

Learning by Local Entropy Maximization: the effective landscape of neural networks learning algorithms

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*Radboud University
Nijmegen*

Plan of the talk

- Geometrical structure of minima in non-convex random optimization and learning problems
 - Clustering and symmetry breaking
 - The **Local Entropy Measure** reveals the existence of subdominant *high local density regions in weight space*.
 - Accessibility and Local Bayesian predictions
- Algorithms from a local entropy measure
 - The Robust Ensemble: an “out-of-equilibrium” measure
 - Real replicas algorithms: MCMC,SGD and Belief Propagation
 - Connections with DNNs
 - ...

What makes a constraint satisfaction problem or a learning problem extracted from a *natural distribution* hard to solve?

Basic example: Random K-SAT

- Let $C_K(N)$ be the set of all $2^K \binom{N}{K}$ possible K-clauses on x_1, x_2, \dots, x_N
- Select uniformly, independently and with replacements $M = \alpha N$ clauses from $C_K(N)$ to generate a K-cnf formula $F_N(K, \alpha)$

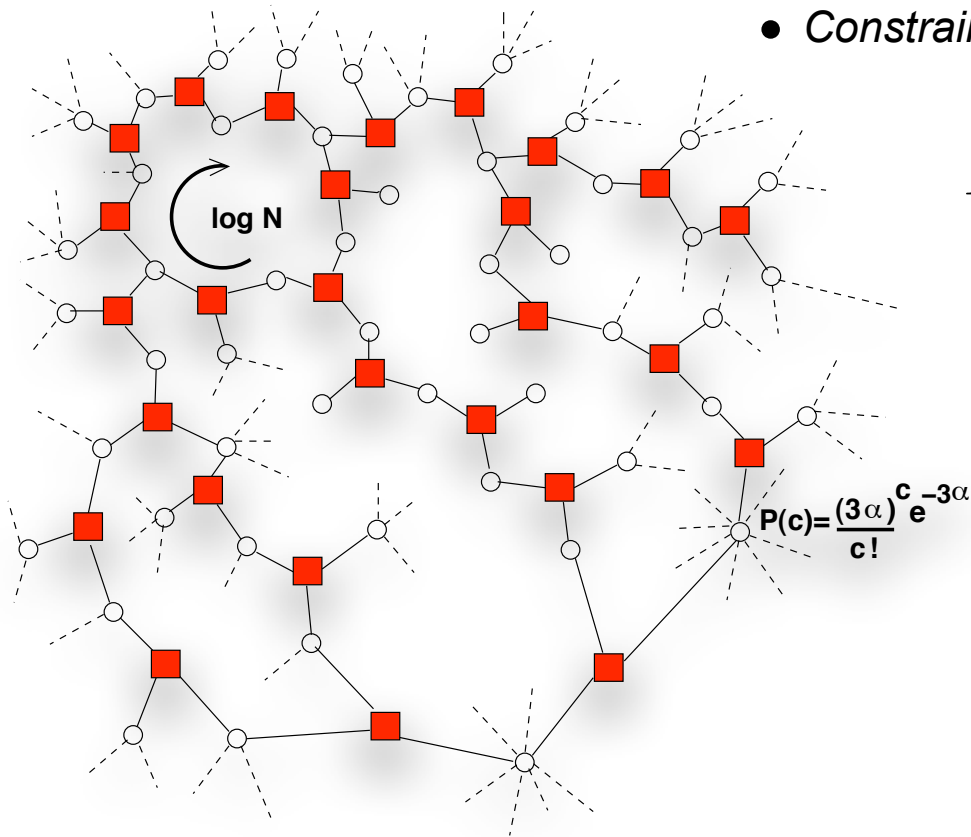
$$F = (x_1 \vee x_{27} \vee \bar{x}_3) \wedge (\bar{x}_{11} \vee x_3 \vee x_2) \wedge \dots \wedge (x_9 \vee \bar{x}_8 \vee \bar{x}_{30})$$

Question: does $F_N(K, \alpha)$ have a truth assignment?

Factor Graphs for CSPs

- N discrete variables $\{x_i\}$, e.g., Boolean, spins, colors
- Constraints E_a , $a = 1, \dots, M$ involving vars $\{x_{i(a)}\}$

$$E_a = \begin{cases} 0 & \text{if } \{x_{i(a)}\} \text{ satisfy constraint} \\ 1 & \text{otherwise} \end{cases}$$

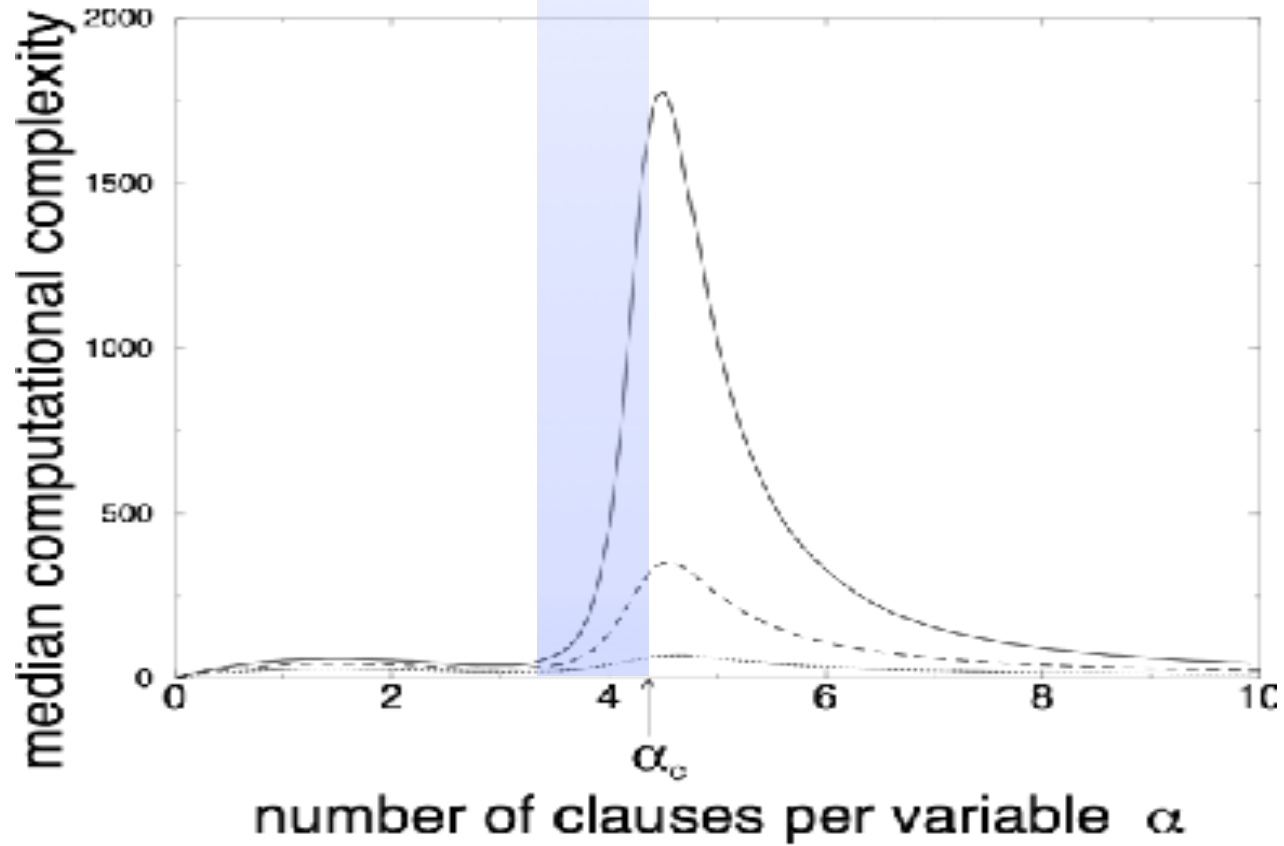
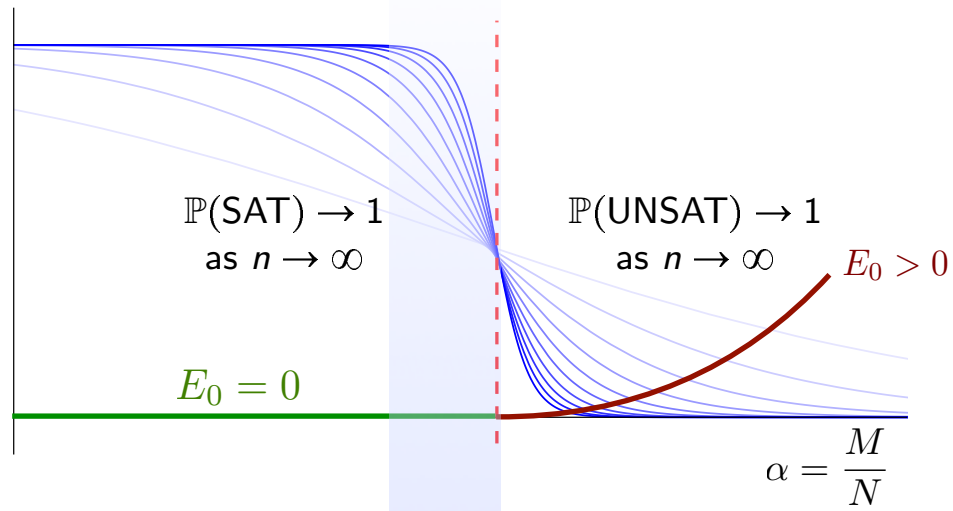


