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Optimal capacity of graded-response perceptrons: a replica-symmetry-breaking solution

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Abstract. Optimal capacities of perceptrons with graded input–output relations are studied within the first-step replica-symmetry-breaking Gardner approach. Input-data errors and a limited output precision are allowed. In particular, the role of non-monotonicity in the input–output relations on the breaking and on the overall performance is determined.

1. Introduction

In recent years non-monotonic neural networks, mostly with binary output neurons, have received some interest [1–7]. A first reason is that they are seen to permit a larger storage capacity than the limiting value $\alpha_c = 2$ found by Gardner [8] for monotonic transfer functions. Furthermore, it is argued that the computational capabilities of non-monotonic networks are improved through a dynamic selection of optimal subnetworks allowing, for example, better storage of correlated patterns. Finally, in extremely diluted non-monotonic models the retrieval quality is better in the sense that the domains of attraction of the retrieval states are enlarged.

In the framework of the Gardner theory [8, 9], optimal storage capacities have been analysed for multi-state monotonic networks (see [10–12] and references therein) and networks with graded (continuous) input–output relations [13], allowing input-data errors and a limited input–output precision. The investigation of the latter network is motivated especially by the fact that graded-response perceptrons constitute the basic building blocks of layered architectures trained by the backpropagation algorithm. Such systems are very frequently used in practical applications.

In most of the works mentioned so far the assumption of replica symmetry (RS) is an important ingredient in the computations. In [2] a first-step replica-symmetry-breaking (RSB) calculation has been performed for a simple fully connected non-monotonic network with binary neurons.

The purpose of the present paper is to extend previous analysis of optimal capacities for graded-response perceptrons [13] in two non-trivial directions. First, besides the influence of the desired output precision and the stability with respect to input errors, the role of increasing non-monotonicity in the input–output relations is analysed and discussed. Second, since it is shown that already in the monotonic case [13] the results obtained are not always stable against RSB, the additional effects of first-step RSB are examined in some detail. These

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effects are shown to be important and in some examples even the qualitative behaviour of the network is changed.

The rest of this paper is organized as follows. In section 2 we formulate the problem in a way that allows us to apply the first-step RSB Gardner-type analysis in a relatively straightforward manner. We give the RS approximation for the capacity and the local field distribution, then discuss its stability and finally work out the corresponding formula in a first-step RSB treatment. In section 3 we present and discuss our main results for a set of representative examples for both monotonic and non-monotonic input–output relations for different values of the input stability and output tolerance. Section 4, finally, contains some concluding remarks.

2. Replica analysis of the problem

We consider a graded-response perceptron mapping a collection of input patterns $\{\xi_i^\mu; 1 \leqslant i \leqslant N\}$, $1 \leqslant \mu \leqslant p$, onto a corresponding set of outputs ζ^μ, $1 \leqslant \mu \leqslant p$, via

$$\zeta^\mu = g\,(\gamma h^\mu) \tag{1}$$

$$h^\mu = \frac{1}{\sqrt{N}} \sum_j J_j \xi_j^\mu \,. \tag{2}$$

Here g is the input–output relation of the perceptron, which may be largely arbitrary. In particular, g need not be monotone non-decreasing, or invertible for our general line of reasoning to be applicable. In equation (1), γ denotes a gain parameter and h^μ is the local field generated by the inputs $\{\xi_i^\mu\}$ as specified in (2). The J_j are couplings of an architecture of perceptron type. We restrict our attention to general unbiased input patterns specified by $\langle \xi_i^\mu \rangle = 0$ and $\langle \xi_i^\mu \xi_j^\nu \rangle = \delta_{\mu,\nu}\delta_{i,j} C$. Since the effect of C in (1) can be absorbed in the gain parameter we take $C = 1$ in the following.

2.1. Replica-symmetric approximation

We start by briefly reviewing the RS Gardner-type analysis of [13], thereby generalizing the final results to non-monotonic input–output relations. We furthermore check the validity of local stability of the RS solution using the arguments of [14].

