Finite Size Scaling of Perceptron

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Abstract

We study the first-order phase transition in the model of a simple perceptron with continuous weights and large, but finite value of the inputs. Making the analogy with the usual finite-size physical systems, we calculate the shift and the rounding exponents near the transition point. In the case of a general perceptron with larger variety of outputs, the analysis gives only bounds for the exponents.

PACS numbers: 87.10.+e 02.70.Lq. 05.50.+q 64.60.Cn
keywords: neural networks, perceptrons, finite-size scaling, critical exponents, first-order phase transitions

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Some time ago W.Nadler and W.Fink [1] showed, for the model of the perceptron, that the transition from storable to unstorable pattern set sizes obeys finite-size scaling (FSS) behavior. This transition is characterized by the absence of an intrinsic length scale as is the correlation length for the usual phase transitions.

Similar "geometrical" phase transitions without intrinsic length, are the satisfiability of random boolean expressions [2], [3], the connectivity of random graphs [4], the quasispecies model of molecular evolution [5], etc. All these models exhibit a sharp transitions for large values of the size of the corresponding system, characterized by universal scaling functions, which describe the size-dependent effects near the threshold. Recently it was also shown that the statistical mechanics study of the K-SAT model is very useful for solving the hard computational NP-complete problem, as it represents, since the nature of the transitions which occur in it may help for the improvement of the efficiency of the search algorithms [6].

In the present letter we study the FSS behavior of perceptrons in the context of the usual FSS study known from different physical systems [7]-[9]. For this purpose we use some of the current definitions for shift and rounding of the transition, which occur when the size of the system is finite.

The system, we are interested on, is a singe-layer perceptron storing a set of input patterns \( \{\xi_i^\mu\}, i = 1, \ldots, N; \mu = 1, \ldots, p\), drawn from a Gaussian distribution. By \( N \) and \( p \) we denote the numbers of the inputs and the patterns, respectively.

It is well known [10]-[12] that for the system with one output unit, Gaussian inputs and continuous couplings, the fraction of all the possible input-output relations of size \( \alpha = p/N \) that can be stored, called \( P(\alpha, N) \), exhibits a smooth transition for finite value of \( N \), which becomes discontinuous (step-like) at \( \alpha_c = 2 \) and in the thermodynamic limit \( N \to \infty \) (see Fig. 5.11 in ref.[11] or Fig.3.4 in ref.[12]). The exact analytical expression for \( P(\alpha, N) \) is [10]:

\[
P(\alpha, N) = 2^{1-p \sum_{i=0}^{N-1} (p - 1\ i)}.
\]

(1)

When the size of the system \( N \) is large, eq.(1) takes the asymptotic form:

\[
P(\alpha, N) \approx \frac{1}{2} \left( 1 + Erf \left( \sqrt{\frac{N}{2\alpha}}(2 - \alpha) \right) \right),
\]

(2)

revealing a FSS behavior with a scaling parameter

\[
y = (\alpha - \alpha_c)N^{1/\nu}
\]

(3)

and a scaling exponent \( \nu = 2 \) near the transition point \( \alpha_c = 2 \). The plot of \( P(\alpha, N) \) in terms of the scaling parameter \( y \) leads to the fall of all the curves with different \( N \) onto a single one [1].

Because of the mean-field character of the model, the usual concept of length and dimensionality become ambiguous. To avoid the lack of natural geometric description in this case, one can choose the number of particles (or the number of inputs in our
case) $N$ as a finite-size parameter and the dimensionality of the system can be considered as arbitrary. Note that the standard finite size scaling hypotheses, involving the notion of correlation length, need a suitable extension for such systems \[13\]. It is easy to make the analogy between the scaling parameter $y$ for the perceptron and the corresponding scaling parameter for infinitely coordinated systems \[13\], defined by the coherence number, which replaces the usual correlation length. The relation between the two models leads to the same scaling form, eq.(3), expressed in terms of the corresponding critical parameter.

Following the analogy with the conventional first-order transitions \[7\]-\[9\], we define as a transition point $\alpha_c(N)$ this value of the parameter $\alpha$, for which the derivative $\frac{\partial P(\alpha,N)}{\partial \alpha}$ shows a maximum for large but finite values of $N$ ($N$ being the size of the system) \[14\]. This derivative becomes divergent in the thermodynamic limit at $\alpha_c = 2$.

