An exact learning algorithm for autoassociative neural networks with binary couplings

Exact learning in binary neuronal networks

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Abstract.

Exact solutions for the learning problem of autoassociative networks with binary couplings are determined by a new method: The use of a branch-and-bound algorithm leads to a substantial saving of computing time compared to complete enumeration. As a result, fully connected networks with up to 40 neurons could be investigated. The network capacity is found to be close to 0.83.

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The training of neural networks with binary couplings is believed to belong to the class of NP-complete problems i.e. the average computing time required to find a solution scales exponentially with the number of couplings to determine. This exponential scaling is due to the discrete structure of the space of couplings and is obvious in the case of complete enumeration. However, theoretical and numerical studies showed that it holds as well for heuristic approaches (e.g. simulated annealing). Training by complete enumeration has been carried out for small networks with up to 25 neurons [3, 4, 5]. Heuristic algorithms [2, 6, 7] were used for networks with up to thousand neurons. Still, the main disadvantage of heuristic algorithms consists in the uncertainty about the existence of solutions not found by the algorithm.

Our aim has been to develop an exact algorithm guaranteed to find all possible solutions in considerably less computing time than complete enumeration. In [8], Gardner showed that the space of interactions in neural network models can be treated in a way similar to the phase space of spin glass models. Accordingly, it should be possible to use the branch-and-bound method, already successfully applied to the search for ground states of a Ising spin glass model [9, 10], for the training of neural networks with binary couplings.

Consider an autoassociative network built of $N$ two-state neurons $s_i = \pm 1$ ($i = 1 \ldots N$) and fully connected by binary synaptic couplings that can take on the values $J_{ij} = \pm 1$. The self couplings $J_{ii}$ should be set to zero. The task of the network would be to store a set of patterns $\bar{\xi}_\mu$ ($\mu = 1 \ldots p$) with elements $\xi^\mu_i = \pm 1$. A training
procedure determines couplings that make these patterns attractors of the discrete
network dynamics

\[ s_i^{(t+1)} = \text{sgn} \left( \sum_{j=1}^{N} J_{ij} s_j^{(t)} \right) \quad i = 1 \ldots N. \] (1)

The capacity of the network specifies the number of different patterns that can be
stored simultaneously. It is normally expressed as a critical load \( \alpha_c = p_c / N \).

For good retrieval one is interested in large basins of attraction. As discussed in
[11, 12], these correspond to large values of the pattern stability

\[ \kappa = \min_{\mu} \left( \frac{1}{\sqrt{N}} \sum_{i(i \neq i)} \xi_{\mu_i} J_{ij} \xi_{\mu_j} \right). \] (2)

The maximally stable rule therefore formulates the learning problem as an
optimization task: For a given set of patterns, one has to determine an optimal set of
couplings that maximises the network stability

\[ \kappa = \min_{\mu} (\kappa^\mu). \] (3)

As long as there is no symmetry constraint on the matrix of couplings, the optimization
task separates into the training of \( N \) simple perceptrons with \( N - 1 \) input neurons,
corresponding to the individual rows of the matrix with the self-coupling excluded.
The network stability \( \kappa \) emerges as the minimum of the “perceptron stabilities” \( \kappa_i \).

The new learning algorithm was developed using the branch-and-bound method,
a standard tool of combinatorial optimization theory [13]: To find a row of the matrix
of couplings with maximal stability \( \kappa_i \), complete enumeration would check the \( 2^{(N-1)} \)
possible configurations for optimal ones. Branch-and-bound starts with a division into
a hierarchy of subproblems: each single coupling is tested with both possible values yet
taking into account the state of the previously (on a trial basis) determined couplings,
thus forming a binary tree of “incomplete” configurations. Only the final level of the
tree would contain the “complete” solutions. This division is the ‘branching’ part of
the algorithm. Standing alone it would double the necessary computing time. Here
the ‘bounding’ (and subsequently cutting) part comes into action: for each node of the
binary tree an upper bound for the best possible solution of the remaining subproblem
is evaluated. Starting point is an ideal stability, \( \kappa_{id} = N - 1 \), which is obtained if one
takes all terms in the sum (3) to be positive. (Generally, the maximal stability lies
below this ideal stability which can only be achieved if there is just one pattern to
store.) When testing a coupling \( J_{ij} \), this bound will be corrected, taking into account
the already fixed part of the configuration. If it falls under a pre-set value, e.g. the
stability attained by the use of the clipped Hebb rule, the binary tree is “cut” at this
node, i.e. the subtree of this node does not need to be considered. As a result, only a
small percentage of the nodes has to be checked. For \( N = 25 \) we found that only \( 10^{-4} \)
to 8 percent of the nodes were evaluated, depending on, e.g., the number of patterns
to store.