$$E_a = (x_{i_1} \vee \bar{x}_{i_2} \vee x_{i_3})$$

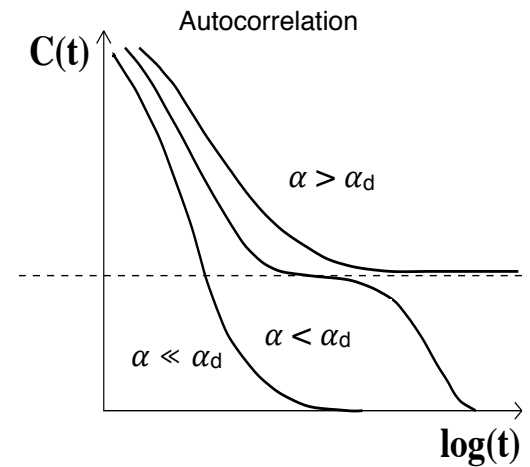
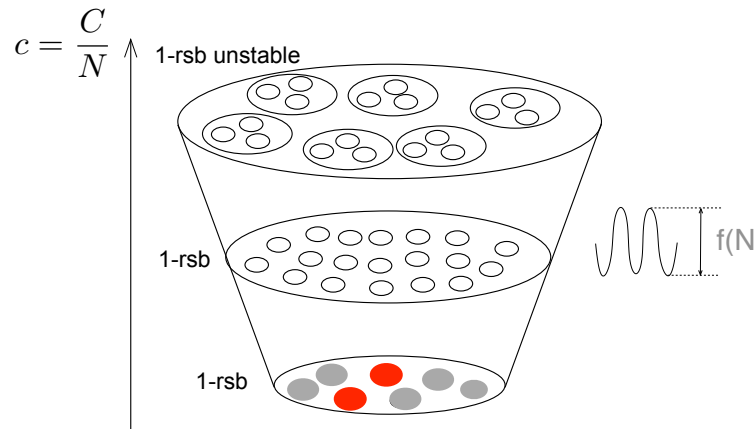
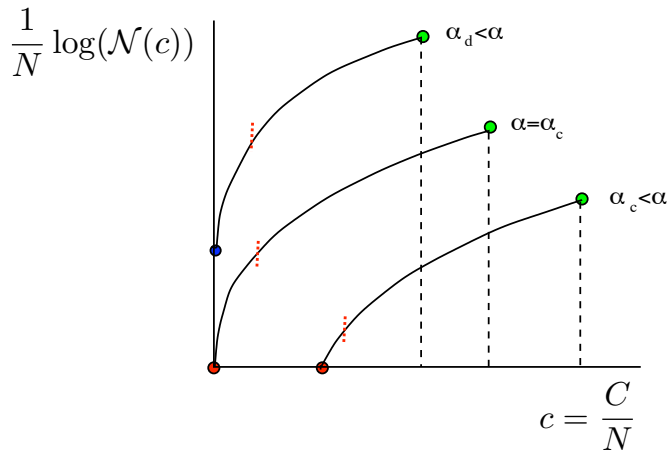
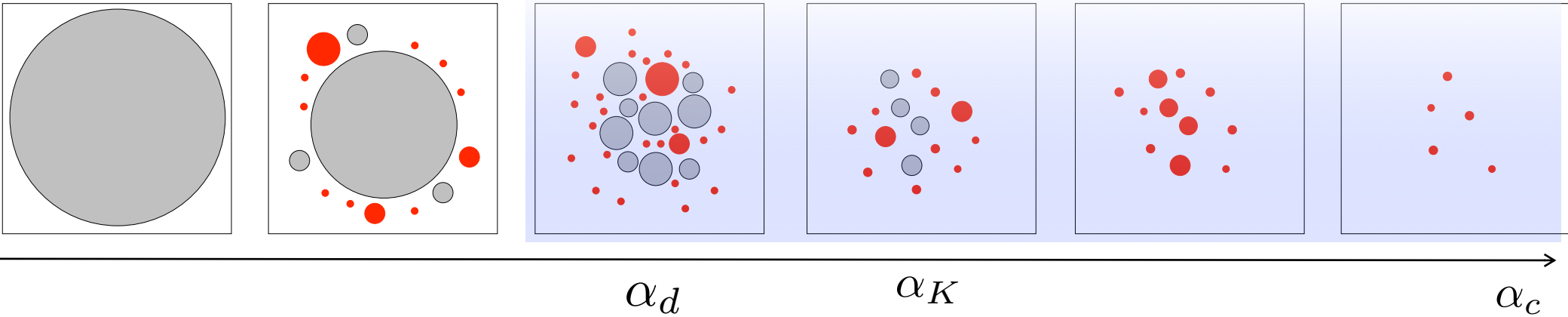
$$M = \alpha N$$

Cost/Energy function:

$$E = \sum_{a=1}^{\alpha N} E_a[\{x_{i(a)}\}]$$



Geometry of solutions in random Constraint Satisfaction Problems: Gibbs measure decomposition



Finding isolated solutions is hard. In the last 15 years many physicists, mathematicians and CS have contributed to various aspects of these results ... the scenario is by now rigorously established

