Learning multilayer perceptrons efficiently

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A learning algorithm for multilayer perceptrons is presented which is based on finding the principal components of a correlation matrix computed from the example inputs and their target outputs. For large networks our procedure needs far fewer examples to achieve good generalization than traditional on-line algorithms.

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Multilayer neural networks achieve the ability to approximate any reasonable function arbitrarily well by interconnecting sufficiently many architecturally identical processing elements, the perceptrons. This replication of identical elements invariably leads to symmetries in the multilayer architecture which need to be broken during training to achieve good generalization. In the dynamics of gradient based training procedures the symmetries give rise to suboptimal fixed points and slow convergence. In particular this holds for stochastic gradient descent methods which to date have been the method of choice for training large networks because, at each time step, the update of the network parameters is based on the presentation of only a single training example and hence computationally cheap. Such stochastic gradient descent methods have been intensively studied in the framework of on-line learning, where each of the training examples is used just once by the network. This is attractive because there is no need to store the entire set of training examples, and the approach also works for nonstationary problems. However, in the on-line framework the number of required training examples is coupled to the slow temporal evolution caused by the symmetries and thus unreasonably large training sets are necessary. In fact the ratio of the number of examples needed for good generalization to the number of free parameters in the network diverges with the network size. While there have been investigations into optimizing the on-line dynamics, these have not lead to practical algorithms since the optimized procedures assume that the symmetry breaking provided by the initial conditions is macroscopic and known to the learning algorithm.

In this letter we present a learning algorithm which has many of the attractive features of the traditional on-line procedures but yields good generalization using a much smaller number of training examples. Further an exact analysis of the algorithm’s performance shows that the ratio of required examples to the number of free parameters in the networks does stay finite in the thermodynamic limit.

The multilayer architecture we analyze is a committee machine with $K$ hidden units defined by

$$
\tau(\xi) = g \left( K^{-1/2} \sum_{i=1}^{K} h(B_i^T \xi) \right),
$$

where $\xi \in \mathbb{R}^N$ is the input and the $B_i \in \mathbb{R}^N$ are the unknown parameter vectors. The goal of learning is to estimate these parameter vectors, which we shall refer to as teacher vectors, from a training set of $P$ examples $(\xi^\mu, \tau(\xi^\mu))$ of the input/output relationship. We shall initially focus on regression problems and later sketch the modifications to our procedure needed for classification tasks. For regression, the output function $g$ is usually assumed invertible, and this easily reduces to the linear case by applying the inverse function to the target outputs. So in this case we simply assume $g(x) = x$. For brevity we also assume that the $B_i$ are orthonormal.

In its simplest form our procedure can be seen as generalizing Hebbian learning. There the parameter vector $J^P$ of a simple perceptron approximating the target function $\tau(\xi)$ is obtained as the average

$$
J^P = P^{-1} \sum_{\mu=1}^{P} \tau(\xi^\mu) \xi^\mu.
$$

Our basic observation is that when $\tau(\xi)$ is given by a multilayer perceptron it is important to not only consider the empirical mean of the distribution of $\tau(\xi^\mu)\xi^\mu$ as in plain Hebbian learning but also its correlation matrix. In particular some of the eigenvectors of the correlation matrix correspond to the parameter vectors $B_i$ and thus the supervised learning task is mapped onto the well understood problem of principal component analysis. While this mapping by itself does not solve the original problem, it does provide a crucial reduction in its dimensionality, such that the remaining problem becomes almost trivial in the thermodynamic limit $N \to \infty$.

We shall consider the general correlation matrix

$$
C^P = P^{-1} \sum_{\mu=1}^{P} F(\tau(\xi^\mu)) \xi^\mu \xi^{\mu T}
$$

where

$$
F(\tau(\xi)) = \begin{cases} 
1 & \text{if } \tau(\xi) \geq 0 \\
0 & \text{otherwise}
\end{cases}
$$