The beginning of the computational strategy is to require stability with respect to input-data errors and to allow a limited output precision in the mapping (1). In other words the output that results when the input layer is in the state $\{\xi_i^\mu\}$ is accepted if

$$g(\gamma(h^\mu \pm \kappa)) \in I_{\text{out}}(\zeta^\mu, \epsilon) \equiv [\zeta^\mu - \epsilon, \zeta^\mu + \epsilon] \qquad \mu = 1, \ldots, p \tag{3}$$

where the positive parameters κ and μ denote the required input stability and the allowed output tolerance, respectively. In order to compute the available Gardner volume in J-space satisfying (3) we rewrite this equation as a condition on the local fields

$$h^\mu \in I^\mu \equiv \{x;\; g(\gamma(x \pm \kappa)) \in I_{\text{out}}(\zeta^\mu, \epsilon)\} \qquad \mu = 1, \ldots, p\,. \tag{4}$$

In general, the sets I^μ form a collection of intervals

$$I^\mu = \cup_{i=1}^{n^\mu} I_i^\mu = \cup_{i=1}^{n^\mu} \left[l_i^\mu, u_i^\mu \right] \tag{5}$$

where l_i^μ and u_i^μ denote upper and lower bounds of the ith subinterval I_i^μ, respectively, and n^μ is the total number of subintervals defined by the pattern ζ^μ. In contrast with the case of monotonic non-decreasing input–output relations treated in [13], the sets I^μ are no longer simply connected intervals when we allow general non-monotonic input–output functions.

Of course, for each output ζ^μ, $I_{\rm out}(\zeta^\mu,\epsilon)$ should have a non-empty intersection with the range of g in order to have $\alpha_c > 0$. Furthermore, for convenience from the technical point of view we also assume that the I^μ contain no isolated points.

We then have for the fractional volume

$$V = \frac{\int \prod_i \mathrm{d}J_i \delta\left(N - \sum_i J_i^2\right) \prod_\mu \int_{I^\mu} \mathrm{d}y^\mu \delta\left(y^\mu - h^\mu\right)}{\int \prod_i \mathrm{d}J_i \delta\left(N - \sum_i J_i^2\right)} \,. \tag{6}$$

We remark that we use explicitly the mean spherical normalization $\sum_i J_i^2 = N$ in order to fix a scale for the gain parameter γ of the input–output relations. Following Gardner [8], we use the replica technique to evaluate $v = \lim_{N\to\infty} N^{-1}\langle\langle \ln V\rangle\rangle$, where $\langle\langle\cdots\rangle\rangle$ denotes an average over the statistics of inputs $\{\xi_i^\mu\}$ and outputs $\{\zeta^\mu\}$. The standard order parameter occurring in this calculation is the overlap between two distinct replicas in coupling space

$$q_{\lambda\lambda'} \equiv \frac{1}{N}\sum_{i=1}^{N} J_i^\lambda J_i^{\lambda'} \qquad \lambda < \lambda' \qquad \lambda, \lambda' = 1, \ldots, n\,. \tag{7}$$

Assuming that replica symmetry is not broken, i.e. $q_{\lambda\lambda'} \equiv q$, a straightforward but tedious calculation following [13] leads to the following result in the relevant RS Gardner limit $q \to 1$:

$$\alpha_{\rm RS}^{-1} = \left\langle \sum_{i=1}^{n^\mu}\left(\int_{\frac{1}{2}(u_{i-1}^\mu + l_i^\mu)}^{l_i^\mu} \mathrm{D}t\,(l_i^\mu - t)^2 + \int_{u_i^\mu}^{\frac{1}{2}(u_i^\mu + l_{i+1}^\mu)} \mathrm{D}t\,(u_i^\mu - t)^2\right)\right\rangle_{\zeta^\mu} \tag{8}$$

where $\mathrm{D}t = (\mathrm{d}t/\sqrt{2\pi})\exp(-t^2/2)$ is the Gaussian measure and where $u_0^\mu = -\infty$ and $l_{n^\mu+1}^\mu = +\infty$ for all μ. The optimal capacity is a function of both ϵ and κ because l_i^μ and u_i^μ are (see equation (4)). Moreover it depends on g, γ and the statistics of the desired ζ^μ, the average over which remains to be done.