Gibbs measure decomposition

$$P(\mathbf{w}) = \frac{1}{Z} \prod_{a=1}^M \Psi_a(\{w_{(ij) \in a}\})$$

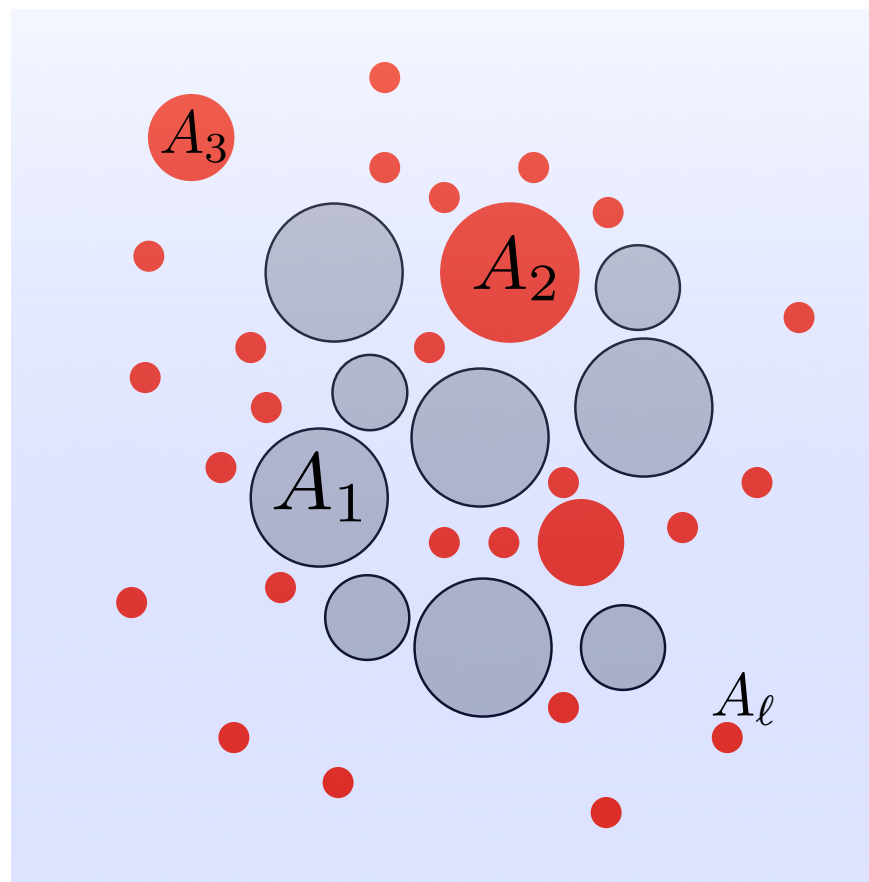
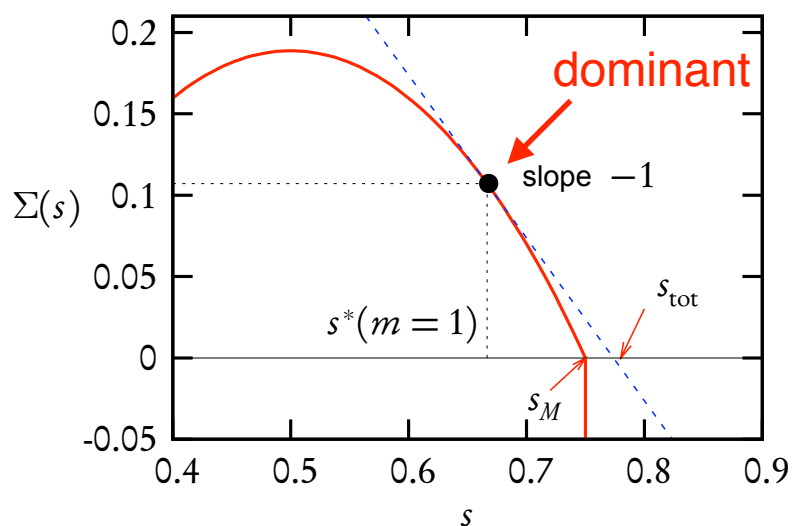
$$P_\ell = \sum_{\{\mathbf{w} \in A_\ell\}} P(\mathbf{w})$$

RS: $P_1 = 1$

$$P_1 > P_2 > P_3 > \dots$$

1RSB-d: $\mathcal{N} = e^{\Sigma N}$

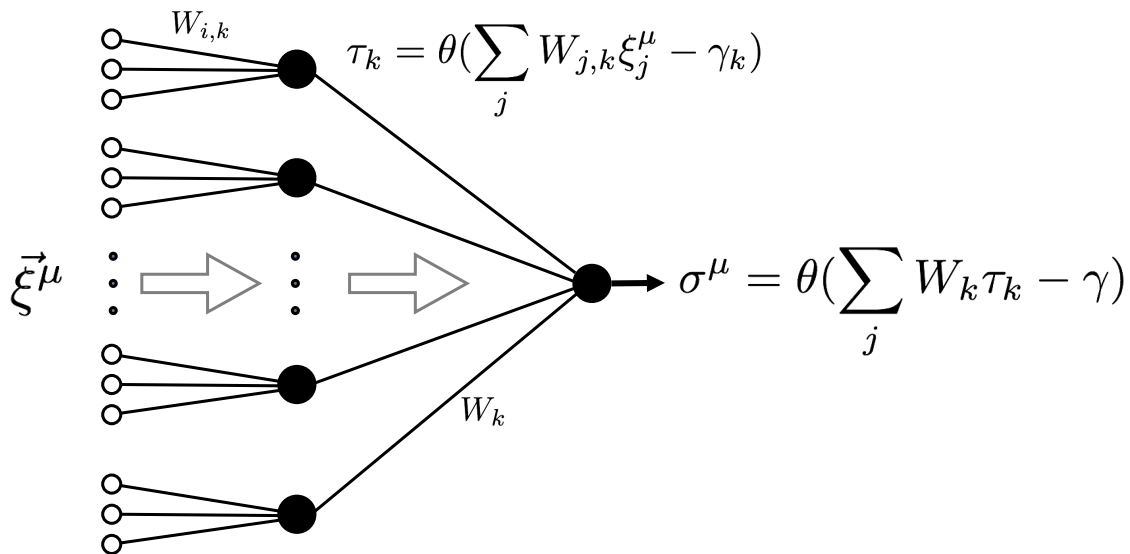
1RSB-s: $\mathcal{N} = \text{sub-exp}$



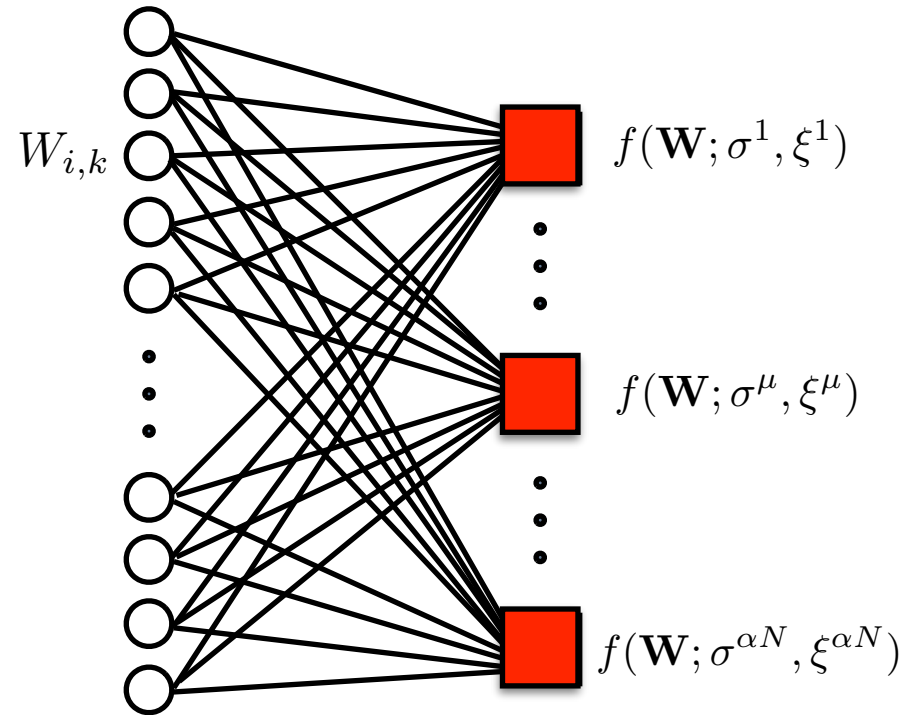
Learning as a CSP problem

Constraints: one for each pattern

$$f(\mathbf{W}; \sigma^\mu, \xi^\mu) = \delta(\sigma^\mu; \sigma(\mathbf{W}, \xi^\mu))$$

