





# STATISTICAL PHYSICS OF LEARNING A RULE: DECADES OLD STORY CONTINUED



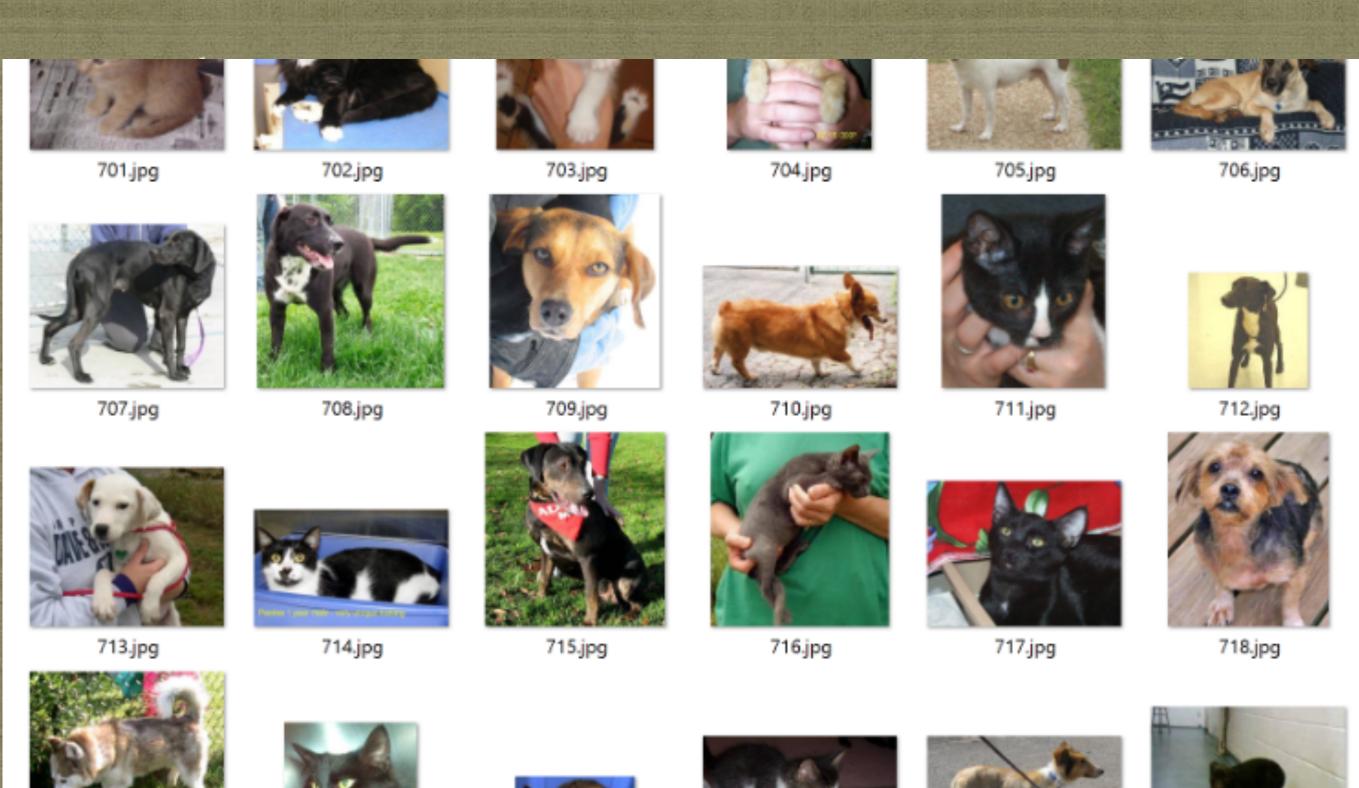
Lenka Zdeborová (IPhT, CEA Saclay, France)



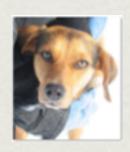
With: F. Krzakala, M. Mezard, N. Macris, J. Barbier, F. Caltagirone, A. Manoel, L. Miolane, F. Sausset, C. Schulke, Y. Sun, E. Tramel,

Memory Formation Conference, KITP, February 12-16, 2018.

# LEARNING A RULE



# LEARNING A RULE



 $= F_{\mu} = (01001010 \ 01110011 \ 10001100 \ 01001011$  01110000 10000 10001100 ..... all the pixels ....)

Goal: Find a function f so that

$$f(F_{\mu}) = +1$$

for a picture of a cat.

$$f(F_{\mu}) = -1$$

for a picture of a dog.

Today this can be done with deep neural networks.

(causing excitement in many areas of interest, in science, in business ...).

### STATISTICAL PHYSICS OF LEARNING A RULE

M "pictures" 
$$F_{\mu} \in \mathbb{R}^{N}$$
  $\mu = 1, ..., M$  A rule:  $f : F_{\mu} \to y_{\mu} \in \{+1, -1\}$ 

A rule: 
$$f: F_{\mu} \to y_{\mu} \in \{+1, -1\}$$

Model B in Gardner, Derrida'88: (teacher-student perceptron)

Elements of F (matrix) generated as iid random Gaussians.

Rule/teacher x\* so that

$$y_{\mu} = \operatorname{sign}(\sum_{i=1}^{N} F_{\mu i} x_{i}^{*})$$

J. Phys. A: Math. Gen. 22 (1989) 1983-1994. Printed in the UK.

### Three unfinished works on the optimal storage capacity of networks

#### E Gardner and B Derrida

The Institute for Advanced Studies, The Hebrew University of Jerusalem, Jerusalem, Israel and Service de Physique Théorique de Saclay\*, F-91191 Gif-sur-Yvette Cedex, France

Received 13 December 1988

Abstract. The optimal storage properties of three different neural network models are studied. For two of these models the architecture of the network is a perceptron with  $\pm J$ interactions, whereas for the third model the output can be an arbitrary function of the inputs. Analytic bounds and numerical estimates of the optimal capacities and of the minimal fraction of errors are obtained for the first two models. The third model can be solved exactly and the exact solution is compared to the bounds and to the results of numerical simulations used for the two other models.