We immediately remark that these results are not always stable against RSB. Following standard considerations [9, 15] we find that in order to check this stability it is sufficient to look at the sign of the product of the eigenvalues of the matrix of transverse fluctuations, the so-called replicon eigenvalue $\lambda_{\rm R}$. The evaluation of $\lambda_{\rm R}$ can be done using an analogous argumentation to the one given in [14]. We obtain again in the RS Gardner limit $q \to 1$

$$\lambda_{\rm R} = \alpha\left\langle \int_{-\infty}^{+\infty} \mathrm{D}t \left(\frac{\mathrm{d}}{\mathrm{d}t}[\lambda_0(t,\sigma) - t]\right)^2\right\rangle_{\zeta^\mu} - 1 < 0 \tag{9}$$

where for the case at hand we have to look at the value of $\lambda_0(t,\sigma)$ in the limit $\sigma \to \infty$. For general input–output relations these values read

$$\lambda_0(t) = \begin{cases} t & \text{for} \quad l_i^\mu < t < u_i^\mu \\ u_i^\mu & \text{for} \quad u_i^\mu < t < \frac{1}{2}(u_i^\mu + l_{i+1}^\mu) \\ l_{i+1}^\mu & \text{for} \quad \frac{1}{2}(u_i^\mu + l_{i+1}^\mu) < t < l_{i+1}^\mu \\ t & \text{for} \quad l_{i+1}^\mu < t < u_{i+1}^\mu \end{cases} \tag{10}$$

for $i = 1, \ldots, n^\mu$. It follows immediately that for monotonic non-decreasing input–output relations (the case of a simply connected interval) RS stability is guaranteed if

$$\lambda_{\rm R} = \alpha_{\rm RS}\left\langle \int_{-\infty}^{l^\mu} \mathrm{D}t + \int_{u^\mu}^{\infty} \mathrm{D}t\right\rangle_{\zeta^\mu} - 1 < 0 \tag{11}$$

in agreement with [13]. However, for non-monotonic input–output relations discontinuities occur at the endpoints of the subintervals in (10) such that the eigenvalue is infinite and hence replica symmetry is unstable. This extends the result of [2] to general non-monotonic input–output relations.

At this point it is instructive to calculate the distribution of the local fields corresponding to a specific output pattern ζ^μ. The result reads (compare [11, 12])

$$\rho_{\mathrm{RS}}(h^\mu) = \sum_{i=1}^{n^\mu} \Bigg[\delta(h^\mu - l_i^\mu) \int_{\frac{1}{2}(u_{i-1}^\mu + l_i^\mu)}^{l_i^\mu} \mathrm{D}t + \delta(h^\mu - u_i^\mu) \int_{u_i^\mu}^{\frac{1}{2}(u_i^\mu + l_{i+1}^\mu)} \mathrm{D}t + \left(\theta(h^\mu - l_i^\mu) - \theta(h^\mu - u_i^\mu)\right) \frac{1}{\sqrt{2\pi}} \exp\left[-\tfrac{1}{2}(h^\mu)^2\right] \Bigg]. \tag{12}$$

Due to the summation over the subintervals I_i^μ a gap structure emerges in equation (12), in agreement with [14]. Finally, we remark that the distribution of the couplings is always Gaussian.

2.2. Replica-symmetry breaking

From the observations presented above and related results in the literature [2, 13] we expect a strong RSB effect. So we want to improve the RS results by applying the first step of Parisi's RSB scheme [16]. We therefore introduce the following order parameters

$$q_{\lambda\lambda'} = q_{\beta_1\beta_2}^{\alpha_1\alpha_2} = \begin{cases} q_1 & \text{if} \quad \alpha_1 = \beta_1 \\ q_0 & \text{if} \quad \alpha_1 \neq \beta_1 \end{cases} \tag{13}$$

