Statistical Physics of Feedforward Neural Networks

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Abstract

The article is a lightly edited version of my habilitation thesis at the University Würzburg. My aim is to give a self contained, if concise, introduction to the formal methods used when off-line learning in feedforward networks is analyzed by statistical physics. However, due to its origin, the article is not a comprehensive review of the field but is highly skewed towards reporting my own research.
Preface

This thesis summarizes my postdoctoral research insofar as it dealt with supervised learning in feedforward neural networks. This research was carried out at the University of Würzburg and at Aston University, Birmingham.

In Würzburg, I wish to thank Wolfgang Kinzel for giving me the opportunity to work in the stimulating atmosphere of his group. I also acknowledge many interesting discussions with Georg Reents and Michael Biehl. Michael deserves special thanks for taking trouble to comment on the introductory chapters of this work. In Birmingham my thanks go to David Saad and Manfred Opper, both for fruitful discussions and for doing their best to make my stay in England more enjoyable.

Obviously, there are many more people I need to thank - I have not even mentioned all of my coauthors. As a catch all, let me extend my warm thanks to everyone I am omitting to thank. I do, however, wish to explicitly acknowledge the support of the Deutsche Forschungsgemeinschaft which funded a substantial part of the research reported below.
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Chapter 1

Capacity of the perceptron

Choosing a weight vector $J \in \mathbb{R}^N$ defines a dichotomy of the $P$ inputs $\xi^\mu \in \mathbb{R}^N$ by classifying an input as $\text{sgn}(J^T \xi^\mu)$. We now calculate the number $C(P, N)$ of dichotomies which can be obtained in this manner by an inductive argument due to Schl"afli.\footnote{To simplify the argument, we only count the dichotomies which can be obtained with a $J$ satisfying $J^T \xi^\mu \neq 0$ for all $\mu$.} Let $\xi$ be an additional input and assume that all points are in general position. Let $D$ be the number of dichotomies on $\xi^1, \ldots, \xi^P$ which can be represented by a weight vector $J$ satisfying $J^T \xi = 0$. For any such dichotomy we obtain two dichotomies differing only on $\xi$ by replacing $J$ with $J' = J \pm \epsilon \xi$ and choosing $\epsilon$ sufficiently small. Hence $C(P+1, N) = C(P, N) + D$. Further $J^T \xi = 0$, the constraint defining $D$, means that $J$ is confined to an $N-1$ dimensional subspace, so $D = C(P, N-1)$. Finally, the recursion

$$C(P+1, N) = C(P, N) + C(P, N-1)$$

with boundary conditions $C(1, N) = C(P, 1) = 2$ has the solution

$$C(P, N) = 2 \sum_{i=0}^{N-1} \left( \begin{array}{c} P-1 \\ i \end{array} \right).$$

In particular the perceptron can implement all possible dichotomies, $C(P, N) = 2^P$, only if $P \leq N$. But considering large $N$ and scaling $P$ as $P = \alpha N$ one finds

$$\lim_{N \to \infty} \frac{C(\alpha N, N)}{2^{\alpha N}} = \begin{cases} 1 & \text{if } \alpha < 2 \\ 0 & \text{if } \alpha > 2. \end{cases}$$

(1.1)

So in the limit of large $N$ almost all possible dichotomies can be implemented as long as $P/N < 2$.

The above result was rederived by Elisabeth Gardner using the very different approach of Statistical Physics. While Gardner’s calculation is more involved, it can be
adapted to many related scenarios and in particular is a starting point for analyzing learning in multilayer networks.

For a given dichotomy, let \( \tau^\mu \in \{-1, 1\} \) be the labels of the inputs \( \xi^\mu \) and we shall call the input/output pairs \( \mathbb{D} = \{(\xi^\mu, \tau^\mu)\}_{\mu=1}^P \) the training set. A perceptron with weight vector \( J \) implements the dichotomy if \( \tau^\mu J^T \xi^\mu > 0 \) for all \( \mu \) and for convenience we may assume that the Euclidian norm of \( J \) equals 1. In terms of the Heaviside step function

\[
\Theta(x) = \begin{cases} 
0 & \text{if } x \leq 0 \\
1 & \text{if } x > 0 
\end{cases}
\]

the volume \( V(\mathbb{D}) \) of the weight vectors implementing the dichotomy can then be written as

\[
V(\mathbb{D}) = \int dJ \prod_{\mu=1}^P \Theta(\tau^\mu J^T \xi^\mu).
\]

The integration is over the unit sphere in \( \mathbb{R}^N \) and we normalize the measure such that \( V(\emptyset) = 1 \).

In statistical mechanics one is interested in the properties of \( V(\mathbb{D}) \) given a distribution of training sets \( \mathbb{D} \). We shall always assume that the patterns \( (\xi^\mu, \tau^\mu) \) in a training set are obtained by independently sampling a random variable \( (\xi, \tau) \) with values in \( \mathbb{R}^N \times \{-1, 1\} \). For the storage capacity problem considered by Gardner \( \tau \) is further assumed independent of \( \xi \), and \( \tau^\mu = \pm 1 \) with equal probability. When averaging over all training sets \( \mathbb{D} \) of size \( P \) one then obtains

\[
\langle V(\mathbb{D}) \rangle_{\mathbb{D}} = \langle V(\{(\xi, \tau)\}) \rangle_{(\xi, \tau)} = 2^{-P}.
\]

Despite its simplicity this result is remarkable when compared to Eq. (1.1). For large \( N \) and \( P > 2N \) Eq. (1.1) means that for almost all training sets \( V(\mathbb{D}) = 0 \). This is not at all reflected in the behavior of \( \langle V(\mathbb{D}) \rangle_{\mathbb{D}} \); so there must be a few training sets for which \( V(\mathbb{D}) \) is very large compared to \( 2^{-P} \). Instead of averaging \( V(\mathbb{D}) \), one thus has to consider quantities such as \( \langle \Theta(\tau^\mu J^T \xi^\mu) \rangle_{(\tau^\mu)} \), the probability that a dichotomy can be implemented, or \( \langle \ln V(\mathbb{D}) \rangle_{\mathbb{D}} \), which will diverge if the probability that \( V(\mathbb{D}) = 0 \) is finite. Calculating these averages analytically is, however, quite difficult, but they could easily be obtained if one knew \( \langle V^n(\mathbb{D}) \rangle_{\mathbb{D}} \) for all real \( n \).

The basic idea of the replica method is to calculate the moments of \( V(\mathbb{D}) \), that is to consider \( \langle V^n(\mathbb{D}) \rangle_{\mathbb{D}} \) for the special case that \( n \) is a natural number. In contrast to general \( n \in \mathbb{R} \), this case is tractable and it turns out that the expression \( g(n) \) for the \( n \)-th moment thus found can be evaluated for real \( n \) and is even an analytical function of \( n \). So assuming this analytical continuation to be correct, i.e. \( \langle V^n(\mathbb{D}) \rangle_{\mathbb{D}} = g(n) \) for all positive \( n \), one then for instance obtains the probability that a dichotomy can be implemented as

\[
\langle \Theta(V(\mathbb{D})) \rangle_{\mathbb{D}} = \lim_{n \to +0} g(n).
\]

The replica method is not just applicable when the random variable in question is
a volume and we shall straight away consider the more general form

\[ Z(\Omega) = \int dJ \prod_{\mu=1}^P F(\tau^\mu J^T \xi^\mu) ; \quad (1.3) \]

so \( Z(\Omega) = V(\Omega) \) for the special case that \( F \) is the \( \Theta \)-function. We assume that \( F \) is nonnegative and that the RHS of Eq. (1.3) as well as some related integrals are well defined. The name replica method is motivated by the fact that \( Z^n(\Omega) \) is an \( n \)-fold integral for integer \( n \):

\[ Z^n(\Omega) = \int dJ \prod_{\mu=1}^P \prod_{a=1}^n F(\tau^\mu J^a T \xi^\mu) , \]

where \( dJ \equiv \prod_a dJ^a \). For the moments of \( Z(\Omega) \) one then has

\[ \langle Z^n(\Omega) \rangle_\Omega = \int dJ \left( \prod_{a=1}^n F(\tau J^a T \xi) \right)^P \langle \xi, \tau \rangle , \quad (1.4) \]

since the examples are independent. To evaluate the average one has to make some assumptions about the distribution of the inputs and it is simplest to assume that the components \( \xi_i \) of \( \xi \) are i.i.d. \( \mathcal{N}(0,1) \), that is independent and Gaussian with zero mean and unit variance. Then the distribution of the inner products \( J^a T \xi \) in Eq. (1.4) is Gaussian as well, with zero mean and covariances \( \langle J^a T \xi J^b T \xi \rangle_\xi = J^a T J^b \).

Consequently if \( X(Q) \) is an \( n \)-dimensional Gaussian of zero mean and with a covariance matrix \( Q \) satisfying \( Q_{ab} = J^a T J^b \), one has

\[ \left\langle \prod_{a=1}^n F(\tau J^a T \xi) \right\rangle_{\langle \xi, \tau \rangle} = \left\langle \prod_{a=1}^n F(\tau X_a(Q)) \right\rangle_{X(Q), \tau} = \left\langle \prod_{a=1}^n F(X_a(Q)) \right\rangle_{X(Q)} , \quad (1.5) \]

where the last equality holds because \( X(Q) \) and \( -X(Q) \) have the same distribution. Since the integrand in Eq. (1.4) depends on the weight vectors \( J^a \) only via their overlaps \( J^a T J^b \), it is convenient to transform the integration variables. This is best done by multiplying Eq. (1.4) with

\[ \int dQ \delta(Q - J^T J) := \int dQ \prod_{a<b \leq n} \delta(Q_{ab} - J^a T J^b) = 1 \quad (1.6) \]

and changing the order of integration. The integral over \( Q \) runs over the symmetric and positive definite matrices with \( Q_{aa} = 1 \). Combining Eqs. (1.4,1.3,1.6) then yields

\[ \langle Z^n(\Omega) \rangle_\Omega = \int dQ D_n(Q) \left\langle \prod_{a=1}^n F(X_a(Q)) \right\rangle_{X(Q)} , \]
where \( D_n(Q) = \int dJ \delta(Q - J^T J) \). In the appendix a simple derivation is given that \( D_n(Q) = D_n(1)(\det Q)^{(N-n-1)/2} \) where 1 is the \( n \times n \) identity matrix. Thus, setting \( P = \alpha N \),

\[
\langle Z^n(\mathbb{D}) \rangle_D = D_n(1) \int dQ \left( (\det Q)^{1-(n+1)/N} \prod_{a=1}^{n} F(X_a(Q)) \right)^{\alpha X(Q)}.
\]

Now the integration is over \( n(n-1)/2 \) dimensions and this number does not increase with \( N \). We may thus use that the \( L_N \)-norm converges to the maximum norm with increasing \( N \) to find

\[
\lim_{N \to \infty} N^{-1} \ln \langle Z^n(\mathbb{D}) \rangle_D = \max_Q \frac{1}{2} \ln \det Q + \alpha \ln \left( \prod_{a=1}^{n} F(X_a(Q)) \right)_{X(Q)}.
\]

Solving this extremal problem for general \( Q \) is quite difficult and one thus restricts the search to a small subspace of all possible matrices \( Q \). If one assumes that the extremal problem has a unique solution \( Q^* \), all off diagonal elements of \( Q^* \) must have the same value since the set of solutions is invariant under permutations of the replica indices. This is known as the replica symmetric assumption.

One is thus lead to consider \( n \times n \) matrices \( M_n(u,v) \) with diagonal elements equal to \( u \) and off diagonal elements equal to \( v \). A simple calculation shows that \((1, \ldots, 1)^T \) is an eigenvector of \( M_n(u,v) \) with eigenvalue \( u + (n-1)v \) and that the matrix further has \( n-1 \) linearly independent eigenvectors of the form \((1, 0, \ldots, 0, -1, 0, \ldots, 0)^T \) with eigenvalue \( u - v \). Thus \( \det M_n(u,v) = (u + (n-1)v)(u - v)^{n-1} \). Assuming replica symmetry, \( Q^* = M_n(1,q) \), and we can simplify the first term in Eq. (1.7).