Goal: Learn  $x^*$  from M samples/examples of  $(F_{\mu}, y_{\mu})$ .

# STORAGE CAPACITY

- Main focus of Gardner&Derrida was storage capacity:
  - y iid random, F iid random, (no x\*).
  - Is there an x so that for all  $\mu=1,...,M$ :  $y_{\mu}=\mathrm{sign}(\sum_{i=1}F_{\mu i}x_i)$
- Interesting mathematically (constraint satisfaction problem), but no notion of generalisation error (=when we get a new picture the rule should be able to tell a dog from a cat).
- Back to the learning the rule setting where  $y_{\mu} = \text{sign}(\sum_{i=1}^{\infty} F_{\mu i} x_i^*)$  and we need to find x\* back from (y,F).

### Solved using the replica method in the limit $N \to \infty$ $\alpha = M/N$

RAPID COMMUNICATIONS

PHYSICAL REVIEW A

**VOLUME 41, NUMBER 12** 

15 JUNE 1990

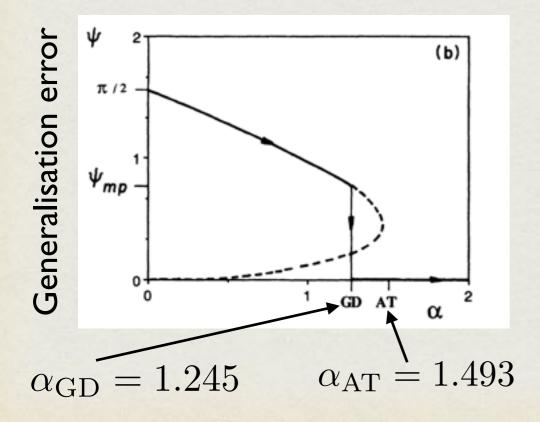
### First-order transition to perfect generalization in a neural network with binary synapses

Géza Györgyi\*

School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430

(Received 9 February 1990)

Learning from examples by a perceptron with binary synaptic parameters is studied. The examples are given by a reference (teacher) perceptron. It is shown that as the number of examples increases, the network undergoes a first-order transition, where it freezes into the state of the reference perceptron. When the transition point is approached from below, the generalization error reaches a minimal positive value, while above that point the error is constantly zero. The transition is found to occur at  $a_{\rm GD} = 1.245$  examples per coupling.



• Binary weights/synapses:

$$x^* \in \{-1, 1\}^N$$

 "The dashed lines represent non-physical segments of the curves." (Gyorgyi'90)

### Learning from Examples in Large Neural Networks

H. Sompolinsky (a) and N. Tishby

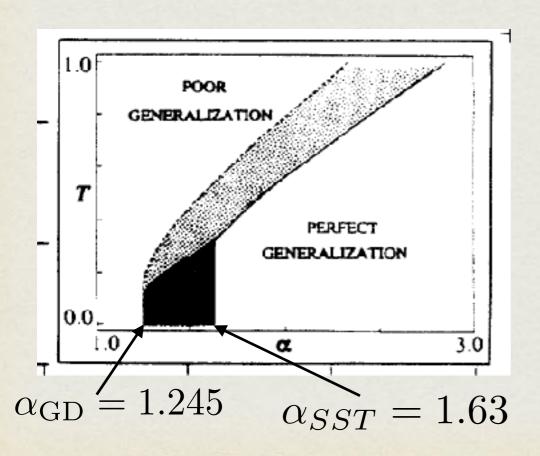
AT&T Bell Laboratories, Murray Hill, New Jersey 07974

### H. S. Seung

Department of Physics, Harvard University, Cambridge, Massachusetts 02138 (Received 29 May 1990)

A statistical mechanical theory of learning from examples in layered networks at finite temperature is studied. When the training error is a smooth function of continuously varying weights the generalization error falls off asymptotically as the inverse number of examples. By analytical and numerical studies of single-layer perceptrons we show that when the weights are discrete the generalization error can exhibit a discontinuous transition to perfect generalization. For intermediate sizes of the example set, the state of perfect generalization coexists with a metastable spin-glass state.

PACS numbers: 87.10.+e, 02.50.+s, 05.20.-y



as  $a \rightarrow 1.24$ . Above a = 1.24 the only ground state, i.e., state with zero training error, is the m = 1 state. <sup>14</sup> However, for  $1.24 < \alpha < 1.63$  metastable states with  $m_0 < 1$  and positive training error exist. Above a = 1.63 the only stable state at T > 0 is that with m = 1, although strictly at T = 0 states that are stable to flips of single weights are expected to be present even at higher a. <sup>15</sup>

In contrast to the high-T limit, in the darker region of the phase diagram the metastable state represents a *spin-glass* phase. The presence of this phase implies that there is an enormous number of metastable states separated by energy barriers which diverge with N, rendering the convergence to m = 1 extremely slow. In

### Mean Field Approach to Bayes Learning in Feed-Forward Neural Networks

### Manfred Opper

Institut für Theoretische Physik, Julius-Maximilians-Universität, Am Hubland, D-97074 Würzburg, Germany

### Ole Winther

CONNECT, The Niels Bohr Institute, Blegdamsvej 17, 2100 Copenhagen Ø, Denmark (Received 6 October 1995)

We propose an algorithm to realize Bayes optimal predictions for feed-forward networks which is based on the Thouless-Anderson-Palmer mean field method developed for the statistical mechanics of disordered systems. We conjecture that our approach will be exact in the thermodynamic limit. The algorithm results in a simple built-in leave-one-out cross validation of the predictions. Simulations for the case of the simple perceptron and the committee machine are in excellent agreement with the results of replica theory.