where $\alpha_1, \beta_1 = 1, \ldots, n/m; \alpha_2, \beta_2 = 1, \ldots, m$ and $1 \leqslant m \leqslant n$. We remark that in the limit $n \to 0$, $0 \leqslant m \leqslant 1$. The fractional volume V becomes a function of the three order parameters q_0, q_1 and m. Analogous to the RS calculation the optimal properties are obtained in the limit $q_1 \to 1^-, m \to 0$ and $0 \leqslant q_0 \leqslant q_1$ with $m/(1-q_1) = M$ a finite value. In this limit the relevant quantity v reads after a standard but tedious calculation

$$(1-q_1)v(q_0, q_1, m) = \frac{1}{2M} \ln[1 + M(1-q_0)] + \frac{q_0}{2[1 + M(1-q_0)]} + \frac{\alpha}{M} \left\langle \int \mathrm{D}z_0 \ln \psi_{I^\mu}(q_0, M, z_0) \right\rangle + \mathcal{O}((1-q_1)\ln(1-q_1)) \tag{14}$$

with

$$\begin{aligned} \psi_{I^\mu}(q_0, M, z_0) = \sum_{i=1}^{n^\mu} \Big[& L\left(q_0, M, z_0; \tfrac{1}{2}(u_{i-1}^\mu + l_i^\mu), l_i^\mu\right) - L\left(q_0, M, z_0; l_i^\mu, l_i^\mu\right) \\ & + L\left(q_0, 0, z_0; l_i^\mu, l_i^\mu\right) - L\left(q_0, 0, z_0; u_i^\mu, u_i^\mu\right) \\ & + L\left(q_0, M, z_0; u_i^\mu, u_i^\mu\right) - L\left(q_0, M, z_0; \tfrac{1}{2}(u_i^\mu + l_{i+1}^\mu), u_i^\mu\right) \Big] \end{aligned} \tag{15}$$

and

$$L(q_0, M, z_0; x, y) = \int_{\frac{x - z_0\sqrt{q_0}}{\sqrt{1-q_0}}}^{\infty} \mathrm{D}z_1 \exp\left[-\frac{M}{2} \left(y - z_0\sqrt{q_0} - z_1\sqrt{1-q_0} \right)^2 \right]. \tag{16}$$

From the saddle-point equations $\partial v/\partial q_0 = 0$, $\partial v/\partial q_1 = 0$ and $\partial v/\partial m = 0$ we obtain, after some algebra, the first-step RSB critical capacity in the form

$$\alpha_{\mathrm{RSB1}} = \min_{q_0, M} \left\{ \frac{-\frac{1}{2}\ln\left[1 + M(1-q_0)\right] - \frac{q_0 M}{2\left[1 + M(1-q_0)\right]}}{\left\langle \int \mathrm{D}z_0 \ln \psi_{I^\mu}(q_0, M, z_0) \right\rangle} \right\}. \tag{17}$$

Explicit results for different input–output relations will be discussed in the next section. Compared with (12) the first-step RSB distribution of the local fields corresponding to the pattern ζ^μ becomes

$$\rho_{\mathrm{RSB1}}(h^\mu) = \sum_{i=1}^{n^\mu} \int \frac{\mathrm{D}z_0}{\psi_{I^\mu}(q_0, M, z_0)} \Big\{ \delta(h^\mu - l_i^\mu) \\ \times \big[L\big(q_0, M, z_0; \tfrac{1}{2}(u_{i-1}^\mu + l_i^\mu), l_i^\mu\big) - L\left(q_0, M, z_0; l_i^\mu, l_i^\mu\right) \big] \\ + \big[\theta(h^\mu - l_i^\mu) - \theta(h^\mu - u_i^\mu)\big] \frac{1}{\sqrt{2\pi(1-q_0)}} \exp\left[-\frac{(h^\mu - z_0\sqrt{q_0})^2}{2(1-q_0)} \right] \\ + \delta(h^\mu - u_i^\mu) \big[L\left(q_0, M, z_0; u_i^\mu, u_i^\mu\right) - L\big(q_0, M, z_0; \tfrac{1}{2}(u_i^\mu + l_{i+1}^\mu), u_i^\mu\big) \big] \Big\}. \tag{18}$$

In contrast to the local field distribution for the RS solution, the continuous part of (18) is non-Gaussian because of the factor $1/\psi_{I^\mu}$. We remark that the distribution for the couplings does not change it is independent of the breaking.