Using the above scheme and eq.(1), we calculated the inflection point of the function $P(\alpha,N)$ with respect to the parameter $\alpha$ for different values of $N$ and we identified the so-called shift exponent \[7\]-\[9\]:

$$\alpha_c(N) - \alpha_c(\infty) \sim \frac{1}{N^\lambda}.$$  \hfill (4)

We obtained the following dependence of the critical storage capacity $\alpha_c(N)$:

$$\alpha_c(N) - \alpha_c(\infty) = \frac{e^{0.0328 - 0.00006N}}{N^{1.00906}},$$  \hfill (5)

for $N$ running between $N = 8$ to $N = 400$ and

$$\alpha_c(N) - \alpha_c(\infty) = \frac{e^{0.00571}}{N^{1.00104}},$$  \hfill (6)

for $N$ between $N = 100$ and $N = 400$, Fig(1).

It becomes evident that for very large $N$, the following scaling dependence takes place:

$$\alpha_c(N) - \alpha_c(\infty) \sim \frac{1}{N}.$$  \hfill (7)

Using the definition of the shift exponent, eq.(3), we obtain $\lambda = 1$.

The other possibility to calculate $\lambda$ is by performing analytical expansions for small values of the shift from the transition point $\alpha_c = 2$, using the asymptotic expression eq.(3). A straightforward calculations leads to the same result for the shift exponent, i.e., $\lambda = 1$. Note that the value of the shift exponent is obtained by defining the shift of the transition point as the position of the maximum of $\frac{\partial P(\alpha,N)}{\partial \alpha}$, as is usually done in FSS analysis of physical systems \[4\]. This value of $\lambda$ does not coincide with the value $1/\nu = 1/2$, as is usually expecting from the analogy with the FSS in physical systems. As we see with the present model, the coincidence of the values of the both exponents is not a necessary condition for the FSS to hold.

\[\text{\textsuperscript{1}Here we would like to mention that the time to find a solution diverges with } N, \text{ reminding of the critical slowing down.}\]
Figure 1: The critical storage capacity $\alpha_c(N)$ for values of $N$ within the interval $[8,400]$.

The finite shift of the critical point shows that the perceptron belongs to the class of systems undergoing asymmetric phase transitions. For symmetric phase transitions the shift is zero and a typical example for such transition is the field-driven transition in the Ising model, where the symmetry for the susceptibility $\chi(h, T, L) = \chi(-h, T, L)$ takes place (here $h$ is the external field and $L$ is the finite size of the system). Obviously, a finite shift in our case means that the above symmetry is broken, which is usually the case of transitions driven by temperature [9].

The result (7) is similar to the well known result for asymmetric temperature-driven first-order transitions in finite $d$-dimensional systems with cubic symmetry, where the location of the shift by the maximal slope scales like $L^{-d}$ ($L$ being the finite size) [7]-[9]. Although our system is effectively finite (with size $N$) in one dimension, we regard this analogy just as a formal one, because of the mean-field character of the interactions of the present model and the absence of any boundary conditions imposed.

Apart of the definition of the transition point by the maximum of $P(\alpha, N)$, there is also another definition of the location of the transition for the first-order transitions, which assumes the equilibrium of various phases near the point of the transition [15]. In contrast to the usual result known for the $q$-state Potts model [4], where the shift is given by $L^{-d}$, $L$ being the size of the system and $d$ its dimension, the definition used in ref. [15] leads to exponentially small corrections for the shift. In the case of a perceptron, however, we can not make the close analogy following the last
scheme, because of the lake of various phases at equilibrium, which is crucial for the application of this definition.

The two classes of transitions, symmetric and asymmetric, also show a rounding behavior for \( N \) finite, which is given by the scaling of the width of the peak of the diverging observable. In other words, it is the interval over which the singularity is smeared out and which becomes increasingly sharp as the finite dimension of the system goes to infinity. In the concrete case of the simple perceptron this is the scaling of the width of \( \frac{\partial P(\alpha,N)}{\partial \alpha} \), which determines the rounding behavior. Using eq.(2), the derivative reads:

\[
\frac{\partial P(\alpha,N)}{\partial \alpha} \sim \sqrt{\frac{N}{2\alpha}} \exp\left\{ -\frac{[N(2-\alpha)]^2}{2\alpha} \right\},
\]

from where the scaling of the variance of the Gaussian distribution gives a rounding exponent \( \theta = \frac{1}{2} \). Note that a similar behavior with \( N \) occurs for the shift and the variance of the generalization error in the case of a Bayesian perceptron with continuous weights \([16]\).