PACS numbers: 87.10.+c, 64.60.Cn

- Spherical weights/synapses  $\sum_{i} x_i^2 = N$
- ▶ But: TAP do not converge for large N.
- ▶ But: Conjecture false for binary weights.

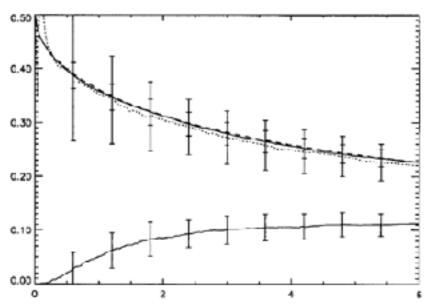


FIG. 1. The Bayes learning curve for the simple perceptron with output noise  $\beta = 0.5$  and N = 50 averaged over 200 runs. The full lines are the simulation results (upper curve shows prediction error and the lower curve shows training error). The dashed line is the theoretical prediction. The dotted line with larger error bars is the moving control estimate.

# A BIT OF HISTORY

- ▶ Very active part of statistical physics in the 90s. Whole section of <u>arxiv.org/</u> cond-mat/ devoted to Disordered Systems and Neural Networks. Hundreds of papers following these studies. Review articles and book:
  - Seung, Sompolinsky, Tishby. Statistical mechanics of learning from examples, Phys. Rev. A, 1992.
  - Watkin, Rau, Biehl. The statistical mechanics of learning a rule, Reviews of Modern Physics, 1993.
  - Engel, Van den Broeck. Statistical Mechanics of Learning, Cambridge University Press, 2001.
- Many questions left open (next slide).
- After 2000, not much activity on \*artificial\* neural networks among statistical physics community.
- ▶ Massive come-back in recent years when Deep Learning became widely known and used.

# OPEN QUESTIONS

- If the optimal generalization error by Gyorgyi & Sompolinsky, Tishby, Seung is correct, can we prove it mathematically rigorously?
- What is the smallest α reachable with tractable algorithms?
- What if the activation function was different (e.g. relu instead of sign)?
- What if the weights were different (e.g. sparse instead of binary)?

All answered in this talk.

## GENERALIZED LINEAR REGRESSION

component-wise function 
$$y=f_{\xi}(Fx^*)$$
 e.g.:  $f_{\xi}(z)=\mathrm{sign}(z)$   $x_i^*\in\{\pm 1\}$ 

labels:  $y \in \mathbb{R}^M$ 

data matrix:  $F \in \mathbb{R}^{M imes N}$ 

ground truth weights:  $x^* \in \mathbb{R}^N$ 

noise:  $\xi \in \mathbb{R}^M$ 

- ▶ Goal: Estimate x from examples  $(F_{\mu},y_{\mu})$ .
- Special cases: Signal reconstruction in computed tomography, magnetic resonance imaging, phase retrieval, compressed sensing, LASSO, superposition error correcting codes, codedivision multiple-access problem, group testing, logistic regression, ...



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### Generalized linear models

P McCullagh - European Journal of Operational Research, 1984 - Elsevier

... where S,cs and S, $\sim$  are the **regression** and residual 290 P. McCullagh / **Generalized linear models** sum of ... A natural **generalization** corresponding to canonical **regression** would be to write 11, = flo + (flVx, )e, (27) but the above **model** is no longer of the gener- alized **linear** type ...

☆ 切り Cited by 32787 Related articles All 15 versions ≫

### Longitudinal data analysis using generalized linear models

KY Liang, SL Zeger - Biometrika, 1986 - academic.oup.com

... With a single observation for each subject (nt =1), a **generalized linear model** (McCullagh & Nelder, 1983) can be applied to obtain such a description ... This paper presents an extension of **generalized linear models** to the analysis of longitudinal data when **regression** is the ...

☆ 切り Cited by 15100 Related articles All 19 versions

### [BOOK] Generalized linear models

JA Nelder, RJ Baker - 1972 - Wiley Online Library

A **statistical model** is the specification of a probability distribution. For example, the **model** implicit in much of **regression** analysis is that the observations have a normal distribution\*, the means being **linearly** related to the covariate values. Similarly, a log-**linear model** for

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### гвоокі Generalized additive models

T Hastie, R Tibshirani - 1990 - Wiley Online Library

... Linearity always remains a special case, and thus simple **linear** relationships can be easily ... Friedman (5) proposed a **generalization** of additive **modeling** that finds interactions among prognostic factors ... Software for fitting **generalized** additive **models** is available as part of the S ...