3. Results

In the following we report the results for a set of representative examples for both monotonic and non-monotonic input–output relations for different values of the output tolerance and input stability.

3.1. Monotonic input–output relations

In order to get a first qualitative idea about RSB in this case, we require all local fields to lie in a fixed finite interval (see equation (4)), in other words we suppose that the output distribution, the input–output relation and the parameters ϵ and κ are such that $I^\mu = [l, u]$ for all patterns ζ^μ.

Roughly speaking, we find that for a small allowed interval the RS result for the critical capacity is stable. When this interval increases the local RS stability breaks down, both the RS and first-step RSB critical capacity increase and their difference also increases. It is seen that this difference in capacity is rather limited. For example, for an asymmetric interval of order unity ($l = 0, u = 1$) it is of the order of 10^{-3}. In contrast, it turns out that for this interval the difference in the RS and the first-step RSB local field distributions is relatively important, as is shown in figure 1. We remark that the coefficients of the δ-part in the distributions (recall equations (12) and (18)) are 0.46 at $h^\mu = 0$ and 0.14 at $h^\mu = 1$ for the RSB solution versus 0.5 and 0.16 for the RS solution. These results indicate that although the RS solution gives a good indication of the critical capacity in this case, it fails in predicting the local field distribution.

Taking a closer look at this relatively simple one-interval case, the details are already very complex. For example, even in the RS analysis it turns out that when the size of a symmetrically chosen interval is greater than a certain critical value, there may be several solutions with non-zero q of the saddle-point equations for given α. In that case additional quantities like the relative entropies have to be compared to pick out the physical one. For more details we refer to [17] where a complete Parisi hierarchical scheme has been worked out for this case.

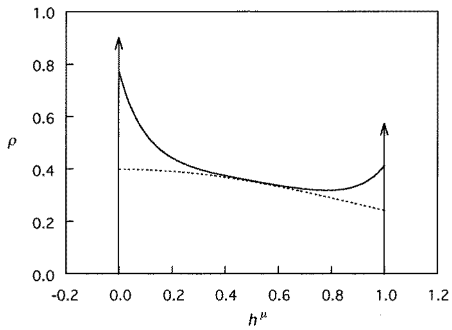

Figure 1. The RS (dotted curve) and RSB (full curve) distributions of the local fields for the allowed interval $[0, +1]$.

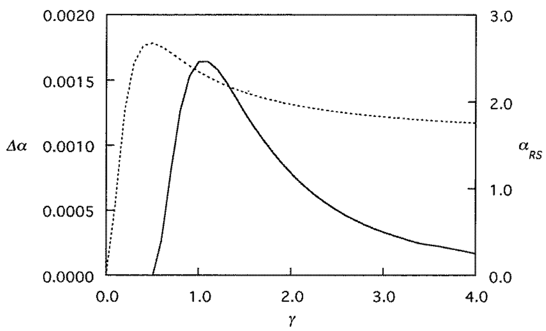

Figure 2. The RS critical capacity (dotted curve) and its difference with the RSB capacity, $\Delta\alpha$, (full curve) for the piecewise linear input–output relation as a function of the gain parameter γ for $\epsilon = 0.7$ and $\kappa = 0$.