Further if the \( n+1 \) random variables \( z_0, \ldots, z_n \) are i.i.d. \( \mathcal{N}(0, 1) \), the covariance matrix of the linear combinations \( X_a = \sqrt{u^2 - v^2} z_a + vz_0, \ a = 1, \ldots, n \), is just \( M_n(u^2, v^2) \). For \( Q^* = M(1,q) \) this observation enables us to factorize the average in Eq. (1.7) as

\[
\left\langle \prod_{a=1}^{n} F(X_a(Q^*)) \right\rangle_{X(Q^*)} = \left\langle \prod_{a=1}^{n} F(\sqrt{1-q} z_a + \sqrt{q} z_0) \right\rangle_{z_0, \ldots, z_n} = \left\langle F(\sqrt{1-q} z_1 + \sqrt{q} z_0)^n \right\rangle_{z_0}.
\]

So in replica symmetry we obtain the important intermediate result

\[
\lim_{N \to \infty} N^{-1} \ln \langle Z^n(\mathbb{D}) \rangle_D = \max_q f(n,q),
\]

where

\[
f(n,q) = \frac{1}{2} \ln(1 + (n-1)q) + \frac{n-1}{2} \ln(1-q) + \alpha \ln \left( \left\langle F(\sqrt{1-q} z_1 + \sqrt{q} z_0)^n \right\rangle_{z_0} \right).
\]
Now \( f(n, q) \) is well defined for any nonnegative value of \( n \) and not just for integer \( n \). We can thus consider the analytical continuation to values of \( n \) close to zero. Here, one has to be rather careful since \( f(n, q) \) does not depend on \( q \) when \( n = 1 \), and in particular \( f(1, q) = -\alpha \ln \langle F(z_0) \rangle_{z_0} \). Expanding \( f(n, q) \) around \( n = 1 \) thus yields
\[
f(n, q) \approx -\alpha \ln \langle F(z_0) \rangle_{z_0} + (n - 1)f_1(1, q)
\]
where \( f_1 \) is the partial derivative of \( f \) w.r.t. to the first argument. So if \( q^* \) maximizes \( f_1(1, q) \) and if \( n \) is greater but close to 1, \( f(n, q^*) \) will be a good approximation to the maximum of \( f(n, q) \). But by the same argument \( f(n, q^*) \) will be a good approximation to the minimum of \( f(n, q) \) when \( n \) is close to but smaller than 1. When looking for a function \( g(n) \) such that \( f(n, g(n)) \) is analytical, one will at least want \( g(n) \) to be continuous at \( n = 1 \). Hence \( f(n, q) \) must be minimized when \( n < 1 \). So for small positive values of \( n \) we obtain
\[
\lim_{N \to \infty} N^{-1} \ln \langle Z^n(D) \rangle_D = \mathcal{O}(n^2) + n \min_q f_1(0, q), \tag{1.10}
\]
and from Eq. \[\text{(1.9)}\]
\[
f_1(0, q) = \frac{1}{2} \left( \frac{q}{1-q} + \ln(1-q) \right) + \alpha \left\langle \ln \left\langle F(\sqrt{1-q}z_1 + \sqrt{q}z_0) \right\rangle_{z_1} \right\rangle_{z_0}.
\]
The first term in the above sum is often called the entropy term since it is determined by the constraints on the weight vectors of the perceptron. In the present case, continuous and normalized weight vectors. The second term, which depends on the choice of \( F \), is called the energy term.

We now specialize to Gardner’s case where \( Z(D) \) is the volume \( V(D) \) and \( F(x) = \Theta(x) \). Introducing the function \( H(x) = \langle \Theta(z_1 - x) \rangle_{z_1} \), which is closely related to the error function, the expression for \( f_1 \) simplifies to
\[
f_1(0, q) = \frac{1}{2} \left( \frac{q}{1-q} + \ln(1-q) \right) + \alpha \left\langle \ln H(-z_0\sqrt{q}/\sqrt{1-q}) \right\rangle_{z_0}. \tag{1.11}
\]

Since the probability that a dichotomy can be implemented by the perceptron is \( \langle \Theta(V(D)) \rangle_D = \lim_{n \to +0} \ln \langle V^n(D) \rangle_D \), by Eq. \[\text{(1.11)}\] this probability approaches 1 in the limit of large \( N \) if \( \min_q f_1(0, q) > -\infty \); otherwise it is 0. Similarly for \( \langle \ln V(D) \rangle_D \), using that this is the derivative w.r.t. to \( n \) of \( \ln \langle V^n(D) \rangle_D \) at \( n = 0 \), one has
\[
\lim_{N \to \infty} N^{-1} \ln \langle V(D) \rangle_D = \min_q f_1(0, q).
\]

To find the critical value \( \alpha_c \) where the minimum of \( f_1(0, q) \) diverges to \(-\infty \), note that \( f_1(0, q) \) only diverges for \( q = 1 \). The average \( \langle \ln H(-z_0\sqrt{q}/\sqrt{1-q}) \rangle_{z_0} \) can be calculated analytically for \( q \to 1 \) using that for large positive arguments \( H(x) \sim \frac{\exp(-x^2)}{x\sqrt{2\pi}} \), whereas \( H(-\infty) = 1 \). This yields that for \( q \to 1 \)
\[
\left\langle \ln H(-z_0\sqrt{q}/\sqrt{1-q}) \right\rangle_{z_0} \sim -\frac{1}{4} \frac{q}{1-q}
\]
and the final result that \( \min_{q} f_1(0, q) \) is only finite if \( \alpha < \alpha_c = 2 \).

In the limit of large \( N \), almost all dichotomies can be implemented by the perceptron up to \( \alpha_c \), but the fraction of implementable dichotomies is vanishingly small when \( \alpha > \alpha_c \). In this sense Gardner's calculation exactly coincides with the result obtained by Schläflí. Further the fact that \( \langle \Theta(V(\mathcal{D})) \rangle \) converges to a step function, implies that \( \Theta(V(\mathcal{D})) \) is selfaveraging: for any \( \epsilon > 0 \) the probability that \( |\Theta(V(\mathcal{D})) - \langle \Theta(V(\mathcal{D})) \rangle| \) vanishes in the large \( N \) limit (except at \( \alpha_c = 2 \)). A simple scaling argument shows that \( N^{-1}\ln V(\mathcal{D}) \) should be selfaveraging as well. The variance of \( \ln V(\mathcal{D}) \) is equal to the second derivative w.r.t. to \( n \) of \( \ln \langle V^n(\mathcal{D}) \rangle \) evaluated at \( n = 0 \). When using replicas to find an analytical continuation to small \( n \), one must obtain that the second derivative of \( N^{-1}\ln \langle (V^n(\mathcal{D})) \rangle_D \) is finite. This yields that the variance of \( N^{-1}\ln V(\mathcal{D}) \) is \( O(1/N) \).

To round off Gardner's calculation we consider the physical interpretation of the parameter \( q \), relating it to the mean of all weight vectors implementing a given dichotomy:

\[
\bar{J}(\mathcal{D}) = V^{-1}(\mathcal{D}) \int dJ J \prod_{\mu=1}^{\alpha N} \Theta(\tau^\mu J^T \xi^\mu).
\]

One can show that \( \langle ||\bar{J}(\mathcal{D})||^2 \rangle_D \rightarrow q^* \) with increasing \( N \), where \( q^* \) is the value minimizing \( f_1(0, q) \). Further, the averaged squared length of \( \bar{J}(\mathcal{D}) \) can be written as

\[
\langle ||\bar{J}(\mathcal{D})||^2 \rangle_D = \left( V^{-2}(\mathcal{D}) \int dJ^1 dJ^2 J^1_T J^2 \prod_{\mu=1}^{P} \prod_{a=1}^{2} \Theta(\tau^\mu J^a_T \xi^\mu) \right)_D.
\]

It can thus also be regarded as the average overlap of two perceptron weight vectors \( J^1 \) and \( J^2 \), picked at random from the set of all perceptrons which implement a given dichotomy. This physical interpretation of \( q \) will be derived in Section 5.3, in the context of discussing the relationship between the parameterization of the matrix \( Q \) and the distribution of the overlaps \( J^1_T J^2 \). As a consequence we shall also find that \( ||\bar{J}(\mathcal{D})||^2 \) is selfaveraging if the replica symmetric parameterization is correct.
Chapter 2

Extensions and Ramifications

2.1 Beyond capacity

If the number of patterns in the training set $\mathbb{D}$ is too large, no perceptron will exist which implements the dichotomy perfectly. One may, however, still try to find a network $\sigma$ which makes few mistakes on $\mathbb{D}$, so $\sigma$ should have a small training error

$$\epsilon_{\mathbb{D}}(\sigma) = P^{-1} \sum_{\mu=1}^{P} \Theta(-\tau^\mu \sigma(\xi^\mu)).$$

(2.1)

To adapt Gardner’s calculation one first defines a probability density on the class of all networks by

$$p(\sigma) = \frac{e^{-P\beta \epsilon_{\mathbb{D}}(\sigma)}}{Z(\mathbb{D})},$$

(2.2)

where the partition function $Z(\mathbb{D})$ assures that the density is normalized. The parameter $\beta$ is called the inverse temperature, and a network drawn from $p(\sigma)$ will have minimal training error in the limit of large $\beta$. Note that one can calculate the average, w.r.t. $p(\sigma)$, of the training error from the derivative of $\ln Z(\mathbb{D})$ with respect to $\beta$.

In the context of a dynamical interpretation, $p(\sigma)$ is the stationary distribution of a suitable Langevin dynamics and $-\beta^{-1}\ln Z(\mathbb{D})$ plays the rôle of a free energy. But I shall not be concerned with such an interpretation here.

Choosing $F$ as

$$F(x) = e^{-\beta \Theta(-x)},$$

in the case of the perceptron yields

$$Z(\mathbb{D}) = \int dJ e^{-P\beta \epsilon_{\mathbb{D}}(\sigma_J)} = \int dJ \prod_{\mu=1}^{P} F(\tau^\mu J^T \xi^\mu).$$

(2.3)
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The second expression is the same as in the definition of $Z(D)$ used in Gardner’s calculation, Eq. (1.3). So, in replica symmetry, we have already calculated $N^{-1} \langle \ln Z(D) \rangle_D$. However, major complications arise from the fact that the assumption of replica symmetry is wrong for $\alpha > \alpha_c$. This is extensively reviewed in [10]. I shall discuss the techniques for dealing with broken replica symmetry in the context of multilayer networks.

Considering the case of finite $\beta$ helps to deal with a technical problem in the above exposition of Gardner’s calculation. From Schlaffi’s result we know that for finite $N$ and $\alpha > 1$ there is a finite probability that $V(D) = 0$. So $\langle \ln V(D) \rangle_D$ diverges, and the expression we found for the large $N$ limit of $N^{-1} \langle \ln V(D) \rangle_D$ is surely incorrect in the range $1 < \alpha < 2$. This is actually quite pleasing since our result reflects the fact that the probability that $V(D) = 0$ vanishes in the large $N$ limit for $\alpha < 2$. To make sense of the calculations, however, one should use Eq. (2.3) at a finite value of $\beta$ and when considering $N^{-1} \langle \ln Z(D) \rangle_D$ first take the limit of large $N$ and then the limit $\beta \to \infty$. In the replica calculation the two limits commute since for finite $N$ we are only calculating the moments of $Z(D)$.