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### GENERALIZED LINEAR REGRESSION

# component-wise function $y=f_{\xi}(Fx^*)$ e.g.: $f_{\xi}(z)=\mathrm{sign}(z)$ $x_i^*\in\{\pm 1\}$

labels: 
$$y \in \mathbb{R}^M$$

data matrix:  $F \in \mathbb{R}^{M imes N}$ 

ground truth weights:  $x^* \in \mathbb{R}^N$ 

noise:  $\xi \in \mathbb{R}^M$ 

- ▶ Goal: Estimate x from examples  $(F_{\mu},y_{\mu})$ .
- Model considered in this talk:
  - F iid of zero mean and variance 1/N;
  - x\* iid random from P<sub>x</sub> (e.g. sparse, binary);
  - High-dimensional limit:  $N, M \to \infty, \alpha \equiv M/N = O(1)$

## BAYES-OPTIMAL ESTIMATION

$$P(x|y,F) = \frac{1}{Z(y,F)} \prod_{\mu=1}^{M} P_{\text{out}}(y_{\mu}|z_{\mu}) \prod_{i=1}^{N} P_{X}(x_{i}) \qquad z_{\mu} = \sum_{i=1}^{N} F_{\mu i} x_{i}$$

- $Arr x^* \sim P_{X;}$  y generated from  $P_{\mathrm{out}}(y|z) = \mathbb{E}_{P_{\xi}}[\delta(y f_{\xi}(z))]$
- Estimate  $x^*$  from (F, y). For a new row,  $F_{new}$ , predict the label  $y_{new}$ .
- Bayes-optimal inference  $\hat{x}_i = \text{marginal mean of } x_i \text{ in } P(x|y,F)$ .

  Optimal because it minimizes  $MSE = \frac{1}{N} \sum_{i=1}^{N} (\hat{x}_i x_i^*)^2$
- Bayes-optimal prediction/generalization:

$$\hat{y}_{\text{new}} = \mathbb{E}_{P(x|y,F),P_{\xi}} \left[ f_{\xi}(F_{\text{new}}x) \right]$$



No over-fitting! No other procedure can be better.

## CLOSING 27 YEARS OLD CONJECTURE

Barbier, Krzakala, Macris, Miolane, LZ arXiv:1708.03395

Def. "quenched" free energy:  $f \equiv \lim_{N \to \infty} \frac{1}{N} \mathbb{E}_{y,F} \log Z(y,F)$   $\alpha = \frac{M}{N}$ 

Theorem 1 (informally): The replica free energy is correct.

$$f = \sup_{m} \inf_{\hat{m}} f_{RS}(m, \hat{m})$$
$$f_{RS}(m, \hat{m}) = \Phi_{P_X}(\hat{m}) + \alpha \Phi_{P_{\text{out}}}(m; \rho) - \frac{m\hat{m}}{2}$$

where

$$\begin{split} & \Phi_{P_X}(\hat{m}) \equiv \mathbb{E}_{z,x_0} \left[ \ln \mathbb{E}_x \left[ e^{\hat{m}xx_0 + \sqrt{\hat{m}}xz - \hat{m}x^2/2} \right] \right] \\ & \Phi_{P_{\text{out}}}(m;\rho) \equiv \mathbb{E}_{v,z} \left[ \int \mathrm{d}y \, P_{\text{out}}(y|\sqrt{m}\,v + \sqrt{\rho - m}\,z) \ln \mathbb{E}_w \left[ P_{\text{out}}(y|\sqrt{m}\,v + \sqrt{\rho - m}\,w) \right] \right] \\ & x, x_0 \sim P_X \qquad \qquad z, v, w \sim \mathcal{N}(0,1) \qquad \qquad \rho = \mathbb{E}_{P_X}(x^2) \end{split}$$

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Theorem 2: Optimal error on estimation of x\* is:

$$MMSE = \rho - m^*$$

where m\* is the extremizer of f<sub>RS</sub>.

$$\rho = \mathbb{E}_{P_X}(x^2)$$

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$$f_{RS}(m, \hat{m}) = \Phi_{P_X}(\hat{m}) + \alpha \Phi_{P_{\text{out}}}(m; \rho) - \frac{m\hat{m}}{2}$$

Theorem 3: Optimal generalisation error is

$$\mathcal{E}_{\mathrm{gen}} = \underset{v,\xi}{\mathbb{E}} \left[ f_{\xi}(\sqrt{\rho} \, v)^2 \right] - \underset{v}{\mathbb{E}} \underset{w,\xi}{\mathbb{E}} \left[ f_{\xi}(\sqrt{m^*} \, v + \sqrt{\rho - m^*} \, w) \right]^2$$
 where m\* is the extremizer of f<sub>RS</sub>. 
$$\rho = \underset{v,w}{\mathbb{E}}_{P_X}(x^2)$$
 
$$v,w \sim \mathcal{N}(0,1)$$
 
$$\xi \sim P_{\varepsilon}$$

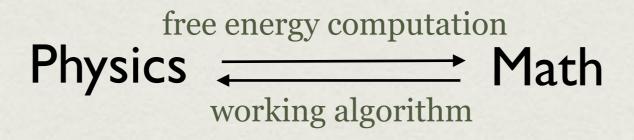
### ONE SLIDE ON THE PROOF

Barbier, Krzakala, Macris, Miolane, LZ arXiv:1708.03395

Guerra-Toninelli interpolation between the original posterior and N + M independent scalar denoising problems.

Novel (more powerful) variant where the interpolation parameter depends is a suitably chosen function of the interpolation "time".

Key property for the proof to work (Nishimori): Under expectations ground truth  $x^*$  is exchangeable for a sample from P(x|y,F).