is the Heaviside function.
calculated exactly in the thermodynamic limit $N \to \infty$ and any vector orthogonal to all teacher vectors $B_i$ is an eigenvector. The eigenvalue $\lambda$ has the single eigenvector $B = K^{-1/2} \sum_{i=1}^{K} B_i$; this eigenvector is of little interest since for large $\hat{P}$ one also has $\hat{B} \propto J^P$, and it is thus simpler to use Hebb’s rule [3] to estimate $\hat{B}$. The important eigenspace is the one of $\lambda_\Delta$ since it is spanned by the $K - 1$ vectors $B_1 - B_j$ ($j = 2, \ldots, K$). The three eigenvalues can be written as averages over independent, zero mean, unit variance, Gaussian random variables $y_i$. For instance one obtains $\lambda_\Delta = \frac{1}{2} \langle F(\tau_y) (y_1 - y_2)^2 \rangle_y$ where $\tau_y = K^{-1/2} \sum_{i=1}^{K} b(y_i)$. The activation function $h$ is sigmoidal (odd, monotonic and bounded), and when stating specific numerical values we will always assume $h(y) = \text{erf}(y)$. Then for the choice $F(x) = x^2$ one finds the ordering $\lambda > \lambda_0 > \lambda_\Delta$ and $\lambda - \lambda_\Delta = \frac{1}{2} (1 - \frac{1}{\sqrt{2}})$.

For a finite number $P$ of training examples the degeneracy in the spectrum is broken by random fluctuations. But a computation of the orthonormal eigenvectors $\Delta^P$ corresponding to the $K - 1$ smallest eigenvalues of $C^P$ nevertheless yields an estimate of the space spanned by the difference vectors $B_1 - B_j$. To measure the success of approximating this space, we introduce the overlap

$$\rho = (K - 1)^{-1/2} \text{Tr}(\Delta^T B B^T \Delta)^{1/2}, \quad (4)$$

where $B$ is the matrix $(B_1, \ldots, B_K)$ of the teacher vectors and $\Delta = (\Delta_1, \ldots, \Delta_{K-1})$. This is a sensible measure because $\rho$ is invariant with respect to the change of an orthonormal basis of the space spanned by the $\Delta_j^P$ and since it attains its maximal value of 1 iff all $\Delta_j^P$ lie in the space spanned by the $B_i$. Simulations showing the overlap $\rho$ as function of the number of examples per free parameter, $\alpha = P/(KN)$, are depicted in Fig. 1. They indicate a second order phase transition from zero to positive $\rho$ at a critical value $\alpha_c$. The evolution of $\rho$ can be calculated exactly in the thermodynamic limit $N \to \infty$. But since up to now we are only estimating the space spanned by the $B_i$, instead of the vectors themselves, we address this problem first and defer the calculation of $\rho$.

Using the above eigenspace procedure, the $B_i$ can be approximated by linear combinations of the $\Delta_j^P$ and $J^P$. Thus the original $KN$ dimensional problem is reduced to $K^2$ dimensions and this is much easier for large $N$. To exploit the dimensionality reduction, we write the possible linear combinations as $\Delta^\Gamma$ where $\Delta = (J^P, \Delta^P_1, \ldots, \Delta^P_{K-1})$, $\Gamma$ is a $K$ by $K$ matrix of tunable parameters, and we define a student network $\sigma_T$ in the restricted space via $\sigma_T(\xi) = g \left( K^{-1/2} \sum_{i=1}^{K} h \left( (\Delta^\Gamma)^T \xi \right) \right)$. We want to choose $\Gamma$ to minimize the generalization error $\epsilon_g = \langle \frac{1}{2} (\tau(\xi) - \sigma_T(\xi))^2 \rangle_\xi$, and to this end $\hat{P}$ additional examples $(\xi^\nu, \tau(\xi^\nu)), \nu = 1, \ldots, \hat{P}$, are used. To simplify the theoretical analysis, the additional examples should be picked independently of the examples used to obtain $\Delta$. We then apply the standard on-line gradient descent procedure $\Gamma^{\nu+1} = \Gamma^{\nu} - \eta \nabla_{\Gamma^{\nu}} \left( \langle \tau(\xi^\nu) - \sigma_T(\xi^\nu) \rangle^2 \right)$. However, by choosing a scaling of the learning rate $\eta$ such that $\eta \ll 1$ for large $N$, the stochasticity drops out of the procedure [6] and in the restricted space it performs gradient descent in $\epsilon_g$. Further we can scale $\hat{P}$ such that $\eta \hat{P} \gg 1$ and then $\Gamma^{\hat{P}}$ will be a minimum of $\epsilon_g$ for large $N$. Finally both scaling conditions can be satisfied while observing $\hat{P} \ll N$, so that the required number of additional examples is negligible compared to the size of the first training set. Note that thanks to the reduced dimensionality the details of the scaling of $\eta$ and $\hat{P}$ only affect finite size effects and not the performance in the thermodynamic limit. Simulations combining the two stages of our algorithm (Fig. 1) show a steady decay in $\epsilon_g$.