2.2 Discrete weight vectors

Upto now we have assumed that the components of the weight vector can take on any real value. In numerical calculations, however, the set of possible values will be finite, even if it can be quite large. We thus assume that the vector $J$ is restricted to lie in a finite subset $L$ of $\mathbb{R}^N$ and consider the number $M_L(D)$ of networks from $L$ that implement a given dichotomy:

$$M_L(D) = \sum_{J \in L} \prod_{\mu=1}^P \Theta(\tau^\mu J^T \xi^\mu).$$

As for continuous weights it is again instructive and simple to calculate the average, 

$$\langle M_L(D) \rangle_D = 2^{-P \text{card} L}. \quad \text{For } P = \alpha N \text{ the average will become zero for large } N \text{ unless the number of networks increases at least exponentially with } N. \text{ We thus assume that there are } L \text{ possible values for each weight and so } \text{card} L = L^N. \text{ Then for large } N \text{ one finds } \langle M_L(D) \rangle_D = 0 \text{ when } \alpha > \log_2 L. \text{ Since the possible values of } M_L(D) \text{ are discrete, for such an } \alpha \text{ the probability that a dichotomy can be implemented by a network in } L \text{ becomes zero. This is sometimes called the information theoretic bound, since any weight vector in } L \text{ can be represented using } N \log_2 L \text{ bits.}

It is interesting that in contrast to continuous weights a simple average of $M_L(D)$ can yield some insight into the critical capacity. But already for $L > 4$ a tighter bound for the perceptron is $\alpha_c \leq 2$, treating the discrete case as a restriction of the continuous one. To improve on the information theoretic bound, let $\phi$ be an orthogonal transformation of $\mathbb{R}^N$ and $\phi L$ the set obtained applying $\phi$ to the elements of $L$. Since
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the distribution of inputs is isotropic, for any function $f$:

$$\langle f(M\xi(D))\rangle_D = \langle f(M\phi\xi(D))\rangle_D .$$

Denote by $\langle \ldots \rangle_\phi$ the average over the uniform density on the orthogonal group of $\mathbb{R}^N$, then for any convex function $f$:

$$\langle f(M\phi\xi(D))\rangle_D \leq \left( \langle f(M\phi\xi(D))\rangle \right)_D .$$

Now $\langle M\phi\xi(D) \rangle_\phi = V(D)\text{card} L$ and we obtain a simple bound in terms of the spherical volume. In particular if $L$ has $L^N$ elements we have $\langle M^n\xi(D) \rangle_D \leq L^{Nn} \langle V^n(D) \rangle_D$ for $0 < n \leq 1$. Since $M\xi(D)$ is integer, $\Theta(M\xi(D)) \leq M_{\xi}(D)$, and we obtain an upper bound on the probability that a dichotomy can be implemented by one of the $L^N$ vectors

$$\langle \Theta(M\xi(D)) \rangle_D \leq L^{Nn} \langle V^n(D) \rangle_D .$$

For $n = 1$ this is just the information theoretic bound but tighter bounds can be obtained by evaluating the RHS for $n < 1$. Using the results for the continuous case, one can easily compute the smallest $\alpha_c(L)$ with the property that for any $\alpha > \alpha_c(L)$ the right hand side decays to zero exponentially with increasing $N$ for some finite value $n(\alpha)$. This yields an upper bound on the critical capacity. For $L = 2$ one obtains $\alpha_c(2) = 0.85$ and this bound is close to the value $\alpha_c = 0.83$ found for $L = \{-1,1\}^N$ by calculating $N^{-1} \langle \ln M\xi(D) \rangle_D$ using replicas \[13\]. The latter value is in good agreement with results from numerical simulations (\[21\]). Further, based on the findings in \[26\] for equidistant weight values, one will expect the bound $\alpha_c(L)$ to be asymptotically tight for large $L$.

From a conceptual point of view the case of discrete weight is nice because an assumption implicit in the interpretation of Gardner’s calculation can be avoided. In identifying the critical capacity with the divergence of $N^{-1} \langle \ln Z(D) \rangle_D$ as well as in commuting the limit $n \to 0$ with $N \to \infty$ in the calculation of $\langle \Theta(V(D)) \rangle_D$, one assumes that for an implementable dichotomy $\ln V(D)$ typically is on the order of $N$. In the discrete case this assumption is not needed. The reason for this is of course that the information theoretic bound guarantees that below the capacity limit $\ln M\xi(D)$ is on the order of $N$.

### 2.3 More general input distributions

Up to now we have assumed that the components of $\xi$ are independent and Gaussian. But in Gardner’s calculation the essential point is not that $\xi$ is Gaussian but that the field $J^T\xi$ is Gaussian. Using the central limit theorem, one can argue that this will also be the case when the input components are not Gaussian but just independent. If further the components have zero mean and unit variance, Gardner’s calculation does not even have to be modified.
It is, however, worthwhile noting that the central limit theorem will not apply for all choices of $J$. While the set of exceptions will have zero measure for large $N$, so does the version space, the set of weight vectors implementing a given dichotomy. Reasonably, one will not expect this to be a problem; but it would be difficult to actually show that all the important contributions to $\langle \ln Z(D) \rangle_D$ do come from the region of state space where the central limit theorem holds.

If one is prepared to live with this, one can argue that the assumption of independent input components is too strong. We consider the characteristic function of $J^T \xi$
\[
e_J(k) = \left\langle e^{i J^T \xi} \right\rangle_{\xi}
\]
and for simplicity assume that $J$ is drawn from a isotropic Gaussian distribution with the normalization $\langle \|J\|^2 \rangle = 1$. Then, for the average value of $c_J(k)$ one immediately finds
\[
\langle c_J(k) \rangle_J = \left\langle e^{-\frac{1}{2} k^2 \|\xi\|^2 / N} \right\rangle_{\xi}.
\]
We now assume that $\|\xi\|^2$ is selfaveraging with mean $N$ and not too malicious, so that $\langle c_J(k) \rangle_J = e^{-\frac{1}{2} k^2}$, i.e. a Gaussian. Generically $c_J(k)$ will thus also be Gaussian if $c_J(k)$ is selfaveraging. For its second moment we obtain
\[
\langle c_J(k)^2 \rangle_J = \left\langle e^{-\frac{1}{2} k^2 (\|\xi^1\|^2 + \|\xi^2\|^2) / N} e^{-\frac{1}{2} k^2 \xi^1 T \xi^2 / N} \right\rangle_{\xi^1, \xi^2},
\]
where $\xi^1$ and $\xi^2$ are independent and have the same distribution as $\xi$. For a large class of distributions, $\xi^1 T \xi^2$ is sufficiently small compared to $N$ so that for large $N$:
\[
\langle c_J(k)^2 \rangle_J \to \left\langle e^{-\frac{1}{2} k^2 (\|\xi^1\|^2 + \|\xi^2\|^2) / N} \right\rangle_{\xi^1, \xi^2} = \langle c_J(k) \rangle^2_J.
\]
In this case, the variance of $c_J(k)$ vanishes for large $N$, $c_J(k)$ is selfaveraging, and typically $J^T \xi$ becomes Gaussian.

Even if one will thus expect that it is not really necessary, in the sequel I shall nevertheless assume i.i.d. $\mathcal{N}(0, 1)$ input components for brevity and simplicity.

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1 The following argument is due to Manfred Opper, personal communication.
Chapter 3

Learning a rule

In the capacity problem one assumes that the outputs in the training set are independent of the inputs. For pattern recognition, however, one is mainly interested in the performance of the network on inputs which were not used for training. This only makes sense if one assumes that the desired output is not random but depends on the input, and that this dependency is learned by the network based on the training examples. So while the training data still consists of $P$ independent samples of the random variable $(\xi, \tau)$, one no longer assumes that $\tau$ is independent of $\xi$. One scenario is that the desired output $\tau$ is a binary function $b(\xi)$ of the input $\xi$, and $b$ is then sometimes called the teacher. One can then measure how well a student, i.e. a network $\sigma$, approximates the input/output relationship by defining the generalization error

$$\epsilon_g(\sigma) = \langle \Theta(-\tau \sigma(\xi)) \rangle_{(\xi,\tau)} ,$$

which is just the probability that $(\xi, \sigma(\xi)) \neq (\xi, \tau)$. Training then amounts to finding a student which makes few mistakes on the examples $\mathbb{D}$, and this is measured by the training error

$$\epsilon_\mathbb{D}(\sigma) = P^{-1} \sum_{\mu=1}^{P} \Theta(-\tau^{\mu} \sigma(\xi^{\mu})) .$$

A key question in formal learning theory is to which extent minimizing $\epsilon_\mathbb{D}$ is conducive to the actual goal of minimizing $\epsilon_g$.

In the case that the network is a perceptron, as simple model is that $b$ can be implemented by a perceptron, i.e.

$$b(\xi) = \text{sgn}(B^T \xi)$$

with a suitable weight vector $B \in \mathbb{R}^N$. If the input components are i.i.d. $N(0,1)$ as in the capacity problem, it is simple to calculate the generalization error of a perceptron
\[ \epsilon_\sigma(\sigma, J) = \langle \Theta(-B^T J^T J) \rangle_{\xi} = \frac{1}{\pi} \arccos B^T J. \]  

(3.2)

Here, and in the sequel, the weight vectors are normalized to 1.

Since the teacher is a perceptron, in contrast to the capacity problem, \( V(D) \) is nonzero for all training set sizes \( P \). One can, however, ask whether a student \( J \) can generalize badly but still achieve zero training error. In view of Eq. (3.2) generalizing badly means that \( B^T J \) is small and one thus considers the restricted volumes

\[ V_R(D) = \int dJ \delta(R - B^T J) \prod_{\mu=1}^P \Theta(\tau^\mu J^T \xi^\mu). \]

When \( \alpha = P/N \) is sufficiently large, one will expect that \( \Theta(V_R(D)) \) vanishes unless \( R \) exceeds a critical value \( R_c \). So a student with zero training error must have a generalization error smaller than \( \frac{1}{\pi} \arccos R_c \) and this is sometimes called the worst case generalization behavior. One may also consider the expected generalization behavior by computing the value \( R^* \) which maximizes \( \ln V_R(D) \). This yields the most probable generalization error of a student picked at random among all perceptrons with zero training error. Since, as in the capacity problem, \( N^{-1} \ln V_R(D) \) is on the order of 1 unless it diverges, for large \( N \) the volume corresponding to \( R^* \) is much larger than that of any other value of \( R \), and the most probable generalization error is in fact observed with probability 1 in this limit.

By the same arguments as in the capacity problem \( \Theta(V_R(D)) \) and \( N^{-1} \ln V_R(D) \) are selfaveraging, and the generalization behavior is obtained by a straightforward adaptation of Gardner’s calculation. We again consider the more general form

\[ Z_R(D) = \int dJ \delta(R - B^T J) \prod_{\mu=1}^P F(\tau^\mu J^T \xi^\mu) \]

and obtain for its moments

\[ \langle Z^n_R(D) \rangle_D = \int dJ \left( \prod_{a=1}^n F(B^T \xi J^a T \xi) \right)^P \prod_{a=1}^n \delta(R - B^T J^a). \]

(3.4)

The \( n+1 \) random variables \( X_{n+1} = B^T \xi \) and \( X_a = J^a T \xi \) are Gaussian with a covariance matrix

\[ \hat{Q} = \begin{pmatrix} Q & R \\ R^T & 1 \end{pmatrix}, \]

here \( Q \) is the \( n \) by \( n \) matrix \( Q_{ab} = J^a T J^b \) and \( R = (R, R, \ldots, R)^T \) is an \( n \)-dimensional vector. So

\[ \langle Z^n_R(D) \rangle_D = \int dQ D_n(Q,R) \left( \prod_{a=1}^n F(X_{n+1}(\hat{Q}) X_a(\hat{Q})) \right)^P_{x(\hat{Q})}, \]
where \( D_n(Q, R) = \int dJ \delta(Q - J^T J) \prod_{a=1}^n \delta(R - B^T J^a) \).

To calculate \( D_n(Q, R) \), note that by rotational symmetry it is invariant to the choice of \( B \) as long as \( \|B\| = 1 \). So averaging over the uniform density on the unit sphere yields

\[
D_n(Q, R) = \int dB \, D_n(Q, R) = D_{n+1}(\hat{Q}) = D_{n+1}(1) (\det \hat{Q})^{(N-n-2)/2}. \tag{3.5}
\]

The expression for \( \det \hat{Q} \) can be simplified since for a square block matrix \((a \ b \ c \ d)\) with invertible square matrices \(a\) and \(d\)

\[
\det(a \ b \\
c \ d) = \det(a - b d^{-1} c) \det d \tag{3.6}
\]

holds. Thus \( \det \hat{Q} = \det(Q - RR^T) \).