# IS THE OPTIMAL ERROR REACHABLE WITH EFFICIENT ALGORITHMS?

Input: y

Initialize:  $\mathbf{a}^0, \mathbf{v}^0, g^0_{\text{out}, \mu}, \mathbf{t} = 1$ 

repeat

AMP Update of  $\omega_{\mu}, V_{\mu}$ 

$$\begin{split} V_{\mu}^t \leftarrow \sum_i F_{\mu i}^2 v_i^{t-1} \\ \omega_{\mu}^t \leftarrow \sum_i F_{\mu i} a_i^{t-1} - V_{\mu}^t g_{\text{out},\mu}^{t-1} \end{split}$$

AMP Update of  $\Sigma_i, R_i, g_{\text{out},\mu}$ 

$$g_{\text{out},\mu}^{t} \leftarrow g_{\text{out}}(\omega_{\mu}^{t}, y_{\mu}, V_{\mu}^{t})$$

$$\Sigma_{i}^{t} \leftarrow \left[ -\sum_{\mu} F_{\mu i}^{2} \partial_{\omega} g_{\text{out}}(\omega_{\mu}^{t}, y_{\mu}, V_{\mu}^{t}) \right]^{-1}$$

$$R_{i}^{t} \leftarrow a_{i}^{t-1} + \Sigma_{i}^{t} \sum_{\mu} F_{\mu i} g_{\text{out},\mu}^{t}$$

AMP Update of the estimated marginals  $a_i, v_i$ 

$$a_i^t \leftarrow f_a(\Sigma_i^t, R_i^t)$$
  
 $v_i^t \leftarrow f_v(\Sigma_i^t, R_i^t)$ 

 $t \leftarrow t + 1$ 

until Convergence on a,v output: a,v.

Simple to implement, only matrix multiplications, O(N2)

$$f_a(\Sigma, R) = \frac{\int \mathrm{d}x \, x \, P_X(x) \, e^{-\frac{(x-R)^2}{2\Sigma}}}{\int \mathrm{d}x \, P_X(x) \, e^{-\frac{(x-R)^2}{2\Sigma}}} \,, \qquad f_v(\Sigma, R) = \Sigma \partial_R f_a(\Sigma, R) \,.$$

$$g_{\rm out}(\omega,y,V) \equiv \frac{\int \mathrm{d}z P_{\rm out}(y|z) \left(z-\omega\right) e^{-\frac{(z-\omega)^2}{2V}}}{V \int \mathrm{d}z P_{\rm out}(y|z) e^{-\frac{(z-\omega)^2}{2V}}} \,.$$

Input: y

Initialize:  $\mathbf{a}^0, \mathbf{v}^0, g^0_{\text{out}, \mu}, \mathbf{t} = 1$ 

repeat

AMP Update of  $\omega_{\mu}, V_{\mu}$ 

$$V_{\mu}^{t} \leftarrow \sum_{i} F_{\mu i}^{2} v_{i}^{t-1}$$

$$\omega_{\mu}^{t} \leftarrow \sum_{i} F_{\mu i} a_{i}^{t-1} - V_{\mu}^{t} g_{\text{out},\mu}^{t-1}$$

AMP Update of  $\Sigma_i, R_i, g_{\text{out},\mu}$ 

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$$a_i^t \leftarrow f_a(\Sigma_i^t, R_i^t)$$
  
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Simple to implement, only matrix multiplications, O(N2)

GAMP for prediction:

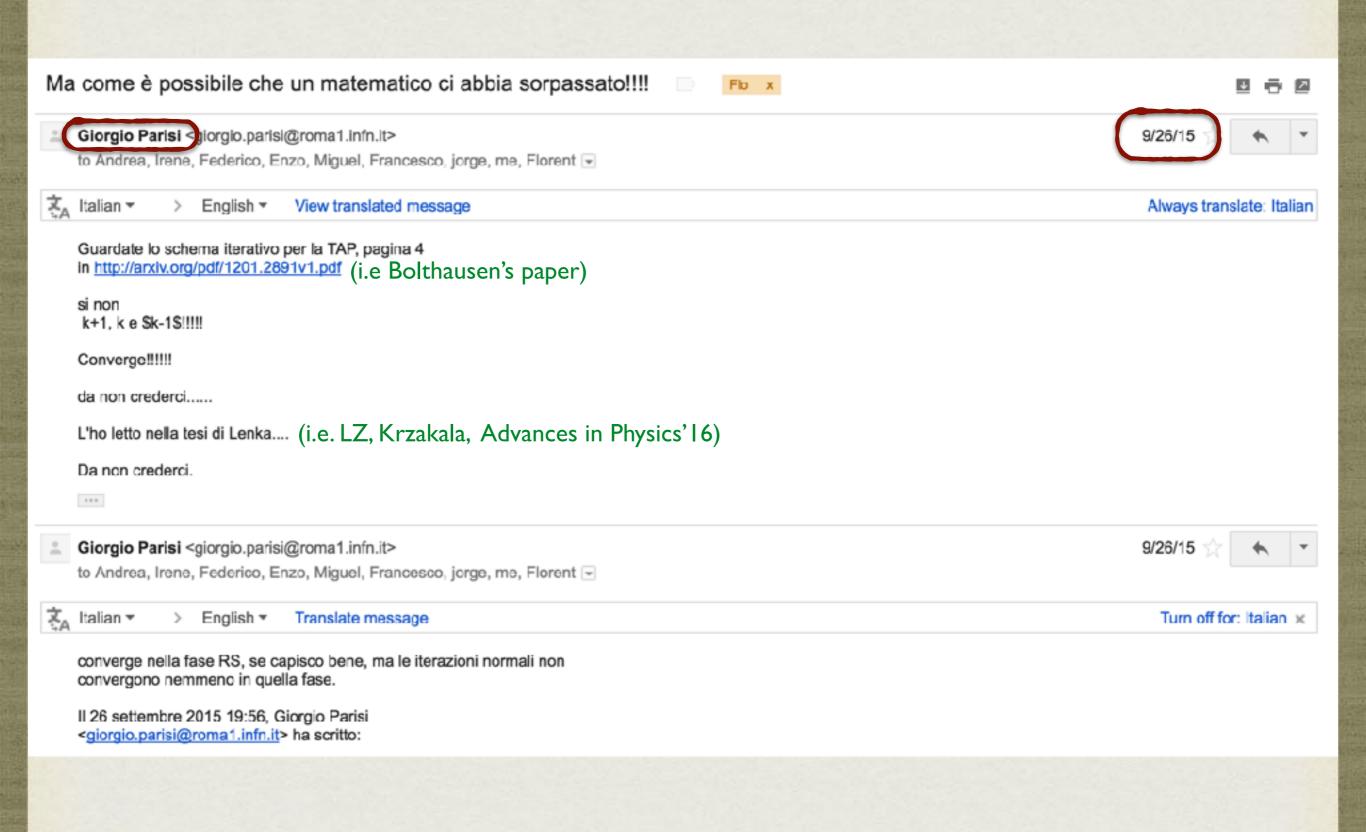
$$\hat{y}_{\text{new}}^{t} = \frac{1}{\sqrt{2\pi V^{t}}} \int dz \, dy \, y P_{\text{out}}(y|z) e^{-\frac{1}{2V^{t}} (z - \sum_{i} F_{\text{new},i} a_{i}^{t-1})^{2}}$$

