(c_1)$ for (from bottom to top): $c_3 = 1, 0.9$, and 0.5 (dashed) and $c_3 = -1, -0.9$ and -0.5 (full). The lines end at the thin line given by $c_3 = 3c_1 - 2$. The symbol corresponds to the machine giving overall output +1 only if exactly one hidden unit is -1.

The symbols in fig.3 refer again to pure cases with $x = \infty$ at α_c corresponding to the MLN summarized in table 3. In addition to the and- and parity-machine we have now the committee-machine and a machine with the Boolean function for which the output is +1 if *exactly one* hidden unit is -1.

symbol in fig.(3)	c_1	c_3	$\alpha_c(x = \infty)$	μ	Boolean function
triangle	1	1	2/3	$\mu < 1$	AND
star	5/12	-3/4	4.02	$\mu = 1$	COMMITTEE
diamond	1/3	-1	3.669	$\mu > 1$	$(- + +), (+ - +), (+ + -)$
circle	0	± 1	10.37	$\mu = \pm \infty$	PARITY

Table 3: *Patterns of correlations for $K = 2$ perceptrons equivalent to two-layer networks with fixed Boolean function between hidden units and output.*

We can again summarize the results in a contour plot showing lines of constant α_c and μ in the c_1 - c_3 -plane fig.4. Only combinations of c_1 and c_3 that belong to the shaded areas are possible, light shade corresponds to $\mu < 1$, dark shade to $\mu > 1$. The arrows at the dashed lines of constant μ point again into

regions of lower α_c , the symbols are those of table 3. Large values of c_1 imply a strong correlation of every perceptron with the common output and gives therefore small α_c and a narrow interval of consistent values of c_3 . Relaxing the constraint on c_1 allows a more efficient “division of labour” between the perceptrons and results in a broader spectrum of c_3 -values and enhanced storage capacity. Accordingly the largest values of α_c are possible for $c_1 = 0$. Then α_c only depends on c_3 and starting from the value 10.37 for the parity machine at $c_3 = \pm 1$ it increases without bound with decreasing $|c_3|$.

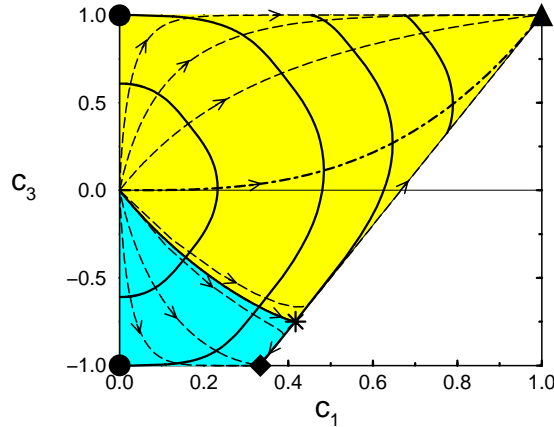


Figure 4: **Contour map of $\alpha_c(c_1, c_3)$ and $\mu(c_1, c_3)$ for $K = 3$ correlated perceptrons.** Full lines correspond to $\alpha_c = 100, 10.37 = \alpha_c^{PAR}, 4.02 = \alpha_c^{COM}$ and 2. (from left to right), dashed lines to $\mu = -10, -2, -1, 0, 0.99, 1.01, 2,$ and 10 (from bottom to top). Symbols denote the same MLN as in table (3).

A new aspect of the case $K = 3$ is that there is a correlation coefficient, c_2 , that was not prescribed (since we put $\mu_2 = 0$). It is nevertheless of interest to know the value of c_2 that corresponds to different choices of c_1 and c_3 . The easiest way to obtain c_2 is via a maximum entropy argument. This is sketched in appendix C. The result is

$$c_2 = -\frac{1}{2} + \sqrt{\frac{1}{4} + c_1^2 + c_1 c_3} \quad (20)$$

It is interesting to note that for the values $c_1 = 5/12$ and $c_3 = -3/4$ characteristic for the committee-machine this formula gives $c_2 = -1/6$ which is in fact the correct result [14]. The committee function for $K = 3$ does hence not imply constraints on c_2 and is already uniquely characterized by the values of c_1 and c_3 .