We now turn to the theoretical calculation of $\rho$ in the important first stage of the algorithm. The smallest eigenvalue of $C^P$ can be found by minimizing $\int dJ C^P \chi$ under the constraint $|J| = 1$. Hence we consider the partition function $Z = \int dJ \exp(-\beta P J^T C^P J)$ where the integration is over the $N$-dimensional unit sphere. For large $N$ the typical properties of the minimization problem are found by calculating the training set average $\langle \ln Z \rangle$ and taking the limit $\beta \to \infty$. Using replicas, one introduces the $K$ dimensional order parameter $R$, the typical overlap $B^T J$ of the teacher vectors with a vector $J$ drawn from the Gibbs distribution $Z^{-1} \exp(-\beta P J^T C^P J)$, and further the replica symmetric scalar order parameter $q$ which is the overlap $J^T P$ of two vectors drawn from this distribution. For $P > N$ the correlation matrix $C^P$ is nonsingular, $q$ approaches 1 with increasing $\beta$, and the relevant scaling is $\chi = \beta (1 - q) = \mathcal{O}(1)$. Then for the quenched averaged of $\ln Z$ one finds in the limit $\beta \to \infty$

$$\langle \ln Z \rangle \frac{\beta N}{\partial R} = \text{extr} \left. R^T A(\alpha, \chi) R + a(\alpha, \chi) \right|_{R, \chi}. \quad (5)$$

Here $a(\alpha, \chi) = -\alpha K \langle G(\tau_\chi) \rangle_y + \frac{1}{2\chi}$, the $K$ by $K$ matrix $A(\alpha, \chi)$ has entries

$$A_{jk}(\alpha, \chi) = -\alpha K \langle G(\tau_\chi) (y_j y_k - \delta_{jk}) \rangle_y - \frac{\delta_{jk}}{2\chi}, \quad (6)$$

and $G(\tau_\chi) = F(\tau_\chi)/(1 + 2\chi F(\tau_\chi))$. Since Eq. (5) is quadratic in $R$ the extremal problem can only have a solution $R \neq 0$ if the matrix $A$ is singular. From the symmetries one easily obtains that $A$ has just two eigenvalues. The first can be written as $A_{11} = A_{12}$, it is the relevant eigenvalue in our case [6] and its eigenspace is spanned by the vectors $e_1 - e_j$ ($j = 2, \ldots, K$), where
\( e_1, \ldots, e_K \) denote the standard basis of \( \mathbb{R}^K \). This degeneracy shows that the difference between the \( K-1 \) smallest eigenvalues of the correlation matrix vanishes for large \( N \). So the simple procedure of analyzing the properties of the single vector \( J \) minimizing \( JTCPJ \), in fact yields the properties of the \( K-1 \) eigenvectors vectors of \( CP \) with smallest eigenvalues in the thermodynamic limit.

Due to the degeneracy, we can reparametrize setting \( R = \rho (e_1 - e_j)/\sqrt{2} \) and obtain an extremal problem with only two variables \( \rho \) and \( \chi \). Note that \( \rho \) is indeed the parameter introduced in the analysis of the numerical simulations. Its evolution is now obtained by solving (3) and this confirms the continuous phase transition found in the simulations from \( \rho = 0 \) to positive \( \rho \) at a critical value \( \alpha_c \). For \( K = 2 \) one finds \( \alpha_c = 4.49 \) and for \( K = 3 \) the result is \( \alpha_c = 8.70 \). As shown in Fig. 1 beyond the phase transition there is excellent agreement between the theoretical prediction and the simulations.