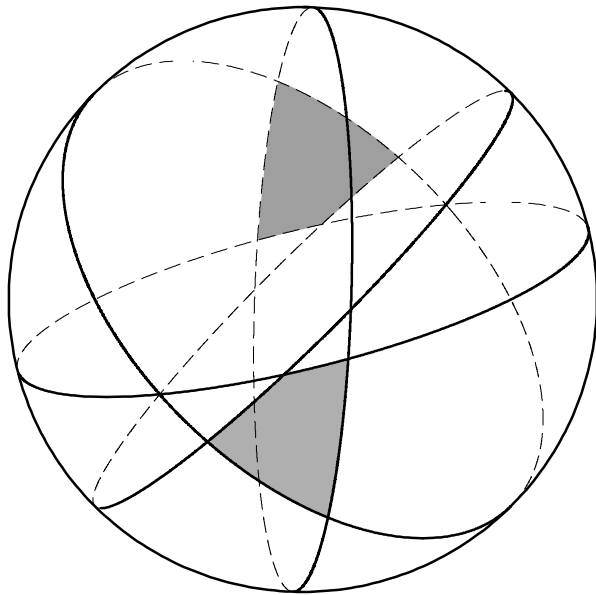


Fully connected factor graph



“Old” (90s) statistical physics results: a relatively similar scenario

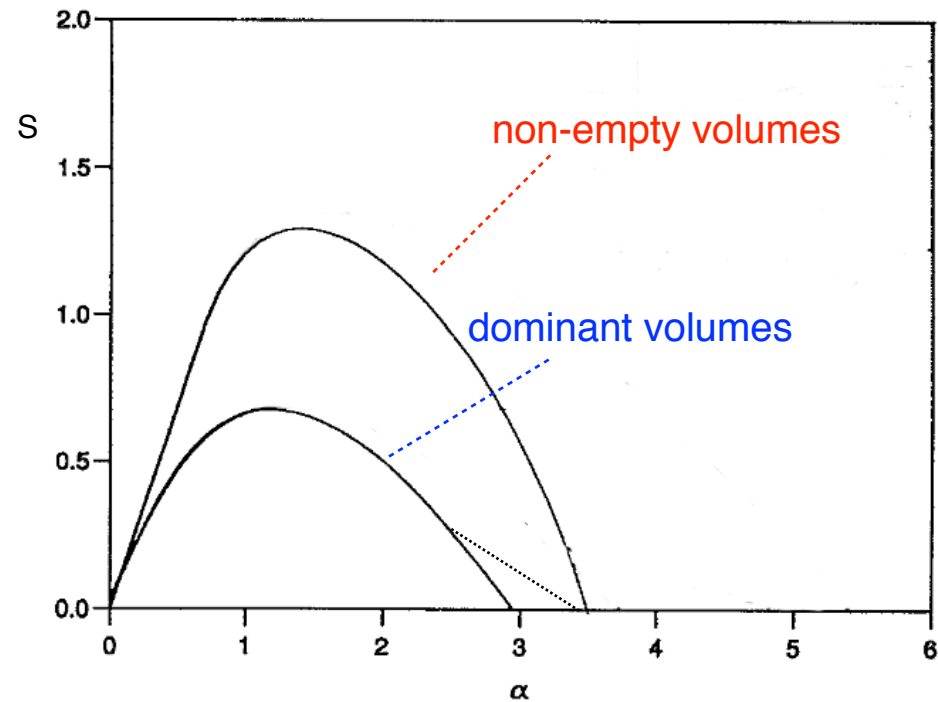
Geometry of space of solution and internal representations in MLP learning random patterns with continuous weights (zero errors landscape)



Fractional volume of weights storing the patterns

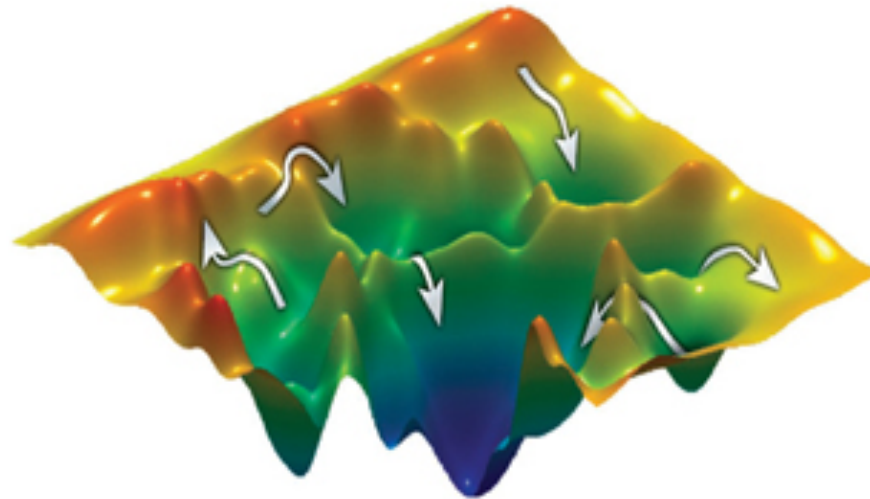
$$V = \frac{\int d\mathbf{w} \delta(\mathbf{w}^2 - 1) \prod_{\mu} \delta(\sigma^{\mu}; \sigma(\mathbf{w}, \xi^{\mu}))}{\int d\mathbf{w} \delta(\mathbf{w}^2 - 1)}$$

one hidden layer committee NN



How does learning take place in large scale DNNs?

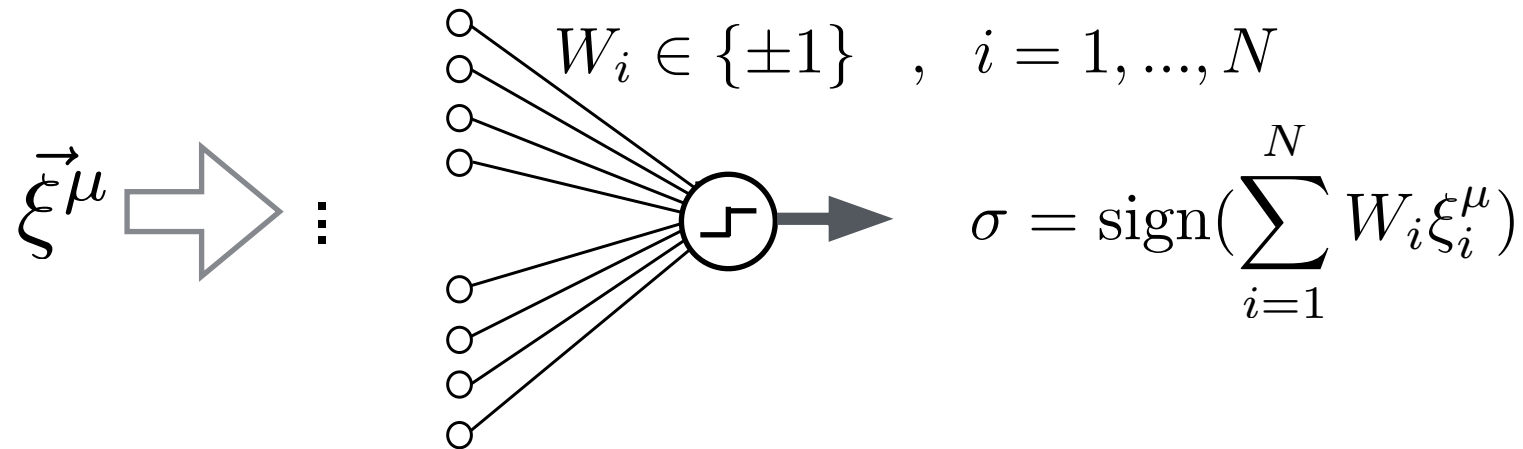
Learning algorithms: Variants of **gradient back-propagation**