To evaluate Eq. \((3.4)\) for large \( N \) and \( P = \alpha N \), we again assume that the value of \( Q \) maximizing the integrand is replica symmetric, i.e. \( Q = M_n(1, q) \). So it is straightforward to evaluate \( D_n(Q, R) \) since \( \det \hat{Q} = \det M_n(1 - R^2, q - R^2) \). Further, at the maximum \( X(Q) \) can be rewritten in terms of i.i.d. \( N(0, 1) \) random variables \( z_1, z_0, \ldots, z_n \) as

\[
X_a(\hat{Q}) = Rz_1 + \sqrt{q - R^2 z_0 + \sqrt{1 - q} z_1} \quad \text{and} \quad X_{n+1}(\hat{Q}) = z_1.
\]

Then at the maximum the average in Eq. \((3.4)\) simplifies to

\[
\left\langle \prod_{a=1}^n F(X_{n+1}(\hat{Q}), X_a(\hat{Q})) \right\rangle_{X(\hat{Q})} = \left\langle \left( F(z_1(Rz_1 + \sqrt{q - R^2 z_0 + \sqrt{1 - q} z_1})) \right)^n \right\rangle_{z_1, z_0},
\]

where the second expression makes sense also for noninteger \( n \).

As in the capacity problem one now uses an analytical continuation to find for small \( n \)

\[
\lim_{N \to \infty} N^{-1} \ln \langle Z^n_R(\mathbb{D}) \rangle_D = \mathcal{O}(n^2) + n \min_q g(R, q), \tag{3.7}
\]

with

\[
g(R, q) = \frac{1}{2} \left( \frac{q - R^2}{1 - q} + \ln(1 - q) \right) + \alpha \left\langle \ln \left( F(z_1(Rz_1 + \sqrt{q - R^2 z_0 + \sqrt{1 - q} z_1})) \right) \right\rangle_{z_1, z_0}.
\]

\footnote{Note that \((1 \ -b \ c \ 1) = (1 - bc \ 0 \ c \ 1) \). In this equation, it is trivial to obtain the determinant of two matrices, and thus the third. Hence, the same statement applies to \((a^{-1} \ 0 \ d^{-1} \ 0) \ (a \ b \ c \ d) = (d^{-1} \ 1) \ (a^{-1} \ 0) \).}
Specializing to the case that $F(x) = \Theta(x)$ allows the minor simplification of rewriting the $z_1$-average in terms of $H(x)$. Then the analysis of (3.7) shows that the generalization error decays to zero as $1/\alpha$ in the worst case as well as in the expected case and that only the pre-factor differs in the two cases [5, 11]. However, a much larger difference between the two scenarios has been found for some multilayer networks (29).

That the teacher is a perceptron, is a rather unrealistic assumption. In a more general case it may be impossible to find a network which has zero training error. A reasonable strategy is then to look for a network with minimal training error.

A simple model of such a situation is that student and teacher are perceptrons but the output of the teacher is corrupted by noise. The cases of additive and multiplicative noise have been widely analyzed [11, 18, 18, 32]. In the first case $\tau = \text{sgn}(B^T \xi + \eta)$ where the noise term $\eta$ is independent of $\xi$ and typically assumed $N(0, \nu)$. For multiplicative noise $\tau = \text{sgn}(B^T \xi) \eta$, $\eta$ is $\pm 1$ and again independent of $\xi$. In this case one will reasonably assume that the mean of $\eta$ is positive so that $\tau$ equals the uncorrupted output $\text{sgn}(B^T \xi)$ with a probability greater than $1/2$.

It is easy to apply the above analysis to the noisy cases since the generalization error of a perceptron $\sigma_J$ is still just a function of the overlap $R = B^T J$. To consider the Gibbs density $p(\sigma)$ given by Eq. (2.2) we use $F(x) = e^{-\beta \Theta(-x)}$ in the definition of $Z_R(D)$. The partition function then is $Z(D) = \int_0^1 dR Z_R(D)$. Now the probability that the weight vector of a student $\sigma_J$ drawn from $p$ has an overlap $R = B^T J$ with the teacher is $Z_R(D)/Z(D)$, and the most probable value $R^*$ of $R$ is obtained by maximizing $Z_R(D)$. Since $N^{-1}\ln Z_R(D)$ and hence $N^{-1}\ln Z(D)$ are selfaveraging, in the thermodynamic limit $R^*$ is again obtained by maximizing $\langle N^{-1}\ln Z_R(D) \rangle_D$.

Major complications arise from the fact that the replica symmetric assumption is invalid for sufficiently high $\beta$ if no student with zero training error exist [11]. This problem can probably be avoided within the framework of a Bayesian analysis, which yields that in the presence of noise the training error should not be minimized when aiming for good generalization. Instead, in the case of multiplicative noise, one uses a carefully chosen finite value of the inverse temperature. Unfortunately this value depends not only on $\alpha$ but also on the noise level [13, 18]. Since the Bayesian strategy involves many assumptions about what is being learned, one may wish to stick with the suboptimal but generally applicable strategy of minimizing $\epsilon_D$, and I shall shortly describe techniques for dealing with the broken replica symmetry.
Chapter 4
Multilayer perceptrons

As mentioned in the introduction a general two layer network is given by

\[ \sigma_{J,w}(\xi) = g \left( \sum_{k=1}^{K} w_k h(\xi^T J_k) \right), \]

and such networks have found many applications both in regression and classification problems. In statistical physics it has only been possible to analyze these networks in the limit where the number of input dimensions \( N \) is much larger than the number of hidden units \( K \). In this limit one will not expect the few adaptable hidden to output couplings \( w_k \) to play a major rôle. Hence one considers so called committee machines where the \( w_k \) are constant and equal 1. (Sometimes, for the sake of normalization, one assumes \( w_k = 1/\sqrt{K} \) instead.)

Formally, the analysis of regression and classification is very similar, and for brevity I shall consider only classification here, results for regression can be found in the papers 7 and 8. For classification the output function is \( g(x) = \text{sgn}(x) \) and I shall also assume that \( h \) is the sign function. So in the sequel the term committee machine (CM) refers to the class of functions

\[ \sigma_J(\xi) = \text{sgn} \left( \sum_{k=1}^{K} \text{sgn}(\xi^T J_k) \right). \] (4.1)

Note that, as for a real committee, the output is decided by the majority vote of the \( K \) hidden units, and we shall assume that \( K \) is odd to avoid a draw. Sometimes it is convenient to consider a simplified architecture the so called tree committee machine (TCM). For the tree the input \( \xi \) is \( NK \) dimensional, composed of \( K \) vectors \( \xi_k \in \mathbb{R}^N \), and

\[ \sigma_J(\xi) = \text{sgn} \left( \sum_{k=1}^{K} \text{sgn}(\xi_k^T J_k) \right). \] (4.2)
This is simpler because the fields $\xi^T J_k$ are now statistically independent if all input components are independent.\footnote{In much of the literature the definition of the tree committee assumes $N/K$ dimensional $J_k$ and $\xi_k$, so that the number of free parameters is $N$ and not $NK$ as in the above definition. But this difference is immaterial as long as final results are expressed in terms of the ratio of examples to free parameters.}

For the committee machine (CM) it is interesting to consider the effect of correlations between the fields $\xi^T J_k$. Let us assume that $J_k = p w_0 + \sqrt{1 - p^2} w_k$ with orthonormal vectors $w_j$ and $p > 0$. Then one will expect that quite often $\sigma_J(\xi) = \text{sgn}(\xi^T w_0)$. Indeed, by the law of large numbers, $\sigma_J(\xi) = \text{sgn}(\xi^T w_0)$, will hold with a probability approaching 1 in the limit of large $K$ if the input components are i.i.d. $N(0, 1)$. So for any finite value of the correlation $p$ the output of the committee becomes identical to that of a perceptron with weight vector $w_0$ in this limit. Hence in many contexts one will expect $p$ to be small when $K$ is large.

We now turn to the capacity problem for these architectures setting

$$Z(\mathbb{D}) = \int dJ \prod_{\mu=1}^P F(\tau^\mu \sigma_J(\xi^\mu)), \quad (4.3)$$

and as for the perceptron

$$\langle Z^n(\mathbb{D}) \rangle_B = \int dJ \left\langle \prod_{a=1}^n F(\tau \sigma_{J_a}(\xi)) \right\rangle_{(\xi, \tau)}^P.$$

Now $dJ$ refers to an integration over $Kn$ unit spheres in $\mathbb{R}^N$. Further we define the $Kn$ by $Kn$ order parameter matrix $Q$ as $Q_{ab}^{kl} = J_a^k J_b^l$ for $a, b = 1, \ldots, n$ and $k, l = 1, \ldots, K$ and an $Kn$ dimensional Gaussian $X(Q)$ with zero mean and covariances

$$\langle X_a^k(Q) X_b^l(Q) \rangle = \begin{cases} Q_{ab}^{kl} & \text{CM} \\ \delta_{kl} Q_{ab}^{kl} & \text{TCM}. \end{cases}$$

The value of $\sigma_{J_a}(\xi)$ is determined by the values of $\xi^T J_a^k$ for the CM and by $\xi^T J_a^k$ for the TCM. Thus

$$\left\langle \prod_{a=1}^n F(\tau \sigma_{J_a}(\xi)) \right\rangle_{(\xi, \tau)} = \left\langle \prod_{a=1}^n F\left( \text{sgn} \left( \sum_{k=1}^K \text{sgn}(X_a^k(Q)) \right) \right) \right\rangle_{X(Q)}.$$

Defining the load parameter as $\alpha = \frac{P}{K N}$ and using the same arguments as in the case of the perceptron yields

$$\lim_{N \to \infty} \frac{\ln \langle Z^n(\mathbb{D}) \rangle_B}{K N} = \max_Q \frac{1}{2K} \ln \det Q + \alpha n \ln \left\langle \prod_{a=1}^n F\left( \text{sgn} \left( \sum_{k=1}^K \text{sgn}(X_a^k(Q)) \right) \right) \right\rangle_{X(Q)}.$$

\footnote{In much of the literature the definition of the tree committee assumes $N/K$ dimensional $J_k$ and $\xi_k$, so that the number of free parameters is $N$ and not $NK$ as in the above definition. But this difference is immaterial as long as final results are expressed in terms of the ratio of examples to free parameters.}
In principle one could now adopt an, e.g., replica symmetric parameterization of $Q$ and obtain an analytic continuation to small $n$. One then still has a large number of order parameters and the extremal problem involves a $K$-fold integral which has to be done numerically. While it would probably be feasible to solve this problem for $K = 3$, to my knowledge no one has done this.

To simplify the extremal problem, it is convenient to view $Q$ as a $K$ by $K$ block matrix indexed by the site indices $k, l$ and consisting of blocks which are $n$ by $n$ matrices. For the TCM the energy term does not depend on $Q^{ab}_{kl}$ if $k \neq l$ and thus in this case at the maximum $Q^{ab}_{kl} = 0$. For both architectures we now make the site symmetric assumption that at the extremum:

$$Q^{ab}_{kl} = \delta_{kl} Q^{ab} + P^{ab} / K, \quad (4.5)$$

which can be more concisely written in block form: $Q = M_K(Q + P/K, P/K)$. As just noted $P = 0$ for the TCM.

Now $\det Q$ can be evaluated in a way which is analogous to the calculation of $M_n(u, v)$. Let $U, V$ be $n$ by $n$ matrices and $x \in \mathbb{R}^N$ then

$$M_K(U, V) \begin{pmatrix} x \\ x \\ \vdots \\ x \end{pmatrix} = \begin{pmatrix} (U + (K - 1)V)x \\ (U + (K - 1)V)x \\ \vdots \\ (U + (K - 1)V)x \end{pmatrix} \{ \text{K rows} \}$$

as well as

$$M_K(U, V) \begin{pmatrix} x \\ -x \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} (U - V)x \\ -(U - V)x \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$ 

The last equation stays valid if the rows of the argument vector and the resulting vector are permuted. We thus obtain a decomposition of $\mathbb{R}^{Kn}$ into a direct sum of $K$ $n$-dimensional eigenspaces of $M_K(U, V)$ and the determinant of $M_K(U, V)$ is just the product of the determinants on the eigenspaces:

$$\det M_K(U, V) = \det(U + (K - 1)V) \det(U - V)^{K-1}, \quad (4.6)$$

and in particular

$$\det Q = \det(Q + P) \det Q^{K-1}. \quad (4.7)$$

---

2 It suffices to show this for a symmetric 2 by 2 block matrix $U = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$, the extension to general $K$ is then by induction. Using (4.6) one has $\det U = \det(\begin{pmatrix} a & b \\ b & c \end{pmatrix})$. So over the positive definite matrices, $0 = \arg \max_c \det(\begin{pmatrix} a & b \\ b & c \end{pmatrix})$, since $\ln \det U$ is a convex function on these matrices. The convexity can be shown by rewriting $(\det(\lambda U + (1 - \lambda)V))^{-1/2}$ as a Gaussian integral and applying Hölders inequality.
CHAPTER 4. MULTILAYER PERCEPTRONS

Equations (4.4, 4.7) form the basis for the following discussion of committee machines. I shall first consider a limiting scenario in which for large $K$ the summation over hidden units is exploited to simplify the energy term using the central limit theorem. This leads to a very simple Gaussian theory which is formally similar to the one for the perceptron. The main result is that the storage capacity diverges with $K$, but the theory only yields limited insight into the rate of divergence. But this approach is highly suited to the analysis of learning problems where the target outputs are not random but given by a rule (see [23, 25, 24, 22, 28, 27] and [31]). As in the case of the perceptron, adapting the capacity calculations to a learning problem is relatively straightforward and I shall not dwell on this. Instead, in the next chapter, I shall consider the more precise capacity calculation obtained by taking the $n \to 0$ limit for fixed $K$ and the interpretation of the replica symmetry breaking found in this calculation in terms of the internal representations of the committee machine.