To obtain generic results for large \( K \) note that the contributions of \( y_1 \) and \( y_2 \) to the target output \( \tau \) will be small in this limit. Decomposing \( \tau \) as \( \tau = \tau_0^* + \delta \sqrt{K} \) where \( \delta = h(y_1) + h(y_2) \), and expanding \( G(\tau) \) up to second order for large \( K \) simplifies Eq. (3) to:

\[
\frac{(\ln Z)}{\beta N} = \frac{\alpha \rho^2}{4} \langle G(\tau) \rangle \langle \delta^2(y_1 - y_2)^2 \rangle - \alpha K \langle G(\tau) \rangle + 1 - \frac{\rho^2}{2\chi}.
\]

(7)

On the one hand, applying the central limit theorem, the multiple integrals \( \langle G(\tau) \rangle \langle \delta^2 \rangle \) can now be replaced by a single average, on the other hand the structure of (3) shows that \( \chi \) approaches zero with increasing \( K \). These observations yield the very simple result that \( \rho^2 = 1 - \alpha_c/\alpha \) for large \( K \) and \( \alpha > \alpha_c \). The value of \( \alpha_c \) is obtained as

\[
\alpha_c = \frac{4K}{\langle F^2(\mu) \rangle} \left( \frac{1}{\langle z^2 h^2(z) \rangle} - \mu^2 - 2 \langle z h(z) \rangle^2 \right)^2.
\]

where \( \mu^2 = \langle h^2(z) \rangle \), and the distribution of \( z \) is Gaussian with zero mean and unit variance. It is now straightforward to derive the optimal choice of \( F \) from Eq. (3) by noting that in the denominator \( \langle F^2(\mu) \rangle \) is \( \mu^{-2} \langle (z^2 - 1) \rangle \). Applying the Cauchy-Schwarz inequality to \( \langle F^2(\mu) \rangle / \langle F^2(\mu) \rangle \) then yields that the optimal choice is \( F(x) = x^2 - \mu^2 \). For this choice the eigenvalue \( \lambda_0 \) of the correlation matrix \( C^T \) vanishes for large \( P \). So the optimal \( F \) maximizes the signal to noise ratio between the eigenspace of difference vectors we want to estimate and the orthogonal space.

For the activation function \( h(x) = \text{erf}(x) \) one finds that \( \alpha_c = 1.96K \) when \( F \) is optimal, whereas the simple choice \( F(x) = x^2 \) yields a critical \( \alpha \) which is one and a half times higher. Simulation results for \( K = 7 \) plotted in Fig. 2 show that the large \( K \) theory provides a reasonable approximation already for networks with quite few hidden units.

To round off the analysis of the regression problem, we obtain a theoretical prediction for the generalization error achieved by combining the two stages of our procedure. A simple calculation shows that the overlap \( r \) of the Hebbian vector \( J \) with \( \bar{B} = r B^T J \), for large \( N \) satisfies \( r = (1 + \arcsin(2/3)K)^{-1/2} \). Further, using the explicit expression for \( e_\rho \) given in (3) and the values \( r \) and \( \rho \), we can calculate the minimum of \( e_\rho \) in the restricted space and find a theoretical prediction for the generalization error obtained by the second stage. This prediction is compared to the simulations in Fig. 1 and 2.

We next consider classification problems, that is we assume that the output function of the network given by Eq. (3) is \( g(x) = \text{sgn}(x) \). Then, since the output is binary, \( \lambda_0 = \overline{\lambda} \) holds for any choice of the weight function \( F \), and our procedure cannot immediately be applied. However, it is possible to gain information about the target rule by not just considering its output \( \tau \) but by comparing the output to the value \( B^T \xi \) which would have been obtained by the linearized network, \( g(x) = h(x) = x \). This is feasible since, even for classification, \( B \) can be estimated by the Hebbian vector \( J \) defined by (3). We are thus lead to consider more general correlation matrices of the form

\[
C^T = P^{-1} \sum_{\mu=1}^P F \left( \tau(\xi^\mu), \overline{J} \xi^\mu \right) \overline{\xi}^\mu \overline{\xi}^\mu^T.
\]

A reasonable way of choosing \( F \) is to focus on inputs \( \xi^\mu \) where the target output has a different sign than the output of the linearized network. So we consider \( F(x, y) = \Theta(-xy)-\mu \), where \( \Theta \) is the Heaviside step function.

In the large \( P \) limit, the matrix \( C^T \) has the same eigenspaces as in the case of regression and the three eigenvalues will in general be different. For the activation function we choose \( h(x) = \text{sgn}(x) \) to compare our results with the findings for on-line Gibbs learning [10], to our knowledge the only algorithm which has been simulated in any detail for classifications task with a connected committee machine. For this \( h \) one finds \( \lambda_{\Delta} > \lambda_0 > \overline{\lambda} \), and for large \( K \) to leading order \( \lambda_{\Delta} - \lambda_0 = \sqrt{2\pi - 4}/(\pi^2 K) \). Numerical simulations of the procedure are shown in Fig. 3 using \( \mu = \pi^{-1} \arccos(\sqrt{2}/\pi) \). Motivated by our findings in the case of regression, this choice of \( \mu \) yields \( \lambda_0 = 0 \) for large \( K \). While the training sets needed to achieve good generalization are much larger than for regression, they are, for exactly the same architecture, approximately 20-times smaller than for on-line Gibbs learning [10] already for \( N = 150 \).