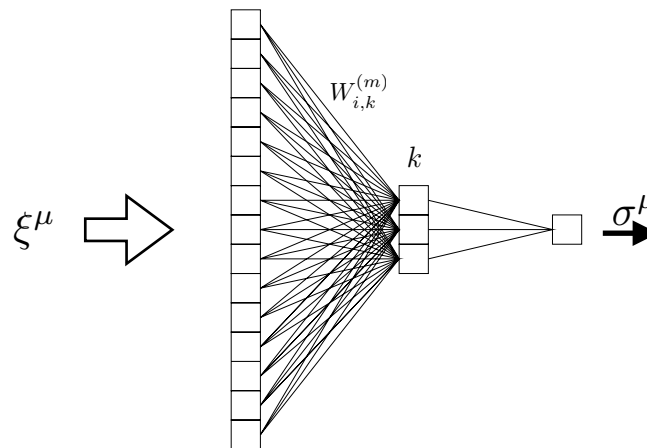
However, successful algorithms never “simply” minimize the loss.

Why?

The simplest non-convex neural device: perceptron with discrete weights



Analytical results generalise to arbitrary
number of levels and multiple layers

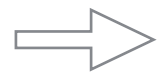


Non-convex minimum “energy” problem

Given a set of i.i.d. random examples ($p=1/2$):

$$\{(\xi_i^\mu = \pm 1, \sigma^\mu = \pm 1)\} \quad i = 1, \dots, N \quad \mu = 1, \dots, \alpha N$$

Find \mathbf{W} such that $\sigma^\mu = \sigma(\mathbf{W}, \xi^\mu) \quad \forall \mu$



αN constraints on $\{W_i\}$

Cost-energy function

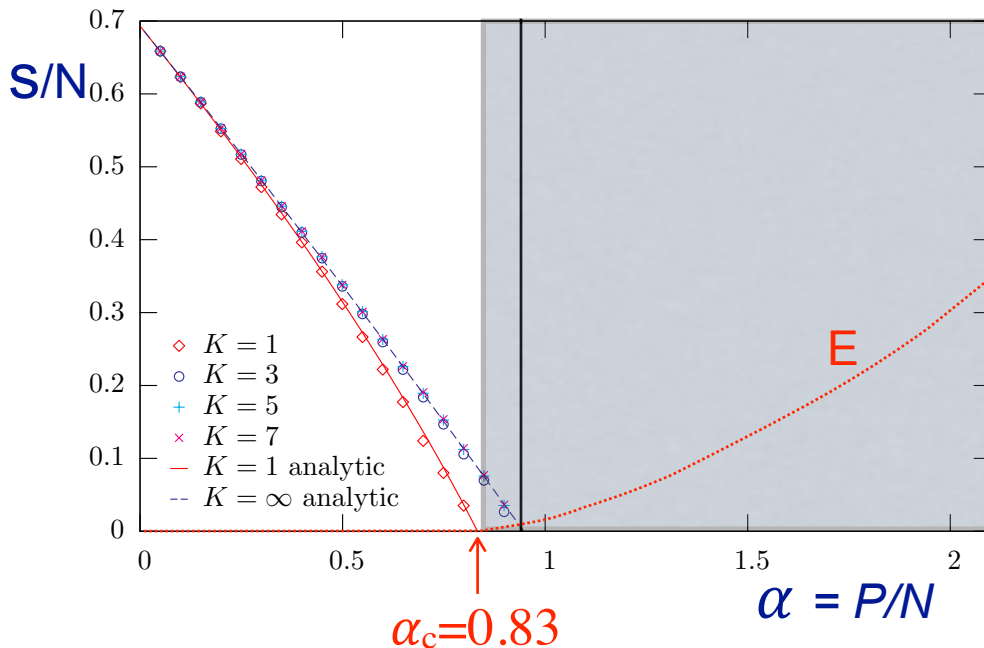
$$E(\mathbf{W}) = \sum_{\mu} \Theta(-\sigma^\mu \text{sgn}(\mathbf{W} \cdot \xi^\mu)) = \# \text{ number of errors}$$

$$\Theta(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}$$

Phase diagram (~1990)

- At $E=0$, minima are very narrow and isolated

$S = \log(\# \text{ optimal } W \text{ assignments})$



some classical papers:

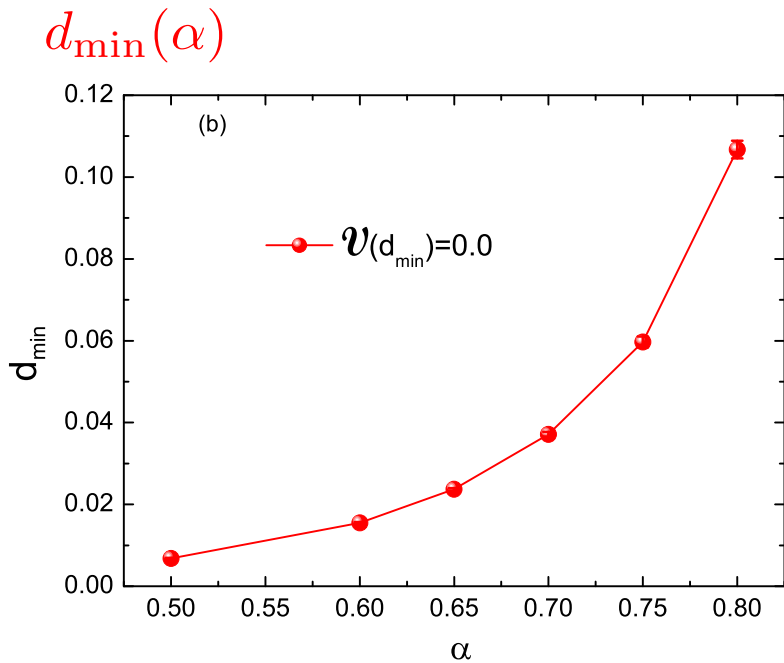
E. Gardner, E. Gardner B. Derrida, +
W. Krauth, M. Mézard, *J. de Physique* **50**, 3057-3066 (1989); E. Barkai, D. Hansel, H. Sompolinsky, *Phys. Rev. A* **45**, 4146-4160 (1992); M. Mezard, *J. Phys. A* **22**, 2181 (1989); H.S. Seung, H. Sompolinsky, N. Tishby, *Phys. Rev. A* **45**, 6056 (1992); E. Barkai, I. Kanter, *Europhys. Lett* **14**, 107 (1991); R. Penney and D. Sherrington, *J. Phys. A* **26**, 6173(1993)
M. Tsodyks, *Mod. Phys. Lett. B* **4**, 713 (1990); D.J. Amit, S. Fusi *NETWORK* **3**, 443 (1992); D.J. Amit, S. Fusi, *Neural Computation* **6**, 957-982 (1994);
H. Horner, *Z. Phys. B* **86**, 291-308 (1992)
...

For decades, heuristic local search algorithms were believed to fail in finding solutions for any extensive number of patterns.