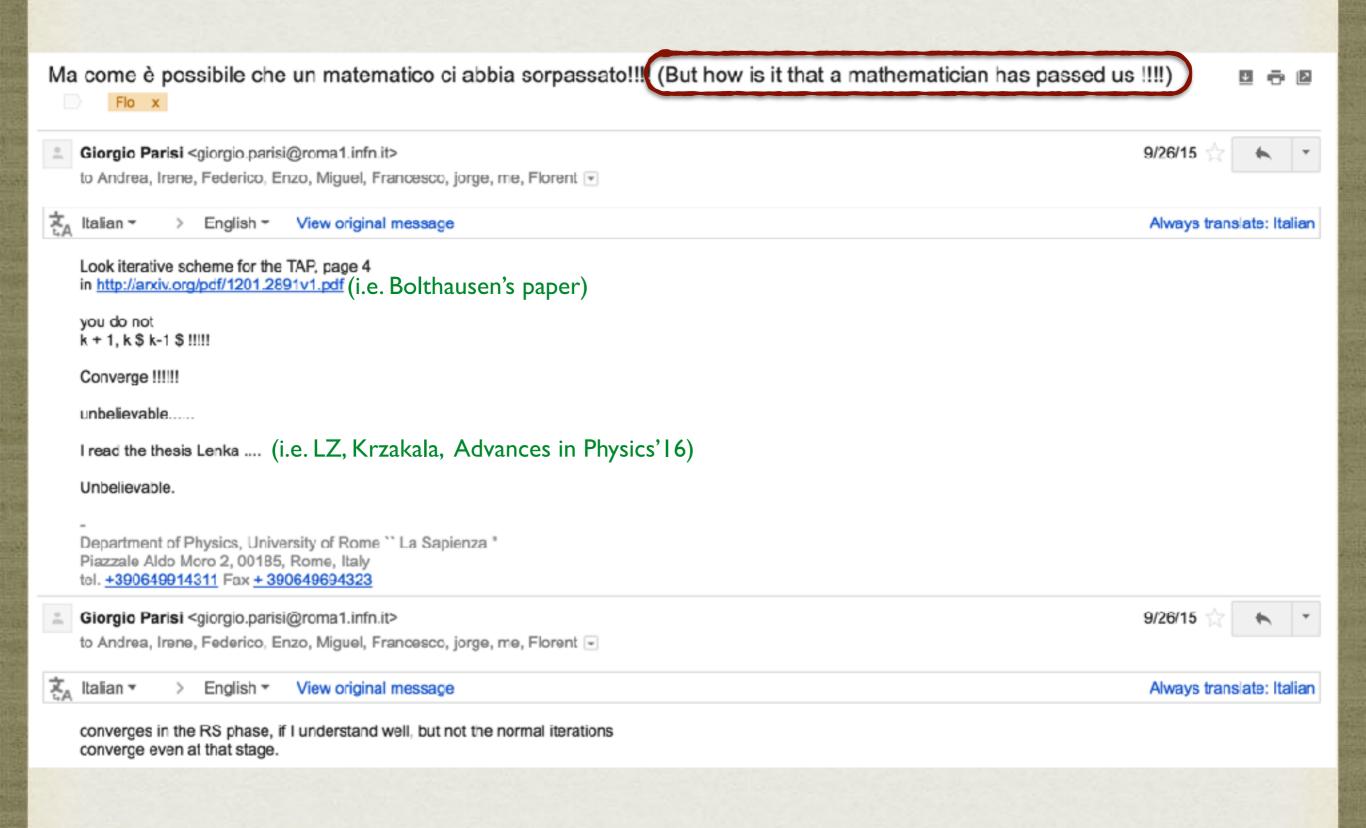
# THE STORY OF GAMP

GAMP is closely related to the Thouless-Anderson-Palmer'76 equations for the Sherrington-Kirkpatrick spin glass. For perceptron written by Mezard'89 as a way to derive the replica result without replicas, not used as an actual algorithm.

TAP was used as an iterative algorithm, but had wrong iteration-indices and consequently did not convergence.

Bolthausen fixed the issue in ~2008 and proved state evolution for the corrected TAP equations.





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Bolthausen fixed the issue in ~2008 and proved state evolution for the corrected TAP equations.

For GAMP state evolution proven by Bayati, Montanari'11, Bayati, Lelarge, Montanari'12, Javanmard, Montanari'13.