7 Conclusions

In the present paper we have considered ensembles of K perceptrons with random inputs and investigated the possibility to choose the couplings such that prescribed correlations c_m between the outputs of the perceptrons occur. For any combinatorically possible combination of c_m there is a critical value $\alpha_c(c_1, \dots, c_K)$ and solutions for the couplings of the perceptrons exist if the number of inputs is less than $N\alpha_c$. These investigation establish a relation between the results for single perceptrons above

their storage capacity and those for several MLN with tree-structure and K hidden units and fixed Boolean function between hidden layer and output. Similar ideas were pursued in [15] and [11] where approximate expressions for the storage capacity of a parity machine and committee machine respectively were obtained from the results of Gardner and Derrida on the minimal fraction of errors of perceptrons beyond saturation and in [22] where analogies between a committee machine and noisy perceptrons were investigated. The new aspect in the present paper is that also the influence of higher correlations that are known to be important for the storage abilities was taken into account. The results show which correlations are difficult to implement and are therefore important for the determination of the storage capacity and which are easy and therefore not very restrictive. A detailed analysis was carried out for $K = 2$ and $K = 3$.

The technique used is a generalization of the canonical phase space analysis introduced by Gardner and Derrida. The results were obtained within the replica symmetric ansatz. They should hence be seen as a mere first orientation since it is well known that replica symmetry breaking (RSB) is crucial for both the description of perceptrons above saturation [21] and the storage abilities of MLN [4, 5, 6]. An investigation of the problem within RSB though highly desirable seems technically rather involved. Also the extension of the analysis to the asymptotic behaviour for $K \rightarrow \infty$ would be very interesting and would hopefully shed some light on the still controversial problem of the storage capacity of MLN in this limit.

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8 Appendix A

In this appendix we outline the calculation of the free energy eq.(6) corresponding to the cost function eq.(4) within replica symmetry. To this end we employ a generalization of the formalism of Griniasty and Gutfreund [19].

To perform the average over the random patterns we use the replica trick

$$f(\mu_2, \dots, \mu_K, \beta) = -\frac{1}{\beta N} \langle \ln \mathcal{Z} \rangle = -\frac{1}{\beta N} \lim_{n \rightarrow 0} \frac{\langle \mathcal{Z}^n \rangle - 1}{n} \quad (21)$$

involving the partition function \mathcal{Z}

$$\begin{aligned} \mathcal{Z} &= \int_{-\infty}^{\infty} \prod_k \frac{d\mathbf{J}_k}{\sqrt{2\pi e}} \delta(\mathbf{J}_k^2 - N/K) \int_{-\infty}^{\infty} \prod_{k\nu} d\lambda_k^\nu \delta(\lambda_k^\nu - \mathbf{J}_k \boldsymbol{\xi}_k^\nu \sqrt{K/N}) e^{-\frac{\beta}{\alpha} \sum_\nu V(\lambda_1^\nu, \dots, \lambda_K^\nu)} \quad (22) \\ V(\lambda_1^\nu, \dots, \lambda_K^\nu) &= -\sum_k \text{sgn}(\lambda_k^\nu) + \mu_2 \sum_{(k,l)} \text{sgn}(\lambda_k^\nu \lambda_l^\nu) + \dots + \mu_K \text{sgn}(\lambda_1^\nu \dots \lambda_K^\nu) \end{aligned}$$