4.1 Gaussian theory of committee machines

The main idea here is to simplify the energy term by arguing that the distribution of $Y_a = K^{-1/2} \sum_{k=1}^{K} \text{sgn}(X^a_k(Q))$ becomes Gaussian for large $K$. For the TCM this is just stating the multidimensional central limit theorem since $X^a_k(Q)$ and $X^b_l(Q)$ are independent if $k \neq l$. This does not hold for the CM, but assuming the site symmetric parameterization it has been shown in [27] that the limiting joint distribution of the $Y_a$ is Gaussian. Nevertheless, to reduce clutter, I shall only consider the TCM in this section.

Obviously the mean of $Y_a$ is zero and for the covariances one has

$$\langle Y_a Y_b \rangle = K^{-1} \sum_{k=1}^{K} \langle \text{sgn}(X^a_k(Q)) \text{sgn}(X^b_k(Q)) \rangle = K^{-1} \sum_{k=1}^{K} \frac{2}{\pi} \arcsin(Q^{ab}_{kk}) = \frac{2}{\pi} \arcsin(Q^{ab}).$$

I have assumed site symmetry for the last equality. So from (4.4, 4.7) we obtain

$$\lim_{K,N \to \infty} \frac{\ln \langle Z^n(D) \rangle_D}{KN} = \max_Q \frac{1}{2} \ln \det Q + \ln \left\langle \prod_{a=1}^{n} F(\text{sgn}(Y_a(Q^e))) \right\rangle_{Y(Q^e)},$$

where $Y(Q^e)$ is an $n$-dimensional Gaussian with zero mean and

$$\langle Y_a(Q^e) Y_b(Q^e) \rangle = (Q^e)^{ab} = \frac{2}{\pi} \arcsin(Q^{ab}).$$

The essential difference to the corresponding expression for the perceptron (1.7) is that in the energy term the correlation matrix $Q$ is replaced by the effective correlations $Q^e$. 
4.1. GAUSSIAN THEORY OF COMMITTEE MACHINES

Adopting a replica symmetric parameterization of $Q$, it is now straightforward to take the limit of small $n$ and for $F = \Theta$ one finds

$$
\lim_{K,N \to \infty} \frac{\langle \ln Z(D) \rangle_D}{KN} = \min_{q} \frac{1}{2} \frac{q}{1 - q} + \frac{1}{2} \ln(1 - q) + \alpha \left\langle \ln H\left(-z_0 \sqrt{q^e} / \sqrt{1 - q^e}\right)\right\rangle_{z_0}
$$

(4.9)

where again the only difference to the corresponding expression for the perceptron (1.11) is the substitution in the energy term of $q$ by $q^e = \frac{2}{\pi} \arcsin q$. This, however, has a drastic effect on the capacity, since the derivative of $\arcsin q$ is singular at $q = 1$.

As a consequence the energy term, $\left\langle \ln H\left(-z_0 \sqrt{q^e} / \sqrt{1 - q^e}\right)\right\rangle_{z_0}$, diverges as $1/\sqrt{1 - q^e}$ in the limit $q \to 1$ instead of the the $1/(1 - q)$ divergence found for the perceptron.

Now the divergence of the entropy term in (4.9) for $q \to 1$ is no longer balanced by the divergence of the energy term. Hence the minimization problem has a solution for all values of $\alpha$ and in particular $1 - q$ scales as $1/\alpha^2$ for large $\alpha$.

So we have found the important result that the storage capacity of the TCM diverges with the number of hidden units $K$, and in this sense the multilayer perceptron is more powerful than the sum of its parts. Unfortunately the calculation yields no information on how quickly the capacity increases with $K$.

To gain some insight into this question let us consider the accuracy of the Gaussian approximation leading to the above result. Going back to Eq. (4.4) we set $S_k = (X^1_k(Q), X^2_k(Q), \ldots, X^n_k(Q))^T$. Then one can show that $G = K^{-1/2} \sum_{k=1}^K S_k$ converges to a Gaussian by calculating the characteristic function $\langle e^{iV^T G} \rangle_{\{S_k\}}$, where $V \in \mathbb{R}^K$. This yields

$$
\langle e^{iV^T G} \rangle_{\{S_k\}} = \left( e^{iV^T S_1 / \sqrt{K}} \right)^K_{S_1} = \left( 1 - \frac{\langle (V^T S_1)^2 \rangle_{S_1}}{2K} + O\left( \frac{\langle (V^T S_1)^4 \rangle_{S_1}}{K^2} \right) \right)^K_{S_1}
$$

(4.10)

as the odd terms in the expansion vanish because $S_1$ and $-S_1$ have the same distribution. One then argues that the higher order term can be neglected for large $K$, and this yields that the characteristic function converges to

$$
e^{-\frac{1}{2} \left\langle (V^T S_1)^2 \right\rangle_{S_1}} = e^{-\frac{1}{2} V^T S_1 S_1^T V} = e^{-\frac{1}{2} V^T Q^e V},$$

and this, being Gaussian, is the characteristic function of a Gaussian. But now assume that the matrix $Q^e$ is close to singular, let $\lambda$ be its smallest eigenvalue and $V$ an eigenvector to $\lambda$. Then in the second term of the expansion (4.10) the average $\left\langle (V^T S_1)^2 \right\rangle_{S_1}$ is on the order of $\lambda$ and quite small and the quadratic term only give the leading correction if $\lambda$ is large compared to $1/K$, that is if $\lambda K \gg 1$. Otherwise, it only make sense to truncate the expansion after the constant term, in essence equating $\lambda$ with zero, or to take the term of higher than quadratic order into account as well.
In the replica symmetric theory the smallest eigenvalue of $Q_e$ is $1 - q^e$ which approaches zero with increasing $\alpha$. It is impossible to equate $1 - q^e$ with zero, since this leads to a divergence of the energy term in Eq. (4.9). So, since the Gaussian approximation ignores the higher than quadratic terms, it can only be trusted if $(1 - q^e)K$ is large, and the scaling of $q$ with $\alpha$ yields that this requires $\alpha \ll \sqrt{K}$.

On the other hand, if $\alpha \ll \sqrt{K}$, the Gaussian approximation is reliable and thus the theory predicts that the capacity of the TCM is at least $\sqrt{K}$. Indeed, using a replica symmetric parameterization of Eq. (4.4) and taking the $n \to 0$ limit before the large $K$ limit, has been shown to yield a $\sqrt{K}$ divergence of the capacity [2, 6]. Unfortunately these results are completely wrong as already noticed in [2, 6]. In [15] rigorous upper bounds on the capacity are derived, which show that the storage capacity of the TCM cannot diverge with $K$ faster than $\log K$.

4.2 Breaking replica symmetry

It turns out that one does not obtain the correct analytical continuation from integer $n$ to $n$ close to zero when using a replica symmetric parameterization of $Q$. Such a phenomenon was first discovered in the quite different context of the infinite range spin glass [14] and, after much soul searching among the involved physicist, Giorgio Parisi came up with a hierarchical scheme for relaxing the replica symmetric assumption. I shall first apply the first level of this scheme to the TCM (one step of replica symmetry breaking or just RSB1) and then discuss the physical implications of the approach.

The basic idea in RSB1 is to partition the $n$ replicas into $n/m$ groups of equal size and parameterize $Q$ by setting $Q_{ab}$ equal to $q_1$ if the different replicas $a$ and $b$ belong to the same group and to $q_0$ else. Formally this amounts to writing $Q$ as the block matrix

$$Q = M_{n/m}(M_m(1, q_1), M_m(q_0, q_0)).$$

(4.11)

It is simple to calculate the determinant of $Q$ by applying Eq. (4.6) to obtain

$$\det Q = \det M_m \left( 1 + \frac{n-m}{m}q_0, q_1 + \frac{n-m}{m}q_0 \right) \det M_m(1 - q_0, q_1 - q_0) \frac{m}{\sqrt{m}}.$$ 

Our next goal is to decompose the $n$-dimensional Gaussian $Y(Q^e)$ in Eq. (4.8). Note that $Q^e$ has the same structure as $Q$ with the $q_i$ replaced by $q^e_i = \frac{2}{\pi} \arcsin q_i$. Because of the partitioning of the replicas, it is convenient to think of the replica index $a$ as a two dimensional index $a = [u, v]$. We define $[u, v] = (u-1)m + v$ for $v = 1, \ldots, m$, and $u = 1, \ldots, n/m$ indexes the different groups of the partition. One can now rewrite $Y^a = Y^{[u, v]}$ in terms of i.i.d. N(0,1) random variables $z, z^u, z^{u,v}$ as

$$Y^{[u, v]} = \sqrt{q^e_0} z + \sqrt{q^e_1 - q^e_0} z^u + \sqrt{1 - q^e_1} z^{u,v}.$$
So for the $Y(Q^r)$ average in the energy term of (4.8) we obtain

$$
\left\langle \prod_{a=1}^{n} F(\text{sgn}(Y_a(Q^r))) \right\rangle_{Y(Q^r)} = \left\langle \prod_{u,v} F(\text{sgn}(\sqrt{q_0^u z} + \sqrt{q_1^u - q_0^u} z^u + \sqrt{1 - q_1^u} z^{u,v})) \right\rangle_{Z^{u,v,z^{u,z}}}
$$

where the last expression makes sense for noninteger $n$ and $m$. So, using this continuation to small $n$ and assuming that $F = \Theta$, from Eq. (4.8) we obtain within the RSB1 Ansatz

$$
\lim_{\alpha \to \infty} \frac{\langle nZ(B) \rangle_B}{KN} = \min_{q_0, q_1, m} G_s(q_0, q_1, m) + G_r(q_0, q_1, m),
$$

where

$$
G_s = \frac{1}{2} \frac{q_0}{1 - q_1 + m(q_1 - q_0)} + \frac{m - 1}{2m} \ln(1 - q_1) + \frac{1}{2m} \ln(1 - q_1 + m(q_1 - q_0)),
$$

$$
G_r = \frac{\alpha}{m} \ln \left\langle H \left( \sqrt{q_0^u z} - \sqrt{q_1^u - q_0^u} z^u + \sqrt{1 - q_1^u} z^{u,v} \right) \right\rangle_{Z^{u,v,z^{u,z}}}
$$

Let us first discuss the ways in which the RSB1 parameterization reduces to the replica symmetric one. The case $q_1 = q_0 = q$ is obvious, then $G_s + G_r$ no longer depends on $m$ and is the same as (4.9). But also for $m = 1$ one finds that $G_s + G_r$ is independent of $q_1$ and equivalent to the replica symmetric expression with $q_0$ playing the role of $q$. While one cannot set $m = 0$, a little algebra shows that in the limit $m \to 0$ the value of $G_s + G_r$ becomes independent of $q_0$ yielding equivalence to the replica symmetric case with $q_1$ playing the role of $q$.