## STATE EVOLUTION

$$m^t \equiv rac{1}{N} \sum_{i=1}^N x_i^* a_i^t$$
 then  $MSE(t) = 
ho - m^t$ 

$$MSE(t) = \rho - m^t$$

mt in the AMP algorithm evolves as:

$$m^{t+1} = 2\partial_{\hat{m}} \Phi_{P_X}(\hat{m}^t)$$

$$\hat{m}^t = 2\alpha \partial_m \Phi_{P_{\text{out}}}(m^t; \rho)$$

Recall the RS free energy

$$f_{RS}(m, \hat{m}) = \Phi_{P_X}(\hat{m}) + \alpha \Phi_{P_{\text{out}}}(m; \rho) - \frac{m\hat{m}}{2}$$



No "state evolution" for naive mean-field, nor MCMC, nor Langevin dynamics (except spherical p-spin, much more complex int.-diff. equations).

# BOTTOMLINE

$$P(x|y,F) = \frac{1}{Z(y,F)} \prod_{\mu=1}^{M} P_{\text{out}}(y_{\mu}|\sum_{i=1}^{N} F_{\mu i}x_i) \prod_{i=1}^{N} P_X(x_i)$$

- x\* is generated from Px, y from Pout. F is random iid.
- lacktriangle The analysis gave us the free energy  $f_{
  m RS}(m)$

$$MMSE = \rho - \operatorname{argmax} f_{RS}(m)$$

 $MSE_{AMP}$  = local extremum of  $f_{RS}(m)$ , reached from un-informed initialisation of state evolution.

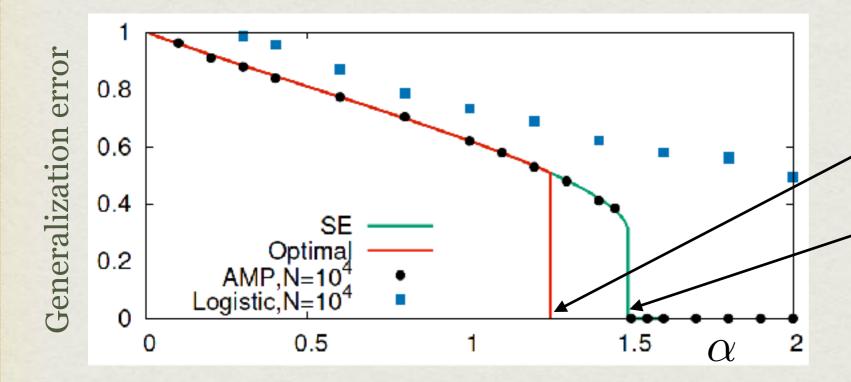
# RESULTS

### BINARY PERCEPTRON

Gardner, Derrida'89, Gyorgyi'90, Sompolinsky, Tishby, Seung'90

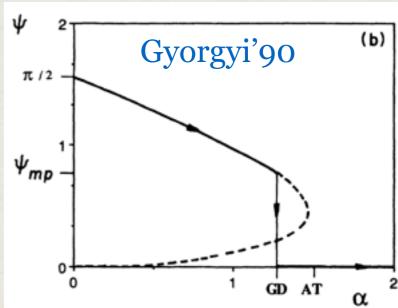
$$y = \operatorname{sign}(Fx^*)$$

$$P_X(x) = \frac{1}{2} [\delta(x-1) + \delta(x+1)]$$

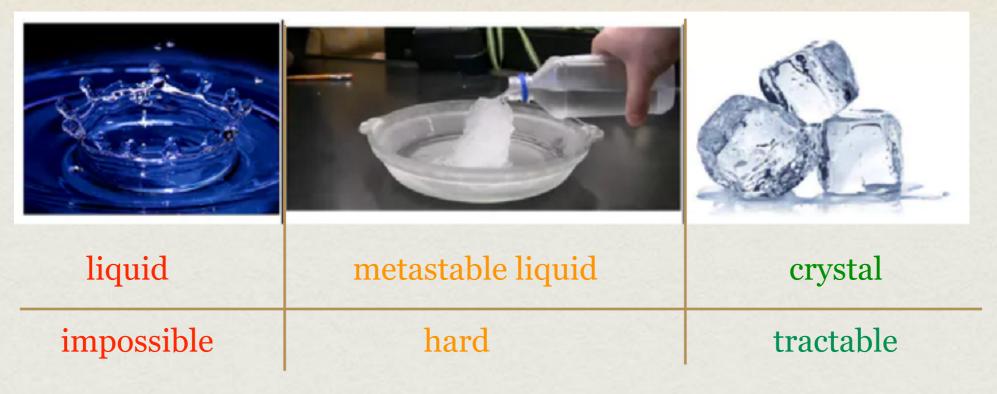


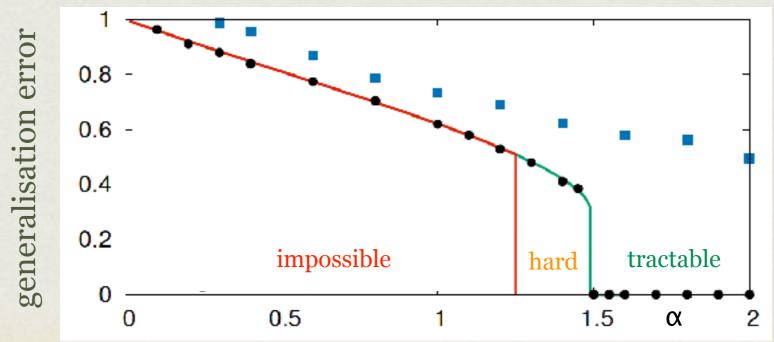
- $\alpha_{\rm IT} = 1.249$
- $\alpha_{\text{Alg}} = 1.493$

- ▶ GAMP is optimal starting from  $\alpha_{Alg}$ .
- Redemption of the "un-physical" branch.