Introducing integral representations for the δ -functions and performing the average over the patterns we

find

$$\begin{aligned} \langle\langle \mathcal{Z}^n \rangle\rangle &= \int_{-\infty}^{\infty} \prod_{a<b;k} dq_k^{ab} \int_{-\infty}^{\infty} \prod_{a<b;k} dF_k^{ab} \frac{N}{2\pi K} \int_{-\infty}^{\infty} \prod_{a;k} \frac{dE_k^a}{4\pi K} \\ &\times \exp\left(\frac{N}{K} \left[\frac{1}{2} \sum_k \text{tr}(Q_k A_k) + G_2(F_k^{ab}, E_k^a) \right] + \alpha N G_1(Q_{1..K})\right) \end{aligned} \quad (23)$$

where

$$G_2(F_k^{ab}, E_k^a) = -\frac{1}{2} \sum_k [n + \text{tr}(\ln A_k)], \quad (24)$$

and

$$G_1(Q_{1..K}) = \ln \left[\int_{-\infty}^{\infty} \prod_k d\lambda_k \int_{-\infty}^{\infty} \prod_k \frac{dy_k}{(2\pi)^n} \exp\left(i \sum_k \mathbf{y}_k \lambda_k - \frac{1}{2} \sum_k \mathbf{y}_k Q_k \mathbf{y}_k^T + \beta \sum_a V(\lambda_1^a, \dots, \lambda_K^a)\right) \right] \quad (25)$$

Here $\lambda_k = (\lambda_k^1, \dots, \lambda_k^n)$ and $\mathbf{y}_k = (y_k^1, \dots, y_k^n)$ and we have used the matrices Q_k and A_k :

$$Q_k = \begin{pmatrix} 1 & q_k^{ab} \\ q_k^{ab} & 1 \end{pmatrix}, \quad A_k = \begin{pmatrix} iE_k^a & -iF_k^{ab} \\ -iF_k^{ab} & iE_k^a \end{pmatrix}, \quad (26)$$

where as usual q_k^{ab} describes the overlap between two replicas a, b in the coupling space of perceptron k ,

$$q_k^{ab} = \mathbf{J}_k^a \mathbf{J}_k^b K/N. \quad (27)$$

The saddlepoint for E_k^a and F_k^{ab} is given by $Q_k^{-1} = A_k$ resulting in

$$\langle\langle \mathcal{Z}^n \rangle\rangle \simeq \int_{-\infty}^{\infty} \prod_{a<b;k} dq_k^{ab} \exp\left(\frac{N}{2K} \sum_k \ln(\det Q_k) + \alpha N G_1(Q_{1..K})\right) \quad (28)$$

To evaluate the remaining saddle point integral we use the replica symmetric ansatz $q_k^{ab} = q_k$ for all $a \neq b$. Moreover we expect permutation symmetry between the different perceptrons implying $q_k = q$ for all $k = 1, \dots, K$. Then $\ln[\det Q] = n(\ln(1-q) + q/(1-q))$ and for $G_1(q_1, \dots, q_K)$ it follows

$$\begin{aligned} G_1(q) &= \\ &= \int_{-\infty}^{\infty} \prod_{a;k} d\lambda_k^a \int_{-\infty}^{\infty} \prod_{a;k} \frac{dy_k^a}{2\pi} \exp\left(i \sum_{a;k} y_k^a \lambda_k^a - \frac{1-q}{2} \sum_{a,k} (y_k^a)^2 - \frac{q}{2} \sum_{a,k} (y_k^a)^2 - \beta V(\lambda_1^a, \dots, \lambda_K^a)\right) \\ &\simeq n \int_{-\infty}^{\infty} \prod_k Dt_k \ln \int_{-\infty}^{\infty} \prod_k \frac{d\lambda_k}{\sqrt{2\pi(1-q)}} \exp\left(-\sum_k \frac{(\lambda_k - t_k \sqrt{q})^2}{2(1-q)} - \beta V(\lambda_1, \dots, \lambda_K)\right). \end{aligned} \quad (29)$$