To solve Eq. (4.12), it helps to first consider the simpler problem of minimizing

$$
F(q_0, q_1, m) = G_s(q_0, q_1, m) + G_r(q_0, q_1, m) - \frac{m - 1}{2m} \ln(1 - q_1) - \frac{1}{2m} \ln m
$$

Setting $q_1 = 1$, one immediately sees that $mF(q, 1, m)$ is independent of $m$ and equal to replica symmetric functional (4.9). Since for any $\alpha > 0$ the latter can be made negative by an appropriate choice of $q$, for this choice of $q$ the value of $F(q, 1, m)$ diverges to $-\infty$ for $m \to +0$. So minimizing $F(q_0, q_1, m)$ is easy.

Due to the divergent $\ln(1 - q_1)$ term in $G_s$, one cannot set $q_1 = 1$ in the function (4.12) we actually want to minimize. But since the divergence is only logarithmic, one will expect the optimal values of $1 - q_1$ and $m$ to be close to 0. Using the asymptotic expansion of $H(x)$ for large arguments, makes it possible to simplify the energy term for $q_1 \to 1$. In the end one finds that the minimization problem has a finite solution for
all values of $\alpha$ and that $q_0 \to q_1 \to 1$ and $m \to 0$ with increasing $\alpha$. The asymptotic scalings are

$$1 - q_0 \propto \alpha^{-2} \quad \text{and} \quad \ln(1 - q_1) \propto \ln m \propto \alpha^2.$$  \hspace{1cm} (4.13)

In spite of the fact that $q_0 \to q_1$ as well as $m \to 0$ are replica symmetric limits, the prediction for the typical volume is completely different. A super-exponential decay is found in RSB1, in contrast to the exponential decay of the volume in the replica symmetric theory.

Most importantly, we obtain a completely different result for the validity of the Gaussian approximation. The smallest Eigenvalue $\lambda$ of $Q^e$ is now $1 - q^e_1$. So in view of (4.13) the $\lambda K \gg 1$ criterion for trusting the central limit theorem translates into $\alpha \ll \sqrt{\ln K}$ and the Gaussian theory now predicts that the critical capacity is at least on the order of $\sqrt{\ln K}$ which is entirely compatible with the rigorous $\ln K$ upper bound.

### 4.3 The physical meaning of RSB

To lighten the notation, I shall discuss the interpretation of RSB in the context of perceptron learning. Since for the perceptron replica symmetry is broken only beyond capacity, the discussion is based on the Gibbs density $p(\sigma J)$ defined by Eq. (2.2). One can then consider the probability density $P_D(q)$ that the weight vectors $J^1_1$ and $J^2_2$ of two perceptrons drawn from the Gibbs density have an overlap $q$. The cumulative distribution function of $P_D(q)$ is

$$C_D(q) = \int_{-1}^{q} dx P_D(x) = \int dJ^1 dJ^2 \Theta(q - J^1T J^2) p(\sigma J^1) p(\sigma J^2)$$

$$= Z(\mathbb{D})^{-2} \int dJ^1 dJ^2 \Theta(q - J^1T J^2) \prod_{a=1}^{P} \prod_{\mu=1}^{P} F(\tau^a J^aT \xi^\mu)$$

We want to calculate the training set average of $C_D(q)$ for large $N$ and to this end consider the related quantity

$$C_\epsilon(q, N, n) = \left\langle Z(\mathbb{D})^{n-2} \int dJ^1 dJ^2 \Theta(\epsilon - J^1T J^2) \prod_{a=1}^{P} \prod_{\mu=1}^{P} F(\tau^a J^aT \xi^\mu) \right\rangle_D$$

where $\Theta_\epsilon(x) = \epsilon + \Theta(x)$. Setting $\epsilon = 0$, for the object of interest to us we have

$$\langle C_D(q) \rangle_D = C_D(q, N, 0).$$  \hspace{1cm} (4.14)

But in the sequel we assume that $\epsilon$ is positive, taking the limit $\epsilon \to 0$ in the end.
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For integer $n \geq 2$ one has

$$C_\epsilon(q, N, n) = \left\langle \int dJ \Theta_\epsilon(q - J^T J) \prod_{a=1}^{n} \prod_{\mu=1}^{P} F(\tau^\mu J_a T \xi^\mu) \right\rangle_D,$$

and, using replicas, we evaluate the RHS for general $n$. To get rid of the special treatment of the first two indices, we introduce the function

$$G_\epsilon(q, Q) = \frac{1}{n(n-1)} \sum_{a \neq b} \Theta_\epsilon(q - Q^{ab})$$

and by symmetry

$$C_\epsilon(q, N, n) = \left\langle \int dJ G_\epsilon(q, J^T J) \prod_{a=1}^{n} \prod_{\mu=1}^{P} F(\tau^\mu J_a T \xi^\mu) \right\rangle_D.$$

Transforming the integral to the order parameter matrix $Q$ yields

$$C_\epsilon(q, N, n) = D_n(1) \int dQ G_\epsilon(q, Q) \left( \left( \det Q \right)^{-\frac{1-(\alpha+1)/2}{N}} \left\langle \prod_{a=1}^{n} F(X_a(Q)) \right\rangle_{X(Q)}^\alpha \right)^N.$$

The integral will decay to zero with increasing $N$, and the asymptotic rate of decay is to leading order found by Laplace’s method [3]. This shows that the decay is determined by the properties of the integrand in arbitrarily small neighborhoods of its maxima. In fact, since $\epsilon$ is positive, $G_\epsilon(q, Q)$ does not vanish, and we need only the neighborhood of a maximum $Q_\ast(n)$ of $(\det Q)^{-\frac{1-(\alpha+1)/2}{N}} \left\langle \prod_{a=1}^{n} F(X_a(Q)) \right\rangle_{X(Q)}^\alpha$ if this maximum is unique up to permutations of the replica indices. Further $G_\epsilon(q, Q)$ is piecewise constant, and in particular $G_\epsilon(q, Q) = G_\epsilon(q, Q_\ast(n))$ holds in a neighborhood of the maximum, except if $q$ is equal to an off-diagonal element of $Q_\ast(n)$. So for a generic value of $q$ we can treat $G_\epsilon(q, Q)$ as a factor constant in $Q$ and find

$$\lim_{N \to \infty} \frac{C_\epsilon(q, N, n)}{C_\epsilon(1, N, n)} = \frac{G_\epsilon(q, Q_\ast(n))}{G_\epsilon(1, Q_\ast(n))}.$$

Thus in any parameterization of $Q_\ast(n)$ which enables us to take $n$ to zero, considering the limit $\epsilon \to 0$, we obtain for the cumulative distribution of $q$

$$\lim_{N \to \infty} \langle C_D(q) \rangle_D = \lim_{n \to 0} G_0(q, Q_\ast(n)).$$

We have used (4.14) and the fact that $G_0(1, Q_\ast(n)) = 1$.

In replica symmetry this yields the simple result that $\langle C_D(q) \rangle_D$ approaches the step function $\Theta(q - q_\ast)$ for large $N$, where $q_\ast$ is the stationary value of the order parameter for small $n$. Further, since $\langle C_D(q) \rangle_D$ converges to a step function with a single step, $C_D(q)$ is selfaveraging.
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If $Q$ is the RSB1 matrix $Q_{RSB1}$, one has $G_0(q, Q) = \frac{n-m}{n-m+1} \Theta(q-q_0) + \frac{m-1}{n-m+1} \Theta(q-q_1)$. So setting $n$ to zero we obtain as the physical interpretation of RSB1 that the cumulative distribution of $q$ has two steps:

$$\lim_{N \to \infty} \langle C_D(q) \rangle_D = m \Theta(q-q_0) + (1-m) \Theta(q-q_1).$$

However, when replica symmetry is broken, $C_D(q)$ is no longer self-averaging $[14, 10]$. So, even for large $N$, not all properties of the single system, can be deduced from those of the training set average in this case.

4.4 Beyond RSB1?

For the TCM discussed in Section 2 the order parameter $q$ refers to the overlap between the weight vectors of the same hidden unit of two TCM’s in version space. So, the RSB1 solution, means that the pattern averaged density of this overlap converges to two $\delta$-peaks. Why not three?

Indeed, it is straightforward two allow for three peaks by parameterizing $Q$ as

$$Q = M_{n/m_1}(R_1(m_1, m_2; 1, q_2, q_1), R_1(m_1, m_2; q_0, q_0, q_0)),$$

where $R_1$ denotes an RSB1-matrix, $R_1(n, m; a, b, c) = M_{n/m}(M_m(a, b), M_m(c, c))$. Of course, one might still think that this RSB2 Ansatz is not general enough, and recursively continue to construct an RSB-$k$ parameterization allowing for $k + 1$ peaks.

Using the techniques discussed for RSB1, it is straightforward, if somewhat tedious, to write down the minimization problem for the typical volume using a, say, RSB2 parameterization. And I would expect, that for sufficiently large but finite $\alpha$ a higher order RSB parameterization does improve on RSB1. But it is not clear that this will affect the capacity result, because the higher order solutions can converge to the RSB1 solution with increasing $\alpha$. One will in fact expect the $q$’s to converge to 1, that is toward a single peak, and already in the RSB1 parameterization, rather extreme scalings are needed to construct a non replica symmetric solution. Unfortunately, it would be extremely complicated, to show analytically, that any RSB2 solution must be degenerate with the RSB1 solution (4.13) in the large $\alpha$ limit. Indeed I have not even proven that the solution (4.13) is the unique global minimum in RSB1 space. But it would perhaps be worthwhile to numerically track a higher order RSB solution to large values of $\alpha$. 

4.5 Storage capacity of the CM

We now obtain an accurate value for the capacity of the CM by taking the limit $n \to 0$ limit for finite $K$. Going back to Eq. (4.4) and using the site symmetry assumption (4.5) we consider the RSB1-theory. Since we are dealing with the fully connected architecture, the matrices $Q$ and $P$ are parameterized as:

$$
Q = M_{n/m}(M_m(1 - \frac{p_2}{K}, q_1), M_m(q_0, q_0)), \quad P = M_{n/m}(M_m(p_2, p_1), M_m(p_0, p_0)).
$$

(4.16)

To decompose the Gaussians $X_k^a(Q)$ in Eq. (4.4), we rewrite $a$ in form of the two dimensional index $[u, v]$ as in Section 4.2, employ the i.i.d. $\mathcal{N}(0, 1)$ Gaussians $z_k, z_k^u, z_k^{u,v}$ and set:

$$
X_k^{[u,v]} = uz_k + vz_k^u + wz_k^{u,v} + \bar{u}z_k + \bar{v}z_k^u + \bar{w}z_k^{u,v}.
$$

(4.17)

Here the parameters $(u, v, \text{etc.})$ have to be chosen so that $Q = M_K(Q + P/K, P/K)$ holds for the covariance matrix $Q$ of the $X_k^a$. The last three summands in (4.17) are needed because the sites can be correlated ($P \neq 0$). In keeping with our usual style of decomposing Gaussians one might expect $\bar{z}, \bar{z}^u, \bar{z}^{u,v}$ to be $\mathcal{N}(0, 1)$ Gaussians independent of each other and the other random variables. However, it turns out that in the relevant regime the sites are anti-correlated, $\langle X_k^a X_l^a \rangle < 0$ for $k \neq l$. If all random variables in the decomposition are independent, such anti-correlations are only possible if, say, $\bar{u}$ is imaginary. This is probably not really a problem because the averages in the energy term lead to $H$-functions which do make sense for complex arguments. However, I find this too murky, $X_k^{[u,v]}$ is after all a real valued Gaussian, and thus adopt a different definition of $\bar{z}, \bar{z}^u, \bar{z}^{u,v}$, setting:

$$
\bar{z} = K^{-1} \sum_{k=1}^K z_k, \quad \bar{z}^u = K^{-1} \sum_{k=1}^K z_k^u, \quad \bar{z}^{u,v} = K^{-1} \sum_{k=1}^K z_k^{u,v}.
$$

Then a simple calculation shows, that the $X_k^a$ have the desired covariances if the parameters satisfy

$$
\begin{align*}
    u^2 &= q_0, & \quad (u + \bar{u})^2 &= p_0 + q_0, \\
    v^2 &= q_1 - q_0, & \quad (v + \bar{v})^2 &= q_1 + p_1 - q_0 - p_0, \\
    w^2 &= 1 - p_2/K - q_1, & \quad (w + \bar{w})^2 &= 1 - p_2/K + p_2 - q_1 - p_1.
\end{align*}
$$

(4.18)
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Using this decomposition the average in the energy term of Eq. (4.4) can be rewritten as:

\[ \langle \prod_{a=1}^{n} F \left( \text{sgn} \left( \sum_{k=1}^{K} \text{sgn} \left( X_{k}^{a} (Q) \right) \right) \right) \rangle_{X(Q)} \]

\[ = \left\langle \left\langle \left\langle F \left( \text{sgn} \left( \sum_{k=1}^{K} \text{sgn} \left( uz_{k} + vz_{k}^{1} + w_{k}^{1,1} + \bar{u} \bar{z}^{1} + \bar{v} \bar{z}^{1,1} \right) \right) \right) \right\rangle_{\{z_{k}^{1,1}\}} \right\rangle_{\{z_{k}\}} \left\rangle_{\{z_{k}\}} \right\rangle_{\{z_{k}\}} \cdot \]

To lighten the notation in the last equation (4.17) is used to write the fields in a more compact form.