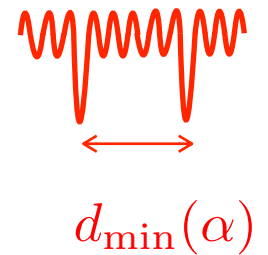
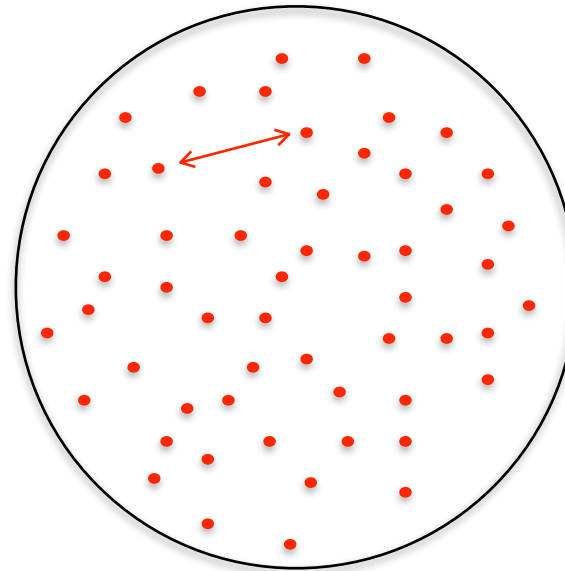
Geometry of the space of solutions in the binary perceptron:

Franz-Parisi potential: entropy at distance \mathbf{d} , sampling from **typical** solution \mathbf{J}

$$F(x) = \left\langle \frac{1}{Z(T')} \sum_{\mathbf{J}} \Theta \left(\frac{1}{\sqrt{N}} \sum_{i=1}^N J_i \xi_i^\mu \right) \ln \sum_{\mathbf{w}} \Theta \left(\frac{1}{\sqrt{N}} \sum_{i=1}^N w_i \xi_i^\mu \right) e^{x \mathbf{J} \cdot \mathbf{w}} \right\rangle_{\xi}$$



$$d_{\min}(\alpha) \sim O(N)$$

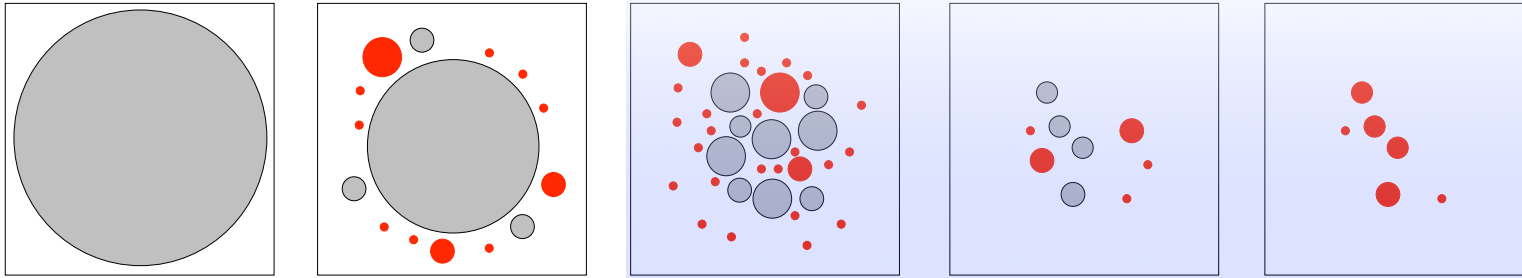


H. Huang, Y. Kabashima (2014) ($q_1=1$ known since the 80's)

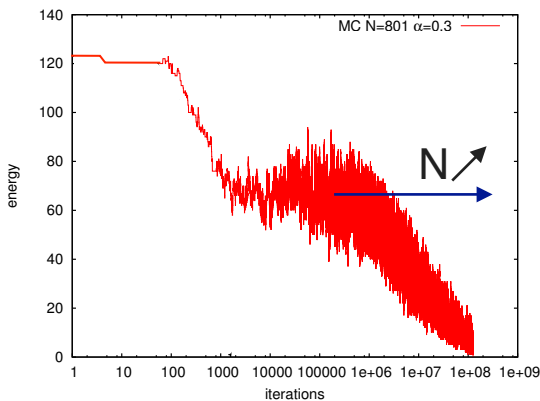
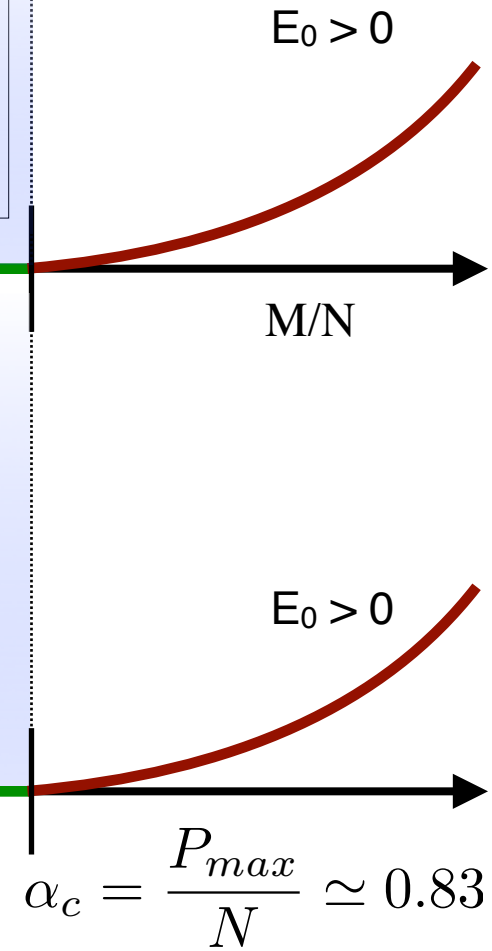
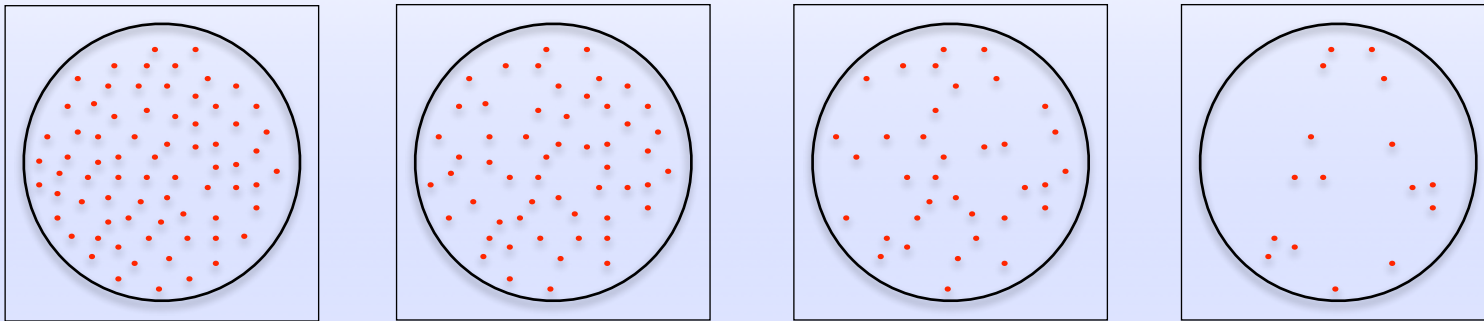
$$\alpha_c = \frac{P_{max}}{N} \simeq 0.83$$

W Krauth, M. Mezard, (1989)