In order to calculate the function $g(\alpha_c, \mu_2, \dots, \mu_K)$ eq.(7) we have to consider the *saturation limit* $\beta \rightarrow \infty$. It is convenient then to use the rescaled saddle point variable $x = \beta(1-q)$ instead of q . In this

way we obtain

$$g(\alpha_c, \mu_2, \dots, \mu_K) = -\min_x \left[\frac{1}{2x} - \alpha_c \int_{-\infty}^{\infty} \prod_k Dt_k F(x, t_1, t_2, \dots, t_K) \right] \quad (30)$$

$$F(x, t_1, t_2, \dots, t_K) = \min_{\lambda_1, \dots, \lambda_K} \left(\sum_k \frac{(\lambda_k - t_k)^2}{2x} + V(\lambda_1, \dots, \lambda_K) \right) \quad (31)$$

which coincides with (10). The saddlepoint equation eq.(13) determining x follows by explicit differentiation of eq.(30) with respect to x .

9 Appendix B

In this appendix we sketch the main steps of the derivation of the saddle point equation (13) and of the free energy (30) for the case that only c_1 and c_K are prescribed. We also give the explicit expressions for c_1 and c_K as a function of α_c and μ .

The calculation of g as given by (30,16) requires minimization of

$$F(x, t_1, t_2, \dots, t_K) = \min_{\lambda_1, \lambda_2, \dots, \lambda_K} \left[\sum_{k=1}^K \frac{(\lambda_k - t_k)^2}{2x} - \sum_{k=1}^K \text{sgn}(\lambda_k) + \mu \prod_{k=1}^K \text{sgn}(\lambda_k) \right]. \quad (32)$$

From eq.(12) we have

$$\text{sgn}(\lambda_k^0) = \begin{cases} \text{sgn}(t_k) & \text{if } \lambda_k^0 = t_k \\ -\text{sgn}(t_k) & \text{else} \end{cases} \quad (33)$$

Eq.(32) then becomes

$$F(x, t_1, t_2, \dots, t_K) = \left[\mu S(\vec{\lambda}^0) - \sum_{k=1}^K \text{sgn}(t_k) + \sum_{\forall_j \lambda_j^0 = 0^\pm} \left(\frac{t_j^2}{2x} + 2 \text{sgn } t_j \right) \right]. \quad (34)$$

Here $S(\vec{\lambda}^0) = \prod_{k=1}^K \text{sgn}(\lambda_k^0) = (-1)^m \prod_{k=1}^K \text{sgn}(t_k)$ where m counts all $\lambda_k^0 \equiv 0$. The last sum in eq.(34) has only contributions from those λ with $\lambda_j^0 = 0^\pm$.

To minimize F for given t_1, \dots, t_K we have hence to find which of the 2^K configurations $\{\lambda_1^0, \dots, \lambda_K^0\}$, $\lambda_k^0 = \{0^\pm, t_k\}$, minimizes eq.(34). A suitable procedure to do this is as follows. We first make the last term in eq.(34) as small as possible. That is for all t_j with $t_j \in (-2\sqrt{x}, 0)$ we choose for a first try $\lambda_j^0 = 0^\pm$. We denote the resulting value for $S(\vec{\lambda}^0)$ by S^* . ($S^* = (-1)^\eta$ where η is the number of all $t_k < -2\sqrt{x}$.) If $\mu S^*(\vec{t}) < 0$ the optimal configuration has already been found because the first summand is at its minimum as well. If on the other hand $\mu S^*(\vec{t}) > 0$ there is competition between the first and the last term in eq.(34). One may then change the sign of $S(\vec{\lambda}^0)$ in order to lower $F(x, t_1, t_2, \dots, t_K)$ by $2|\mu|$ by either setting a single $\lambda_l^0 = 0^\pm$ although $t_l \notin (-2\sqrt{x}, 0)$ or setting a single $\lambda_l^0 = t_l$ for one $t_l \in (-2\sqrt{x}, 0)$. The corresponding changes in F are $2(w(t_l) - |\mu|)$ where

$$w(t) = \begin{cases} t^2/4x - 1 & \text{if } t \in (-\infty, -2\sqrt{x}) \\ -t^2/4x + 1 & \text{if } t \in (-2\sqrt{x}, 0) \\ t^2/4x + 1 & \text{if } t \in (0, \infty) \end{cases}. \quad (35)$$