For the entropy term, we need \( \det Q \) and the determinant is easily calculated by repeatedly applying (4.6). Specializing to \( F = \Theta \), from the small \( n \) limit one then obtains:

\[ \lim_{N \to \infty} \frac{\langle \ln Z(D) \rangle_{D}}{KN} = \frac{1}{m} G_{s} (\{q_{i}\}, \{p_{i}\}, m) + \frac{\alpha}{m} G_{r} (\{q_{i}\}, \{p_{i}\}, m) \quad (4.19) \]

where

\[ G_{s} = \frac{K-1}{2K} S (u^{2}, v^{2}, w^{2}, m) + \frac{1}{2K} S \left( (u + \bar{u})^{2}, (v + \bar{v})^{2}, (w + \bar{w})^{2}, m \right) \]

\[ S(a, b, c, m) = (m-1) \ln c + \ln (c + mb) + \frac{ma}{c + mb} \]

and

\[ G_{r} = \left\langle \ln \left\langle \Theta \left( \text{sgn} \left( \sum_{k=1}^{K} \text{sgn} \left( X_{k}^{[1,1]} \right) \right) \right) \right\rangle_{\{z_{k}^{1,1}\}} \right\rangle_{\{z_{k}\}} \left\rangle_{\{z_{k}\}} \cdot \]

The extremum in Eq. (4.19) means that the function has to be minimized w.r.t to all order parameters except \( p_{0} \). The function has to be maximized w.r.t to \( p_{0} \) since in physical terms \( p_{0} = K J_{k}^{aT} J_{k}^{a} \). So \( p_{0} \) refers to a quantity with a single replica index and is analogous to the student/teacher overlap in the context of learning a rule in the following sense: Instead of considering the full space of networks, we could have focused on sub-shells where \( J_{k}^{aT} J_{k} \) is constant. The capacity of the full space of networks is given by the sub-shell of maximal capacity and this is just what is obtained by maximizing Eq. (4.19) in \( p_{0} \).

It is impractical to calculate \( G_{r} \) in its present form since this involves \( 3K \) Gaussian integrals. To do something about this, we first rewrite (4.19) in terms of the internal
representations $i$ in the committee, that is in terms of the outputs $i_k$ of its hidden units. We use
\[
1 = \text{Tr}_i \prod_{k=1}^{K} \Theta(i_k X_k^{[1,1]}),
\]
where the trace over $i$ denotes a summation over all $i \in \{-1, 1\}^K$. Multiplying the $\Theta$-function in $G_r$ with the above RHS yields:
\[
G_r = \left< \ln \left< \text{Tr}_i \Theta \left( \sum_{k=1}^{K} i_k \prod_{k=1}^{K} \Theta(i_k X_k^{[1,1]}) \right)^m \right> \right>_{\{z^1_k\}}_{\{z_k\}}.
\]
To highlight the dependence of the energy term on $w$ and $\bar{w}$, we now define:
\[
f(\{Y_k\}, \{i_k\}) = \prod_{k=1}^{K} \Theta[\{Y_j + w z_k^{1,1} + \bar{w} \bar{z}^{1,1}\}] \quad \text{and} \quad Y_k = u z_k + \bar{u} \bar{z} + v z_k^{1,1} + \bar{v} \bar{z}^{1,1},
\]
so
\[
G_r = \left< \ln \left< \text{Tr}_i \Theta \left( \sum_{k=1}^{K} i_k \right) f(\{Y_k\}, \{i_k\}) \right> \right>_{\{z^1_k\}}_{\{z_k\}}.
\]
As $\alpha$ approaches the critical capacity the volume of admissible networks vanishes and one will expect that $w, \bar{w} \to 0$. In this limit the trace is dominated by a single term and thus
\[
\left( \text{Tr}_i \Theta \left( \sum_{k=1}^{K} i_k \right) f(\{Y_k\}, \{i_k\}) \right)^m \sim \max_{i} \Theta \left( \sum_{k=1}^{K} i_k \right) f(\{Y_k\}, \{i_k\})^m.
\]
It is too troublesome to locate the maximum as function of the $Y_k$ and hence we replace the maximization in $i$ by a summation over all possible values of $i$. So we use that for $w, \bar{w} \to 0$
\[
\left( \text{Tr}_i \Theta \left( \sum_{k=1}^{K} i_k \right) f(\{Y_k\}, \{i_k\}) \right)^m \leq \text{Tr}_i \Theta(\sum_{k=1}^{K} i_k) f(\{Y_k\}, \{i_k\})^m.
\]
(4.21)
The simplified energy term
\[
\hat{G}_r = \left< \ln \left< \text{Tr}_i \Theta \left( \sum_{k=1}^{K} i_k \right) f(\{Y_k\}, \{i_k\})^m \right> \right>_{\{z^1_k\}}_{\{z_k\}}.
\]
obtained by commuting the trace and the exponentiation with $m$ is an upper bound to the true value of $G_r$ for $w, \bar{w} \to 0$, and we consider the extremal problem

$$\text{extr}_{\{q_i\}, \{p_i\}, m} G_s(\{q_i\}, \{p_i\}, m) + \alpha \hat{G}_r(\{q_i\}, \{p_i\}, m) \quad (4.22)$$

instead of (4.19).

While (4.22) is more accessible than the original extremal problem, the remaining calculations are nevertheless quite involved and they are described in some detail in [30]. Here, I shall just present the key features of the solution. At a critical value $\hat{\alpha}_c(K)$ of $\alpha$ which for large $K$ scales as

$$\hat{\alpha}_c(K) \sim \frac{16}{\pi - 2} \sqrt{\ln K}$$

the solution of (4.22) diverges. At the critical $\alpha$ the stationary values of $w$ and $\bar{w}$ vanish. Consequently the extremal value of (4.22) bounds the extremal value of the original problem (4.19) and $\hat{\alpha}_c(K)$ is an upper bound to the true capacity $\alpha_c(K)$. An interesting question is, whether this upper bound coincides with the critical capacity to leading order in $K$. This is related to the question if the inequality (4.21) is sufficiently tight at the stationary point. Since the trace over the internal representations $\iota$ on its LHS is dominated by a single term due to $w, \bar{w} \to 0$, the inequality would be tight if also on the RHS the trace were dominated by a single term. This, however, is tricky, since as $\alpha$ approaches $\hat{\alpha}_c(K)$ one finds that also $m \to 0$. Consequently as function of $\iota$ the maximum of $f(\{Y_k\}, \{\iota_k\})^m$ on the RHS is not as pronounced as the one of just $f(\{Y_k\}, \{\iota_k\})$ on the LHS of the inequality. So the tightness of the inequality is determined by the ratios of $w, \bar{w}$ and $m$ as they approach zero. These are calculated in [30] and suggest that while a few terms do contribute to the trace on the RHS, their number is not very large, and that the critical capacity to leading order coincides with $\hat{\alpha}_c(K)$. It would however require quite intricate combinatorics to actually show that this is the case.

Finally, it is interesting to compare the results for the connected committee to the ones for the tree architecture. For the TCM entirely analogous calculations [16, 17] yield the smaller capacity of $\frac{16}{\pi} \sqrt{\ln K}$. This difference is due to the fact that at the critical capacity the weight vectors of the CM are anti-correlated, $p_0 = -1$. If one were to artificially restrict the state space of the CM so that the $K$ weight vectors are forced to be orthogonal, this corresponds to $p_0 = 0$, the capacities of the CM and the TCM would be the same. The usefulness of anti-correlated hidden units is related to the fact that in the orthogonal case the output of the CM is quite similar to that of a perceptron. In particular, if one considers the perceptron with weights $\bar{J}$ obtained by averaging the weight vectors $J_k$ of the CM, $\bar{J} = \sum_{k=1}^{K} J_k$, one finds that when $p_0 = 0$ this perceptron gives the same output as the CM for approximately 80% of randomly chosen inputs even when $K$ is large. However, $p_0 = -1$ leads to $\bar{J} = 0$, the approximating perceptron is undefined, and no perceptron improves on random guessing in predicting the output.
of this CM for large $K$. Since the storage capacity of the perceptron is limited, the anti-correlated state maximizes the capacity of the committee.

### 4.6 Counting internal representations

Historically, the capacity of the committee machine was first obtained by counting the typical number of internal representations of a training set [16, 17] and not by the RSB1 calculations of the Gardner volume. To round off the analysis of the CM, I shall describe the close relationship between the two approaches.

Given a training set $\mathbb{D} = \{ (\xi^\mu, \tau^\mu) \}$ one can ask whether outputs $\iota_k^\mu \in \{-1, 1\}$ of the hidden units exist which can be (a) realized by the committee and for which (b) the output of the committee on $\xi^\mu$ is $\tau^\mu$. This amounts to asking whether the volume of weights

$$V_i(\mathbb{D}) = \prod_{\mu=1}^{P} \Theta(\tau^\mu \sum_{k=1}^{K} \iota_k^\mu) \int \mathcal{D} J \prod_{\mu=1}^{P} \prod_{k=1}^{K} \Theta(\iota_k^\mu J_k^T \xi^\mu).$$

(4.23)

associated with the internal representation $i$ is nonzero. There are $2^{(K-1)P}$ internal representations with the property (b), $\tau^\mu \sum_{k=1}^{K} \iota_k^\mu > 0$, but not all of them will be realizable by the committee. So the quantity of interest is the typical number of realizable representations

$$\exp \langle \ln \text{Tr} \Theta (V_i(\mathbb{D})) \rangle_{\mathbb{D}}.$$

To obtain the training set average one uses a double replication. Instead of $\Theta (V_i(\mathbb{D}))$ one considers $V_i(\mathbb{D})^m$ for integer $m$ taking the limit $m \to 0$ in the end; the second replication is used to calculate the logarithm in the usual way. We thus consider

$$S(m) = \frac{1}{KN} \frac{d}{d \hat{n}} \left[ \left\langle \left( \text{Tr} V_i(\mathbb{D})^m \right) \right\rangle_{\mathbb{D}} \right]_{\hat{n}=0}$$

(4.24)

and are mainly interested in $S(0) = \lim_{m \to 0} S(m)$. As long as $S(0)$ is positive, realizable internal representations exist, and the storage capacity of the committee is not exhausted. For $P = \alpha KN$, the smallest value $\alpha_d(K)$ for which $S(0) = 0$ marks the transition to a regime where the number of internal representations is no longer exponential in $N$. So $\alpha_d(K)$ is a lower bound on the capacity and for finite $K$ one will not expect the bound to be tight; for instance $\alpha_d(1) = 0$ but the critical capacity for $K = 1$ is $2$. It is, however, reasonable to expect that $\alpha_d(K)$ for large $K$ yields an asymptotically tight bound since the volume in weight space associated with any single internal representation should vanish in this limit.