Assuming that the evaluation of a node of the binary tree is approximately as
time consuming as checking one possible configuration during complete enumeration,
a comparison of these two methods has been done: As predicted by theory, we still have
an exponential scaling of the algorithm. However, if we set the load \( \alpha = p / N \)
to 0.5 and look for one solution with positive stability, the algorithm scales no longer
with $2^N$ but with $2^{0.46N}$. In the (worst) case of determining all optimal solutions at $\alpha = 1$, the scaling is $3 \times 2^{0.8N}$. (That would mean, the algorithm still optimizes a 30-neuron network in approximately the computing time needed for the complete enumeration of a 25-neuron network.)

We used the branch-and-bound algorithm to determine the capacity of the network storing random uncorrelated patterns. Only one row of the coupling matrix was considered assuming the stability value to be self-averaging in the thermodynamic limit (cf. [8, 3]).

The procedure resembles the one used in [4]: For a given value of $N$, the stability $\kappa^N(\alpha)$ is determined for an increasing number of patterns until its value becomes negative, signifying that it is no longer possible to store all patterns. Then the capacity $\alpha_c(N)$ is determined by a linear interpolation between the last positive $\kappa^N(\alpha_+)$ and the negative $\kappa^N(\alpha_-)$. If the patterns are binary-valued, $\xi_i = \pm 1$, $\kappa^N(\alpha)$ takes on discrete values with a spacing of $2/\sqrt{N}$. For $N$ odd, this discreteness results in two values of $\alpha_c(N)$ corresponding to the first and last occurrence of $\kappa^N(\alpha) = 0$. This procedure was carried out for networks with $N = 4 \ldots 40$. To reduce finite size (discretization and parity) effects, we also used continuous distributed patterns (cf. [3]). We considered a normalized Gaussian distribution as well as patterns with elements evenly distributed in the interval $-1 \leq \xi_i \leq +1$ (box constraint) to examine the influence of the pattern distribution. The figures 1 and 2 show the dependence of this capacity on the network size as well as on the nature of the patterns. The error bars correspond to twice the mean deviation of the average value (statistical error). Sample size varied between 10 000 for small systems and 100 for $N = 40$. The $\pm 1$-patterns exhibit a strong parity effect which should however vanish in the thermodynamic limit. In figure 2, the values for the Gaussian patterns show a periodicity which is probably a result of the linear interpolation as the period of six corresponds to the passing the zero-line of a stability value $\kappa^N(\alpha)$. (Remember that the critical capacity is approximately $5/6$ and $\alpha$ is restricted to rationals $N/p$). Quadratic fits are given as a guideline to the eye (cf. [4]).

![Figure 1. Network capacity in the case of random uncorrelated ±1-patterns](image-url)
Figure 2. Network capacity in the case of continuous distributed patterns

There is no scaling theory for this problem, however, our numerical data suggest that the extrapolation to $N \to \infty$ could not be a linear one. A tentative quadratic extrapolation yields $\alpha_c = 0.834$ for Gaussian distributed patterns, $\alpha_c = 0.832$ for the box constraint and $\alpha_c = 0.827$ for $\pm 1$-patterns and $N$ even. In the case of $\pm 1$-patterns and $N$ odd, a quadratic fit is clearly inadmissible.

A second approach followed the procedure by Krauth and Opper [3] in determining $\kappa_\alpha(N)$ for different values of $\alpha$ and a subsequent extrapolation to $N \to \infty$. The capacity for Gaussian distributed patterns is determined as $\alpha_c = 0.833$.

We aimed to examine the possibilities and limits of combinatorial optimization when used for the training of autoassociative neural networks with binary couplings. The developed branch-and-bound algorithm allowed us to extend the exact investigation to systems with up to 40 neurons. We were not able to leave the region of strong finite size effects but could confirm theoretical [4] and numerical [3, 4] studies with additional numerical evidence. The possibility to determine all solutions of the learning problem also opens the way for an analysis of the space of solutions similar to the one already done for the ground states of the Ising spin glass model [10].

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