Throughout this Letter we have assumed that the inputs are drawn from an isotropic distribution. Typically, in practical applications, the input data itself will have some structure, and in this case the inputs have to be whitened before applying our procedure. To this end one computes the correlations of the inputs by
Then an estimate for the space spanned by the difference vectors is obtained by transforming back, setting \( \Delta_j = R^{-1} \Delta_j \). Numerical simulations for \( F(x) = x^2 \) show that whitening noticeably improves the performance of our algorithm even when the inputs are picked from an isotropic distribution. This is due to the fact that the spectrum of the empirical correlation matrix \( D^P \) has a finite width even when it converges to a delta peak with increasing \( P \).

Fig. 2 showing that the number of hidden units can be determined by inspecting the eigenvalue spectrum of the correlation matrix. So our findings also provide a novel perspective on the problem of model selection. In summary, we have presented the first learning algorithm for a realistic multilayer network which can be exactly analyzed in the thermodynamic limit and yields good generalization already for a finite ratio of training examples to free parameters. This contrasts with the behavior of traditional on-line procedures for target functions such as the ones considered in this Letter. As long as there are on the order of \( N \) on-line steps, the dynamics is exactly described by deterministic differential equations for a set of self-averaging order parameters in the limit of large \( N \). However, even when tuned by choosing a good learning rate, the dynamics is stuck in a badly generalizing plateau on this time scale unless some information about the target function is built into the initial conditions. For the realistic case of randomly chosen initial values, the symmetries are eventually broken due to small initial fluctuations and the accumulation of fluctuations during the dynamics, but only when the number of on-line steps is much larger than \( N \). This symmetry breaking is not adequately described by the deterministic differential equations. When the training set is sampled without replacement, this divergence of the time scale means that large numbers of examples are needed. But even in the recently analyzed scenario of sampling with replacement, the above theoretical problems remain and are compounded since the analysis requires involved techniques such as dynamical replica theory and quite a few approximations already on the time scale \( N \).

Hence, we believe that the findings in this Letter open new avenues for research and that in particular the performance of the algorithm for classification tasks deserves a more detailed analysis. But the perhaps most intriguing aspect of our procedure is that it does not really assume that the number of hidden units in the architecture is known a priori. This is highlighted by the inset of Fig. 2 showing that the number of hidden units can be determined by inspecting the eigenvalue spectrum of the correlation matrix. So our findings also provide a novel perspective on the problem of model selection.

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**FIG. 1.** Results for \( K = 3 \). The evolution of \( \rho \) for \( N = 400 \) (○) and \( N = 1600 \) (●). The right axis relates to the values of \( \epsilon_g \) found when the two stages of our procedure are combined, \( N = 400 \) (□) and \( N = 1600 \) (■). For \( \epsilon_g \) the value of \( \alpha \) refers to the number of examples in both training sets, \( \alpha = (P + \bar{P})/KN \). The full lines show the theoretical prediction for the thermodynamic limit. Where not shown, errorbars are smaller than the symbol size.
FIG. 2. Results for $K = 7$ using the weight function $F(x) = x^2 - \mu^2$. The numerical simulations for $N = 2000$ are compared to the theoretical curves found in the large $K$ limit. Where not shown, errorbars are smaller than the symbol size. The inset shows a histogram of the 200 smallest eigenvalues of $C^P$ for a single training set at $\alpha = 22$. A gap separates the 6 smallest eigenvalues from the rest of the spectrum. The range of the shown eigenvalues is $[-0.1, -0.07]$.

FIG. 3. Numerical simulations of the classification problem for $K = 7, N = 150$ showing the values of $\rho (\bigcirc)$ and $\epsilon_g (\square)$. The errorbars for the $\rho$ values are smaller than the symbol size. Here $\epsilon_g$ is the probability of misclassifying a new input. Training in the restricted space during the second stage of our procedure uses the variant of the perceptron learning rule described in [11] for tree committee machines.