# PHYSICS VS LEARNING





### BINARY PERCEPTRON

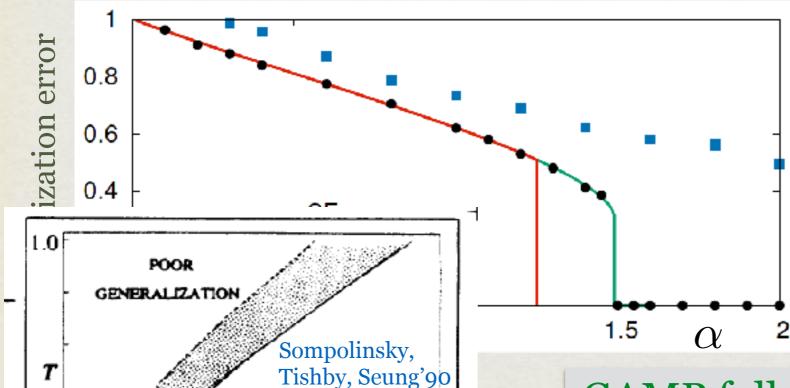
Gardner, Derrida'89, Gyorgyi'90, Sompolinsky, Tishby, Seung'90

$$y = \operatorname{sign}(Fx^*)$$

0.0.

= 1.245

$$P_X(x) = \frac{1}{2} [\delta(x-1) + \delta(x+1)]$$



 $\alpha_{SST} =$ 

$$\alpha_{\rm IT} = 1.249$$

$$\alpha_{\rm Alg} = 1.493$$

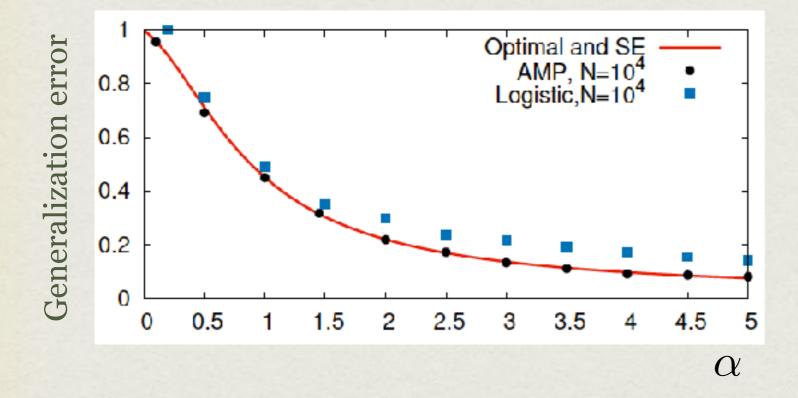
GAMP follows the liquid-spinodal, and ignores the glassiness that slows down MCMC. Can other algorithms match GAMP?

## GAUSS-BERNOULLI PERCEPTRON

$$y = \operatorname{sign}(Fx^*)$$

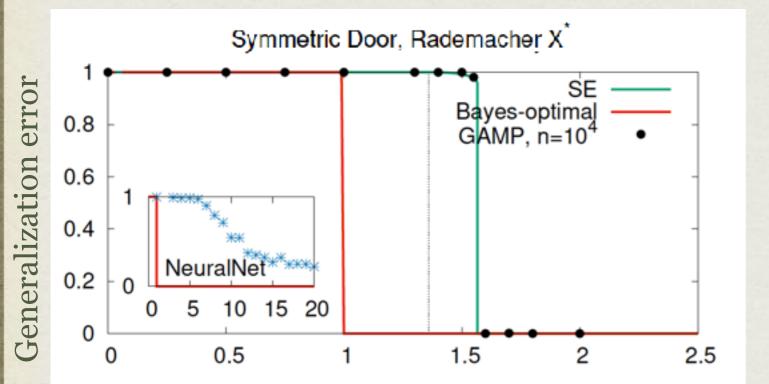
$$P_X(x) = \rho \mathcal{N}(0, 1) + (1 - \rho)\delta(x)$$

$$\rho = 0.2$$



## SYMMETRIC BINARY PERCEPTRON

$$y = \operatorname{sign}(|Fx^*| - K)$$



K chosen so that 
$$P(y=1)=0.5$$

α

$$P_X(x) = \frac{1}{2} [\delta(x-1) + \delta(x+1)]$$

$$\alpha_{\rm IT} = 1$$
 $\alpha_{\rm Alg} = 1.566$ 

Very simple yet very hard benchmark for classification!

from: Barbier, Krzakala, Macris, Miolane, LZ arXiv:1708.03395

# NEW WITH RESPECT TO 1990

- ► Generic P<sub>X</sub> and P<sub>out</sub>, plug-and-go formula/algorithm (Rangan'10; LZ, Krzakala'16)
- ▶ Proof of the optimal error. (Barbier, Krzakala, Macris, Miolane, LZ'17)
- ▶ GAMP with correct time indices (Kabashima'o3; Bolthausen'o8; Donoho, Montanari, Maleki'o9) follows the state evolution. (Bayati, Montanari'11; et al.)
- ▶ GAMP ignores glassiness, it follows the "unphysical" spinodal.
- Conjecture: GAMP optimal among tractable algorithms. (challenge for future work ...)

# ONGOING WORK

- Generalized linear model as an interesting benchmarks for genericpurpose algorithms. How many samples does a deep network need to learn these simple rules?
- Beyond random iid matrices in order to study structured data.
- Beyond separable priors, extending to multiple-layers. With fixed weights (Krzakala, Manoel, Mezard, LZ'17).
- Learning of weights in multiple layers a case where we still have to find the right decoupling to make the replica method work.

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## Thank you for your attention!