Specifying to the monotonic piecewise linear input–output relation

$$g(x) = \begin{cases} x & \text{for} \quad |x| < 1 \\ \text{sign}(x) & \text{elsewhere} \end{cases} \tag{19}$$

as a representative example of the more general situation, and taking the output distribution to be constant homogeneous in this interval $[-1, +1]$, we obtain the following results. In figure 2 the difference between the RS and the first-step RSB critical capacities is shown as a function of the gain parameter γ for the input stability $\kappa = 0$ and the output tolerance $\epsilon = 0.7$. The maximum difference between these capacities turns out to be small for all output tolerances not close to 1. For ϵ increasing from 0 to 0.9, it increases from 0 to 0.028. For ϵ going to 1 it numerically behaves like $(1-\epsilon)^{-1}$. Its peak value occurs for $\gamma > \gamma_{\text{opt}}^{\text{RS}}$ where $\gamma_{\text{opt}}^{\text{RS}}$ is the value of the gain parameter such that, given ϵ and the output statistics, the critical capacity is maximal. This difference between the RS and RSB critical capacities is zero exactly at $\gamma_{\text{opt}}^{\text{RS}}$, confirming that replica symmetry is not broken for $\gamma < \gamma_{\text{opt}}^{\text{RS}}$ [13] and telling us furthermore that the first-step RSB critical capacity attains the same maximum at the same value of γ as the RS one. For $\kappa \neq 0$ the behaviour is similar but in all cases we have examined, the RS breaking occurs beyond the position of the maximum $\gamma_{\text{opt}}^{\text{RS}}$.

3.2. Non-monotonic input–output relations

In this section we describe the results for input–output relations with an increasing degree of non-monotonicity. The prototype of such a function is the ‘saw tooth’ function with an increasing number of teeth. In the course of this discussion we generalize some of the results in [2] and find interesting new behaviour for the graded-response perceptron.

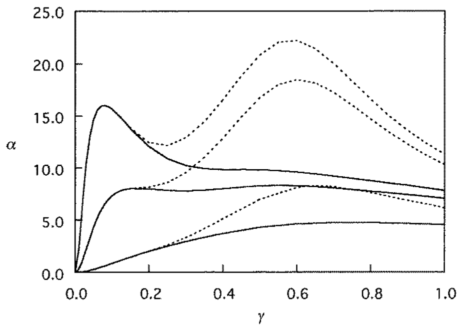

Figure 3. The RS (dotted curve) and RSB (full curve) critical capacities as a function of the gain parameter γ for $\kappa = 0$ and $\epsilon = 0.7$ (lower curves), 0.9 and 0.95 (upper curves).

We start by considering the input–output relation

$$g(x) = \begin{cases} -x & \text{for} \quad |x| < 1 \\ \text{sign}(x) & \text{elsewhere} \end{cases} \tag{20}$$

with a constant homogeneous output distribution. In this case the allowed interval in (4) is no longer connected for the finite fraction of patterns satisfying $|\zeta^\mu| > 1-\epsilon$. For example, the corresponding interval for positive patterns is given by $I^\mu = [-1/\gamma, u^\mu] \cup [1/\gamma, +\infty)$.

We first take $\kappa = 0$. In figure 3 we show the critical capacities for different values of the output tolerance as a function of γ. Compared with the monotonic case we see that the overall difference between the RS and first-step RSB solutions is much bigger. However, for $\gamma \in [0, 0.2]$ it is of the order of 10^{-3} (versus zero for the monotonic case). In this respect we note that for γ close to zero, the input–output relation becomes effectively less non-monotonic. Thinking in terms of the local fields (18) the main contributions concentrate around the origin in one interval, i.e. in the first part of the interval I^μ for the example specified above (namely $[-1/\gamma, u^\mu]$), while the rest of the contributions fall into an interval shifting towards infinity, i.e. in the second part of I^μ specified above (namely $[1/\gamma, +\infty)$). Hence the latter becomes less important and the system almost behaves like a one-interval system.

Furthermore, for small values of γ and $\epsilon \in [0.9, 1]$ a secondary maximum develops in the RS solution. Interestingly, it turns out that this secondary maximum is the only one that survives in the first-step RSB solution. So the peak values in the RS and RSB capacities are very different and occur for very different values of γ. Finally, the RS and RSB local field distributions for the cases we have examined are clearly distinct as in the monotonic case. For $\kappa \neq 0$ all these results are qualitatively the same. We recall that if both ϵ and κ are non-zero then there is an upper bound on γ beyond which $\alpha_c(\epsilon, \kappa, \gamma) = 0$ [13].