To the saddle point equation (13) only regions in the integral contribute for which $\lambda_j^0 \neq t_j$ for at least one j . Formalizing the above consideration we find

$$\begin{aligned} \frac{1}{\alpha_c} &= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} Dt_1 \dots Dt_K \left\{ \sum_{k=1}^K t_{k=1}^2 \Theta_I(t_k) + \right. \\ &\quad \left. + K \Theta(\mu S^*) \Theta(|\mu| - w(t_1)) t_1^2 (-1)^{\Theta_I(t_1)} \prod_{k=2}^K \Theta(w(t_k) - w(t_1)) \right\} \end{aligned} \quad (36)$$

$$\Theta_I(t) = \begin{cases} 1 & \text{if } t \in (-2\sqrt{x}, 0) \\ 0 & \text{else} \end{cases} \quad (37)$$

The first term of eq.(36) stems from our first guess minimizing the last term of eq.(34) only. The various Theta-functions in the term that contributes only for $\mu S^* > 0$ implement the different cases discussed in context with eq.(35). Integration variables can be renamed that always $t_1 < t_2 < \dots < t_K$ with no restriction of generality.

The integrations over t_2, \dots, t_K yields a product of sums of two error functions. Finally the saddlepoint equation reads

$$\frac{1}{K \alpha_c} = \frac{1}{2} - H(2\sqrt{x}) - 2\sqrt{x} \frac{e^{-2x}}{\sqrt{2\pi}} + \frac{1}{2} \left[f_1(|\mu|, x, 1) + f_2(|\mu|, x, 1) \right]. \quad (38)$$

$$f_1(|\mu| < 1, x, L) = [-1]^L \int_{-2\sqrt{x}}^{-2\sqrt{x(1-|\mu|)}} Dt_1 t_1^{2L} \left(\left[H(t_1) + H_m(t_1) \right]^{K-1} + \text{sgn}\mu \left[H(t_1) - H_m(t_1) \right]^{K-1} \right) \quad (39)$$

$$\begin{aligned} f_1(|\mu| > 1, x, L) &= \left\{ \int_0^{2\sqrt{x(|\mu|-1)}} Dt_1 t_1^{2L} \left(\left[H(t_1) + H_p(t_1) \right]^{K-1} + \text{sgn}\mu \left[H(t_1) - H_p(t_1) \right]^{K-1} \right) + \right. \\ &\quad \left. [-1]^L \int_{-2\sqrt{x}}^0 Dt_1 t_1^{2L} \left(\left[H(t_1) + H_m(t_1) \right]^{K-1} + \text{sgn}\mu \left[H(t_1) - H_m(t_1) \right]^{K-1} \right) \right\} \end{aligned} \quad (40)$$

where we introduced the abbreviation $H_p(t_1) = H(\sqrt{8x + t_1^2})$, $H_m(t_1) = H(\sqrt{|8x - t_1^2|})$ and $H_m^-(t_1) = H(-\sqrt{|8x - t_1^2|})$. As usual $H(t) = \int_t^{\infty} Dt$. Similarly

$$f_2(|\mu| < 1, x, L) = \int_{-2\sqrt{x(1+|\mu|)}}^{-2\sqrt{x}} Dt_1 t_1^{2L} \left(\left[H_m^-(t_1) + H(-t_1) \right]^{K-1} - \text{sgn}\mu \left[H_m^-(t_1) - H(-t_1) \right]^{K-1} \right) \quad (41)$$