An interesting problem is what happens in the case of a perceptron with binary weights \([17]\). For this case the numerical analysis for the typical fraction shows a sharper behavior between the two regimes by increasing \( N \), but there is no definitive conclusion about the step-like behavior in the thermodynamic limit \([18]\). An important investigation of the shift of the transition will be a similar calculation of the position of the maximum of the above derivative as we did for the continuous couplings model. This will probably lead to different results, since in the binary case the probabilities of separation as a function of \( \alpha \) for different \( N \) do not intersect at the same point.

In the general case of a perceptron, having a larger variety of outputs \([19]\), and \( p \geq d_{VC} \) (\( d_{VC} \) being the Vapnik-Chervonenkis (VC) dimension), the fraction of all the possible input-output relations obeys the following inequality \([20]\):

\[
P(\alpha,N) \leq 2^{1-p\sum_{i=0}^{d_{VC}} \left( \frac{P-1}{i} \right)}.
\]

It has been shown \([21]\) that in the thermodynamic limit \( N \to \infty \) (\( p, d_{VC} \to \infty \)) and keeping \( \alpha = \frac{p}{N} \), and \( \alpha_{VC} = \frac{d_{VC}}{N} \) fixed, the VC-entropy shows different behavior above and below \( \alpha = 2\alpha_{VC} \), which permits to relate the storage capacity of the network to its VC- dimension via \( \alpha_c \leq 2\alpha_{VC} \) (\( \alpha_c \equiv \alpha_c(\infty) \)) (In the case of a single layer perceptron, treated at the beginning, \( d_{VC} = N, \alpha_{VC} = 1 \) and \( \alpha_c = 2 \)).

Eq.(9) shows that for \( N \)-large, the asymptotic form of the upper bound \( P(\alpha,N) \) of the fraction \( P(\alpha,N) \) is given by:

\[
P(\alpha,N) \leq \bar{P}(\alpha,N) = \frac{1}{2} \left[ 1 + \text{Erf} \left( \sqrt{\frac{N}{2\alpha}}(2\alpha_{VC} - \alpha) \right) \right],
\]

leading to the same values for the shift and the rounding exponents for the upper bound, known from the case of the simple perceptron.
Using the previous conclusion for the upper limit of $P(\alpha, N)$, identifying $2\alpha_{VC}$ with some “upper” critical storage capacity, and using the inequality between $\alpha_{VC}$ and $\alpha_c$, we derive the following relations:

$$|\alpha(N) - \alpha_c| \geq |\alpha(N) - 2\alpha_{VC}| \sim \frac{1}{N^\lambda}$$ \hfill (11)

with $\lambda = 1$ and

$$|\alpha^*(N) - \alpha_c| \geq |\alpha^*(N) - 2\alpha_{VC}| \sim \frac{1}{N^\theta}$$ \hfill (12)

with $\theta = \frac{1}{2}$.

Taking into account the last expressions and the fact that the step-like behavior and the main characteristics of the upper bound persist also in the general case by increasing the size of the system, we conclude that the shift and the rounding exponents for the upper bound, eq. (11), are also upper bounds for the shift and rounding exponents in the general case [21].

In conclusion, in the case of a single-layer perceptron, using the analogy with the usual FSS theory, we derived the shift and the rounding critical exponents $\lambda$ and $\theta$, respectively. Similar analysis in the general case gives results only for the upper limit of the fraction $P(\alpha, N)$. The full understanding of the problem requires additional numerical simulations and an investigation for every concrete case of architecture and machine.

Acknowledgments: E.K. warmly thanks for discussion the Workshop on “Statistical Physics of Neural Networks”, organized by the Max-Planck Institut-Dresden, 1999. This work is supported by the Spanish DGES Project PB97-0076 and the Bulgarian Scientific Foundation Grant F-608.

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