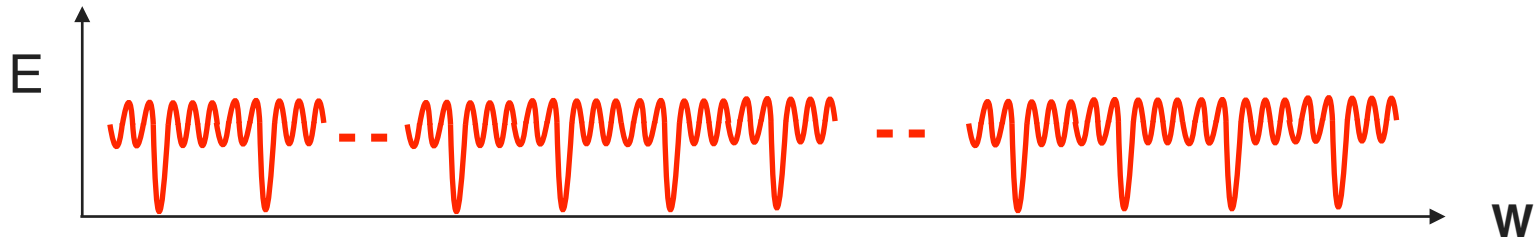
random K-SAT



discrete NN

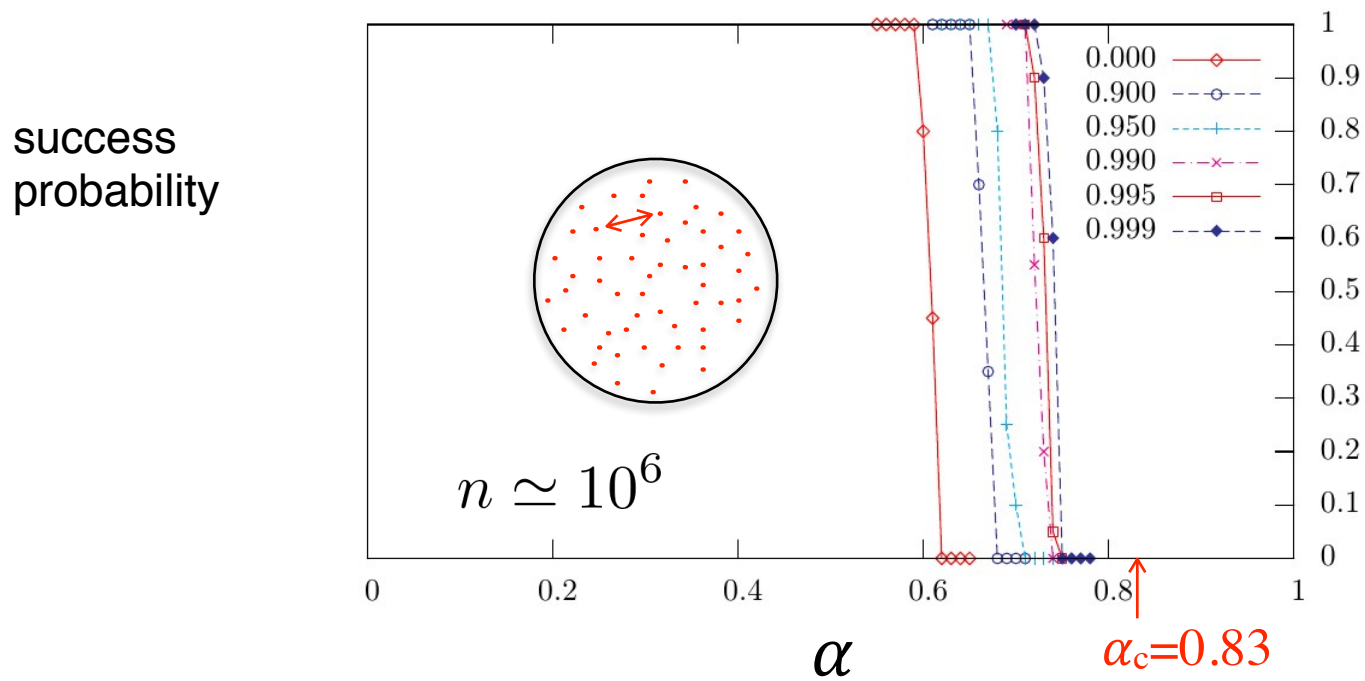


learning impossible
for random patterns ?



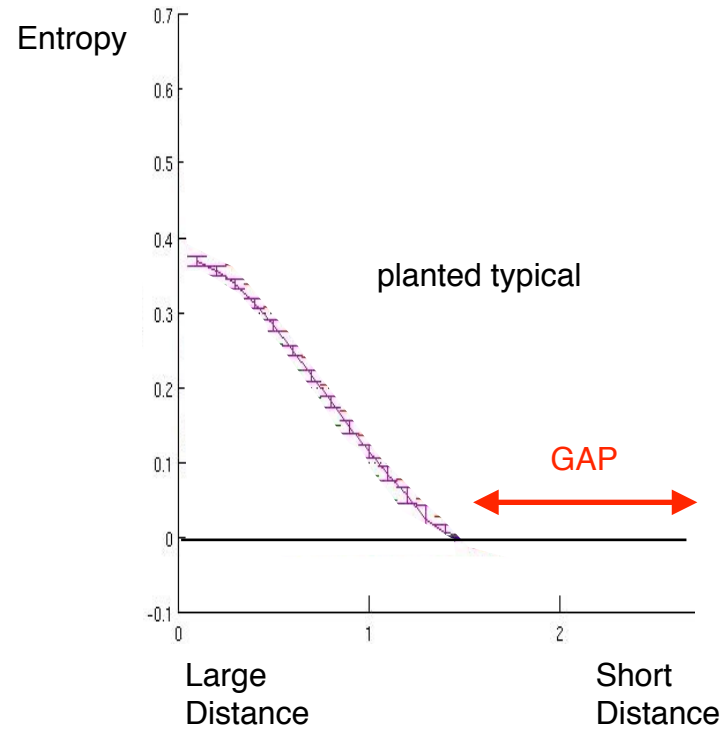
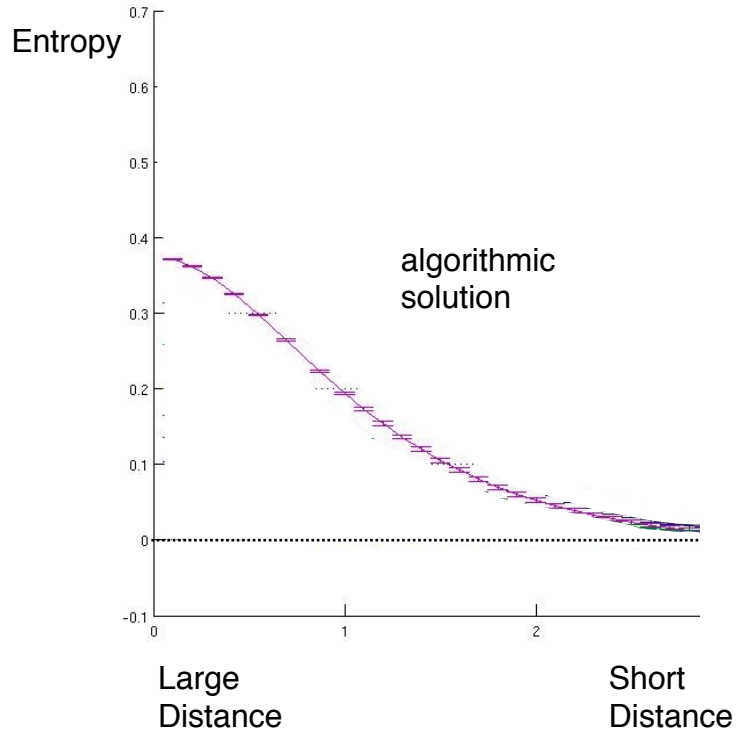
Golf course for any α ? Efficient learning impossible ?