$$\begin{aligned}
f_2(|\mu| > 1, x, L) = & \left\{ \int_{-2\sqrt{2x}}^{-2\sqrt{x}} Dt_1 t_1^{2L} \left(\left[H_m^-(t_1) + H(-t_1) \right]^{K-1} - \text{sgn}\mu \left[H_m^-(t_1) - H(-t_1) \right]^{K-1} \right) \right. \\
& \left. + \int_{-2\sqrt{x(1+|\mu|)}}^{-2\sqrt{2x}} Dt_1 t_1^{2L} \left(\left[H_m(t_1) + H(-t_1) \right]^{K-1} - \text{sgn}\mu \left[H_m(t_1) - H(-t_1) \right]^{K-1} \right) \right\} \quad (42)
\end{aligned}$$

A common feature of eq.(39–42) is that in the binomial expression those terms cancel which correspond to regions with $\mu S^* < 0$.

The calculation of g proceeds along similar lines.

$$\begin{aligned}
g/\alpha_c &= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} Dt_1 \dots Dt_K \left\{ \mu S^* - \sum_{k=1}^K \text{sgn}(t_k) + 2 \sum_{\forall_j \lambda_j^0=0} \text{sgn } t_j \right\} \\
&= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} Dt_1 \dots Dt_K \left\{ \mu S^* - 2 \sum_{k=1}^K \Theta_I(t_k) + 2K \Theta(\mu S^*) \Theta(|\mu| - w(t_1)) \times \right. \\
&\quad \left. \times \left(-\mu S^* + (-1)^{\Theta_I(t_1)} \text{sgn}(t_1) \right) \prod_{k=2}^K \Theta(w(t_k) - w(t_1)) \right\} \quad (43)
\end{aligned}$$

We find

$$\begin{aligned}
g/\alpha_c &= -2K E(2\sqrt{x}) + 2^K \mu E^K(2\sqrt{x}) + \\
&\quad + K \left\{ f_1(|\mu|, x, 0) - f_2(|\mu|, x, 0) - |\mu| \left[f_1(|\mu|, x, 0) + f_2(|\mu|, x, 0) \right] \right\} \quad (44)
\end{aligned}$$

Performing the derivative of g/α_c with respect to μ one realizes that there is no contribution from the μ -dependence of the integration limits in eqs.(39–42). Hence the expression (44) for g/α_c is already of the form $g/\alpha_c = -Kc_1 + \mu c_K$ and we arrive at eq.(17,18) for the correlation coefficients c_1 and c_K .

10 Appendix C

To determine c_2 for given values of c_1 and c_3 we look for the probability distribution $P(\tau_1, \tau_2, \tau_3)$ that for the given values of c_1 and c_3 realizes the maximal entropy. Because of the permutation symmetry between the perceptrons we have only to determine the probabilities p_k of output configurations with k negative outputs where $k = 0, \dots, 3$. Hence we have to maximize

$$\begin{aligned}
S &= -p_0 \log p_0 - 3p_1 \log p_1 - 3p_2 \log p_2 - p_3 \log p_3 \\
&\quad + \lambda_0(p_0 + 3p_1 + 3p_2 + p_3 - 1) \\
&\quad + \lambda_1(p_0 + p_1 - p_2 - p_3 - c_1) \\
&\quad + \lambda_3(p_0 - 3p_1 + 3p_2 - p_3 - c_3)
\end{aligned} \quad (45)$$

where the λ_k are Lagrange multiplier incorporating the constraints. Performing the derivatives with respect to the p_k yields

$$p_0 p_3 = p_1 p_2 \quad (46)$$

Using the constraints to solve for the p_k gives

$$c_2 = -\frac{1}{2} \pm \sqrt{\frac{1}{4} + c_1^2 + c_1 c_3} \quad (47)$$

where only the upper sign give rise to positive values for all p_k .

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