To calculate $S(m)$ we use Eq. (4.23) and obtain in a first step

$$\left( \text{Tr} V_i(\mathbb{D})^m \right) = \int \mathcal{D} J \prod_{\mu,u} \text{Tr} \Theta(\tau^\mu \sum_{k=1}^{K} \iota_k^\mu) \prod_{u,v} \Theta(\iota_k^\mu J_{k,uv}^T \xi^\mu),$$

(4.25)
where the replica index $v$ runs from 1 to $m$, and for the other replica index: $u = 1, \ldots, \hat{n}$. The symbol $dJ$ refers to $K\hat{n}m$ integrations over unit length weight vectors $J_{k}^{uv}$ in $\mathbb{R}^{N}$. We now have to perform the training set average which, after commuting with the weight integral, can be rewritten in terms of zero mean Gaussian random variables $X_{k}^{uv}(Q)$ with covariances

$$
\langle X_{k}^{uv}(Q)X_{k'}^{u'v'}(Q) \rangle = Q_{kk'}^{uu'v'v} = J_{k}^{uu}J_{k'}^{v'v'}
$$

Transforming to an integral over the order parameter matrix then yields

$$
\lim_{N \to \infty} \frac{\langle \text{Tr}_{V}(D)^{m} \rangle_{D}}{KN} = \max_{Q} \alpha \ln \left( \prod_{u} \text{Tr} \Theta \left( \sum_{k=1}^{K} \mu_{k}^{u} \right) \prod_{u,v} \Theta \left( (\mu_{k}^{u}X_{k}^{uv}(Q)) \right) \right)_{X(Q)} + \frac{\ln \det Q}{2K}.
$$

To make further progress we need to parameterize $Q$. Referring back to Eq. (4.25), we see that the weight vectors $J_{k}^{uv}$ and $J_{k'}^{u'v'}$ belong to committee machines which use the same internal representation to store the training set if $u = u'$. So, even when aiming for a replica symmetric parameterization, it makes sense to assume that $Q_{kk'}^{uu'u'v'}$ depends on $\delta_{uu'}$. Further, to control the number of order parameters, we need to assume site symmetry, that is $Q$ depends on $k$ and $k'$ only via $\delta_{kk'}$. These considerations motivate parameterizing $Q$ as $Q = M_{K}(Q + P/K, P/K)$ where

$$
Q = M_{\hat{n}}(M_{m}(1 - \frac{p_{2}}{K}, q_{1}), M_{m}(q_{0}, q_{0})), \quad P = M_{\hat{n}}(M_{m}(p_{2}, p_{1}), M_{m}(p_{0}, p_{0})).
$$

Now, comparing to Eq. (4.16), we see that this is just the RSB1-parameterization used in the Gardner volume calculation for the CM if we equate $\hat{n} = n/m$. So we have already calculated $\det Q$ and the same decomposition of $X(Q)$ into independent contributions as in the preceding section can be used. We then obtain the following remarkable analogy to the calculation of the Gardner volume:

$$
S(m) = \max_{\{q_{i}, \{p_{i}\}\}} G_{s}\{q_{i}\}, \{p_{i}\}, m\} + \alpha \hat{G}_{r}\{q_{i}\}, \{p_{i}\}, m\},
$$

where $G_{s}$ and $\hat{G}_{r}$ are exactly the same as in the preceding section. The critical capacity $\alpha_{c}(K)$ is given by the condition $S(0) = 0$. In the RSB1-calculation the bound $\hat{\alpha}_{c}(K)$ was obtained from the divergence to $-\infty$ of $(G_{s} + \hat{G}_{r})/m$ when this expression was also minimized w.r.t. to $m$. But minimizing in $m$ yielded that $m \to 0$ as $\alpha$ approaches $\hat{\alpha}_{c}(K)$ and this is just the limit needed when counting internal representations. So we obtain the simple result that

$$
\alpha_{d}(K) = \hat{\alpha}_{c}(K) \sim \frac{16}{\pi - 2} \sqrt{\ln K}.
$$
4.6. COUNTING INTERNAL REPRESENTATIONS

In addition we now have a very nice interpretation of the order parameters, e.g. the overlaps \( q_1, p_2 \) refer to networks which use the same internal representation to store the training patterns, whereas networks with differing internal representations yield the overlaps \( q_0, p_1 \).

However, all is not well. By definition \( \alpha_d(K) \) should be a lower bound to the critical capacity, but \( \hat{\alpha}_c(K) \) is an upper bound. This shows that the above (doubly) replica symmetric parameterization is too simple minded, and replica symmetry is broken, presumably for networks which use different internal representations. However, having argued that both \( \alpha_d(K) \) and \( \hat{\alpha}_c(K) \) are tight bounds in the limit of large \( K \), one can reasonably assume that this complication does not invalidate the asymptotic findings. This is supported by results in [17] where the stability of the replica symmetric stationary point was analyzed for the TCM when counting internal representations. The replica symmetric solution was found unstable for finite values of \( K \) but marginally stable in the large \( K \) limit.
Appendix A

The entropy term

We want to calculate a volume of the form

\[ D_n(Q) = \int dJ \, \delta(Q - J^T J) = \int dJ \prod_{a,b=1}^{n} \delta (Q^{ab} - J^a J^b) \quad (A.1) \]

where \( Q \) is a symmetric, positive definite \((n, n)\)-matrix of overlaps and \( J \) is the \((N, n)\)-matrix which is composed of the \( n \) vectors \( J^a \in \mathbb{R}^N \).

For a suitable orthogonal \((n, n)\)-matrix \( o \) and a diagonal \((n, n)\)-matrix \( D \) one can write \( Q = o^T D D o \). We now apply the linear transformation \( J \rightarrow J D o \) to the above integral. Its determinant is \( \det D^N \) and we obtain

\[ D_n(Q) = \int dJ \, \delta(o^T D(1 - J^T J)Do) \, \det D^N. \quad (A.2) \]

The Fourier representation of the \( \delta \)-function yields

\[ \delta(o^T D(1 - J^T J)Do) = C_n \int d\hat{Q} \, \exp \left( i \, \text{Tr} \left[ \hat{Q} o^T D(1 - J^T J)Do \right] \right). \quad (A.3) \]

The integration runs over symmetric \((n, n)\)-matrices and \( C_n = (2\pi)^{-n(n+1)/2}2^{n(n-1)/2} \), where the second factor arises from the fact that the off-diagonal elements are counted twice in the trace. Using

\[ \text{Tr} \left[ \hat{Q} o^T D(1 - J^T J)Do \right] = \text{Tr} \left[ Do \hat{Q} o^T D(1 - J^T J) \right] \]

and transforming \( \hat{Q} \) via \( \hat{Q} \rightarrow o^T D^{-1} \hat{Q} D^{-1} o \) yields

\[ \delta(o^T D(1 - J^T J)Do) = C_n \det D^{-n-1} \int d\hat{Q} \, \exp \left( i \, \text{Tr} \left[ \hat{Q}(1 - J^T J) \right] \right) \]

\[ = C_n \det D^{-n-1} \delta(1 - J^T J) \quad (A.4) \]
and thus $D_n(Q) = \det D^{N-n-1} D_n(1)$. Of course $\det D^2 = \det Q$, so finally

$$D_n(Q) = D_n(1)(\det Q)^{(N-n-1)/2} \quad (A.5)$$

where $D_n(1)$ is just a normalization constant.

The case where one considers an additional $(N, m)$-Matrix $B$ of $m$ teacher vectors and wants to evaluate $\int dJ \ \delta(Q - J^T J) \ \delta(R - J^T B)$ reduces to the above consideration by noting that the integral will not depend on the choice of $B$, as long as the matrix of teacher overlaps $T = B^T B$ is held fixed. Thus, one may in addition integrate over all $B$ which have correlation matrix $T$. 


Bibliography

[1] M. Ahr, M. Biehl, and R. Urbanczik. Statistical physics and practical training of soft-committee machines. *Eur. Phys. J. B*, 10:583–588, 1999.

[2] E. Barkai, D. Hansel, and H. Sompolinsky. Broken symmetries in multilayered perceptrons. *Phys. Rev. A*, 45:4146 – 4161, 1992.

[3] E. Copson. *Asymptotic expansions*. Cambridge University Press, Cambridge, 1965.

[4] A. Engel and C. Van den Broeck. *Statistical Mechanics of Learning*. Cambridge University Press, Cambridge, 2001.

[5] A. Engel and W. Fink. Statistical mechanics calculation of Vapnik-Chervonenkis bounds for the perceptron. *J. Phys. A*, 26:6893 – 6914, 1993.

[6] A. Engel, H.M. Köhler, F. Tschepke, H. Vollmayr, and A. Zippelius. Storage capacity and learning algorithms for two layer neural networks. *Phys. Rev. A*, 45:7590 – 7607, 1992.

[7] E. Gardner. Maximum storage capacity in neural networks. *Europhys. Lett.*, 4:481–485, 1987.

[8] E. Gardner and B. Derrida. The space of interactions in neural network models. *Journal of Physics A*, 21:257–270, 1988.

[9] E. Gardner and B. Derrida. Three unfinished works on the optimal storage capacity of networks. *Journal of Physics A*, 22:1983–1994, 1989.

[10] G. Györgyi. Techniques of replica symmetry breaking and the storage problem of the McCulloch-Pitts neuron. *Physics Reports*, to appear, 2001.

[11] G. Györgyi and N. Tishby. Statistical theory of learning a rule. In K. Thuemann and R. Köberle, editors, *Neural networks and spin glasses*, pages 3–36, Singapore, 1990. World Scientific.

[12] J. Hertz, A. Krogh, and R.G. Palmer. *Introduction to the Theory of Neural Computation*. Addison-Wesley, Redwood City etc., 1991.
BIBLIOGRAPHY

[13] W. Krauth and M. Mézard. Storage capacity of memory networks with binary couplings. J. Phys. France, 50:3057–3066, 1989.

[14] M. Mézard, G. Parisi, and M.A. Virasoro. Spin Glass Theory and Beyond. World Scientific, Singapore, 1987.

[15] G.J. Mitchison and R.M. Durbin. Bounds on the learning capacity of some multilayer networks. Biological Cybernetics, 60:345–356, 1989.

[16] R. Monasson and R. Zecchina. Weight space structure and internal representations: a direct approach to learning and generalization in multilayer neural networks. Phys. Rev. Lett., 75:2432 – 2435, 1995.

[17] R. Monasson and R. Zecchina. Learning and generalization theories of large committee machines. Mod. Phys. Lett. B, 9:1887 – 1897, 1996.

[18] M. Opper and D. Haussler. Calculation of the learning curve of Bayes optimal classification algorithm for learning a perceptron with noise. In L.G. Valiant and M.K. Warmuth, editors, Proceedings of the fourth annual workshop on computational learning theory, pages 75–87, San Mateo, 1991. Morgan Kaufmann.

[19] M. Opper and D. Haussler. Generalization performance of Bayes optimal prediction algorithm for learning a perceptron. Phys. Rev. Lett., 66:2677–2680, 1991.

[20] L. Schlöfli. Theorie der vielfachen Kontinuität. Zürich, 1901.

[21] M. Schröder and R. Urbanczik. Comment on ‘Finite size scaling in neural networks’. Phys. Rev. Lett., 80:4109, 1998.

[22] H. Schwarze. Learning a rule in a multilayer neural network. J. Phys. A, 26:5781 – 5794, 1993.

[23] H. Schwarze and J. Hertz. Generalization in a large committee machine. Europhys. Lett., 20:375 – 380, 1992.

[24] H. Schwarze and J. Hertz. Generalization in fully connected committee machines. Europhys. Lett., 21:785 – 790, 1993.

[25] H. Schwarze, M. Opper, and W. Kinzel. Generalization in a two-layer neural network. Phys. Rev. A, 46:R6185 – R6188, 1992.

[26] R. Urbanczik. Storage capacity of the tree-structured committee machine with discrete weights. Europhys. Lett., 26:233 – 238, 1994.

[27] R. Urbanczik. A fully connected committee machine learning unrealizable rules. J. Phys. A, 28:7097 – 7104, 1995.
[28] R. Urbanczik. A large committee machine learning noisy rules. *Neural Computation*, 8:1267 – 1276, 1996.

[29] R. Urbanczik. Learning in a large committee machine: worst case and average case. *Europhys. Lett.*, 35:553 – 558, 1996.

[30] R. Urbanczik. Storage capacity of the fully connected committee machine. *J. Phys. A*, 30:L387 –L391, 1997.

[31] R. Urbanczik. Multilayer perceptrons may learn simple rules quickly. *Phys. Rev. E*, 58:2298 –2301, 1998.

[32] T. Watkin, A. Rau, and M. Biehl. The statistical mechanics of learning a rule. *Rev. Mod. Phys*, 65:499 – 556, 1993.