Next we extend the discussion to an input–output relation with a stronger non-monotonic behaviour (more 'teeth' in the saw tooth function). To simplify the numerical treatment we fix the output distribution, the input stability and the output tolerance such that the local field for every pattern ζ^μ lies in an interval

$$I = [-ka, -(k-1)a] \cup [-(k-2)a, -(k-3)a] \cup \cdots \cup [(k-2)a, (k-1)a] \cup [ka, \infty] \tag{21}$$

for even k and

$$I = [-\infty, -ka] \cup [-(k-1)a, -(k-2)a] \cup \cdots \cup [(k-3)a, (k-2)a] \cup [(k-1)a, ka] \tag{22}$$

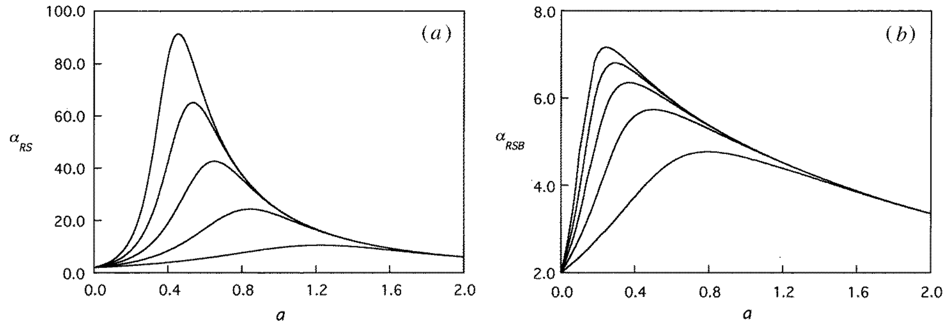

Figure 4. The critical capacity for the k-interval model as a function of the interval width a for $k = 1$ (lower curve) to $k = 5$ (upper curve): (a) RS case; (b) RSB case.

for odd k, where k is an effective measure for the degree of non-monotonicity and a is the width of each subinterval fixed by the choice of κ, γ and ϵ. In figure 4 we show the critical capacities as a function of a for increasing values of k for both the RS and RSB solution. The following remarks have to be made. For $a \to \infty$ the critical capacity goes, of course, to 2. Its maximum increases much faster in the RS case than in the RSB case. Calculations for k up to 100 seem to indicate that the asymptotic behaviour of the maximum is a power law ($\alpha_c^{\max} \approx k^{1.78}$) for the RS solution but only logarithmic for the RSB solution. This teaches us that the effect of the breaking is drastically increasing when the non-monotonicity of the input–output relations gets stronger.

It is interesting to remark that the order parameter q_0 becomes zero for a finite interval width a, indicating that the replica solutions become uncorrelated in J-space. The value of a where this happens decreases with the number of intervals k. Furthermore, the minimum determined in (17) is very flat as a function of q_0 such that it could be calculated with the fixed value $q_0 = 0$. A comparable situation occurs in the parity machine [18] and in the unsupervised learning problem discussed in [19].

4. Concluding remarks

In this paper we have studied the effects of first-step RSB on the performance of the graded-reponse perceptron allowing input-data errors and a limited output precision for both monotonic and non-monotonic input–output relations. Especially in the latter case some interesting new behaviour has been found.

For monotonic input–output relations, where the allowed interval for the local fields is connected, it is found that the effect of the breaking on the critical capacity as a function of the gain parameter is weak as long as the output tolerance is not close to 1. In the neighbourhood of 1 the difference between the symmetric and first-step broken critical capacities diverges. The distribution of the local fields is clearly different in the symmetric versus the first-step broken solution.

However, for non-monotonic input–output relations, where for some fraction of the output patterns the allowed interval is not connected, the overall effect of the breaking on the critical capacity is substantial. The effect on the distribution of the local fields is similar to the monotonic case. It is fair to say that the replica symmetric solution gives wrong results for most values of the gain parameter. When increasing the number of disconnected intervals it even predicts a qualitatively different behaviour.

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