Message-passing algorithms (2006, A. Braunstein RZ) and its simplifications work well



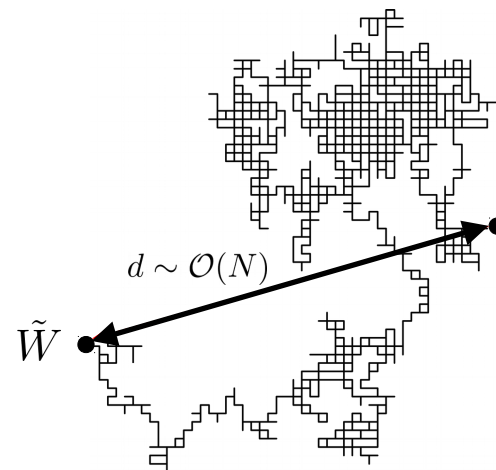
something unclear ...

Weight enumerator functions computed with BP, relative to a solution found by an algorithm and to a typical solution (planted)

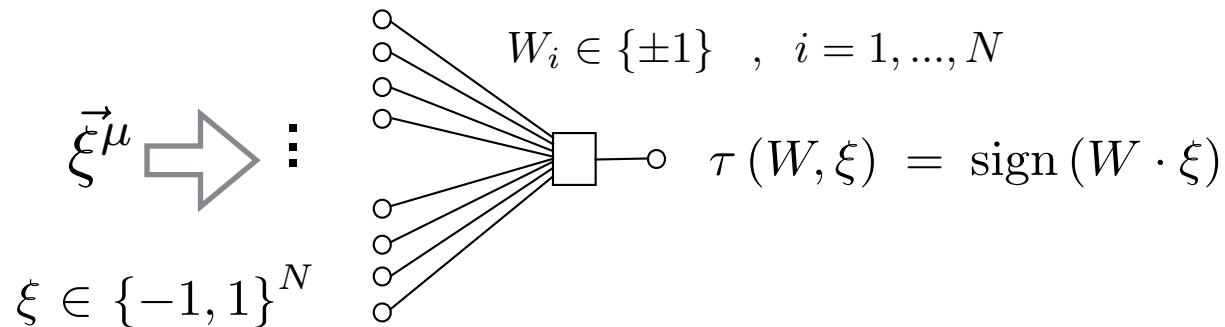


N=1001
samples=50

Evidence for Random Walks analysis:



Learning in rare regions ? Large deviations analysis



Characteristic function:

$$\mathbb{X}_\xi(W) = \prod_{\mu=1}^{\alpha N} \Theta(\sigma^\mu \tau(W, \xi^\mu)) = 1 \text{ iff all patterns are correctly classified}$$

Number of solutions within Hamming distance d from a given weight vector \tilde{W} :

$$\mathcal{N}(\tilde{W}, d) = \sum_{\{W\}} \mathbb{X}_\xi(W) \delta(W \cdot \tilde{W}, N(1 - 2d))$$

$$A \cdot B = \sum_{j=1}^N A_j B_j$$

Local entropy measure

number of solutions within a distance d $\mathcal{N}(\tilde{W}, d) = \sum_{\{W\}} X_{\xi}(W) \delta(W \cdot \tilde{W}, N(1 - 2d))$

“energy” = local entropy

$$\mathcal{E}_d(\tilde{W}) \doteq -\log \mathcal{N}(\tilde{W}, d)$$

Local Entropy Measure

maximally dense for $y \rightarrow \infty$

$$\mathcal{P}(\tilde{W}) \propto e^{-y\mathcal{E}_d(\tilde{W})}$$

normalisation

$$Z(d) = \sum_{\{\tilde{W}\}} X_{\xi}(\tilde{W}) e^{-y\mathcal{E}_d(\tilde{W})}$$

By the replica/cavity method we can compute the expectation of the local entropy in the large N limit

$$\mathcal{S}_I(d, y) = - \left\langle \mathcal{E}(\tilde{W}) \right\rangle_{\xi, \tilde{W}} = \frac{1}{N} \left\langle \log \mathcal{N}(\tilde{W}, d) \right\rangle_{\xi, \tilde{W}}$$

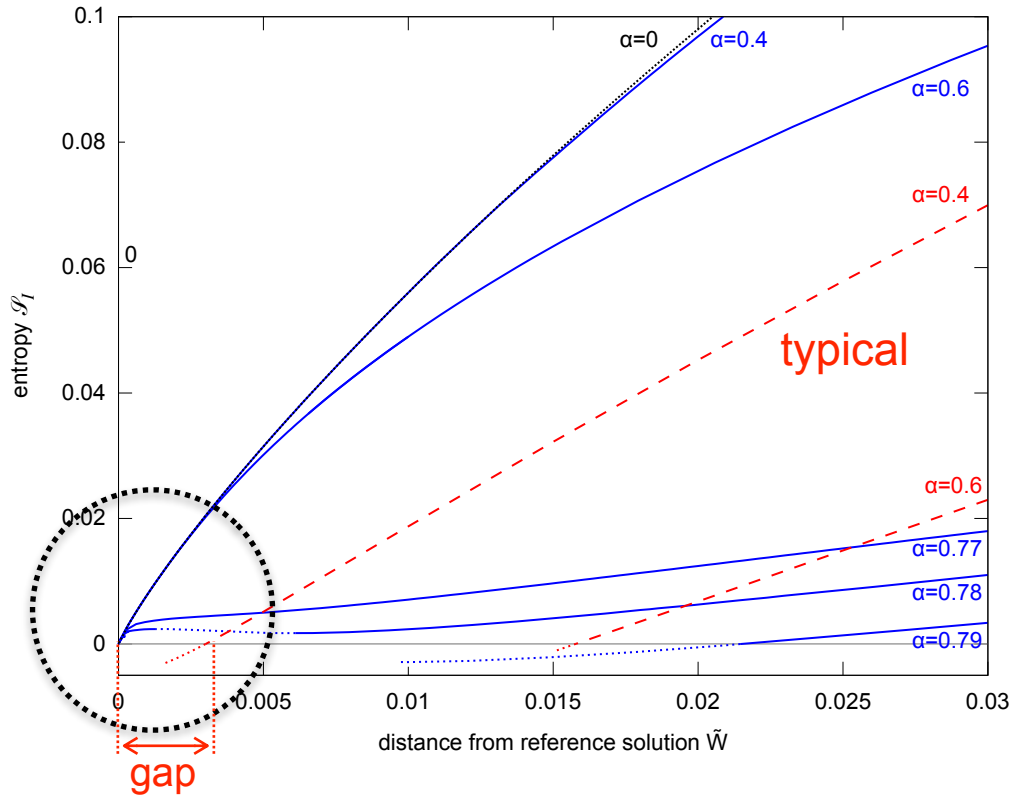
$$\mathcal{S}_I(d, y) = \partial_y (y \mathcal{F}(d, y))$$

internal entropy

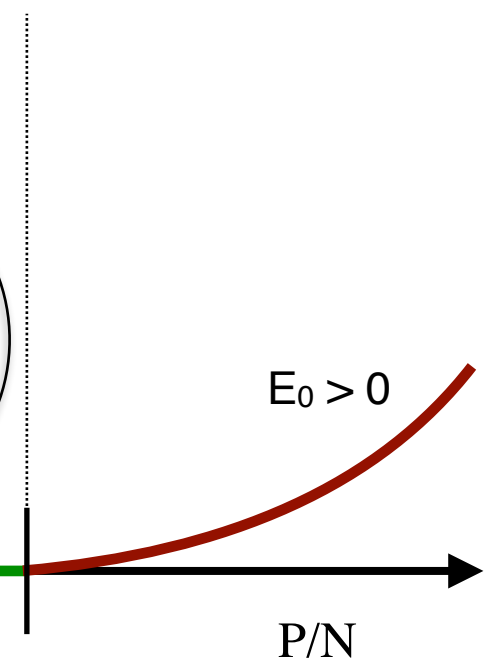
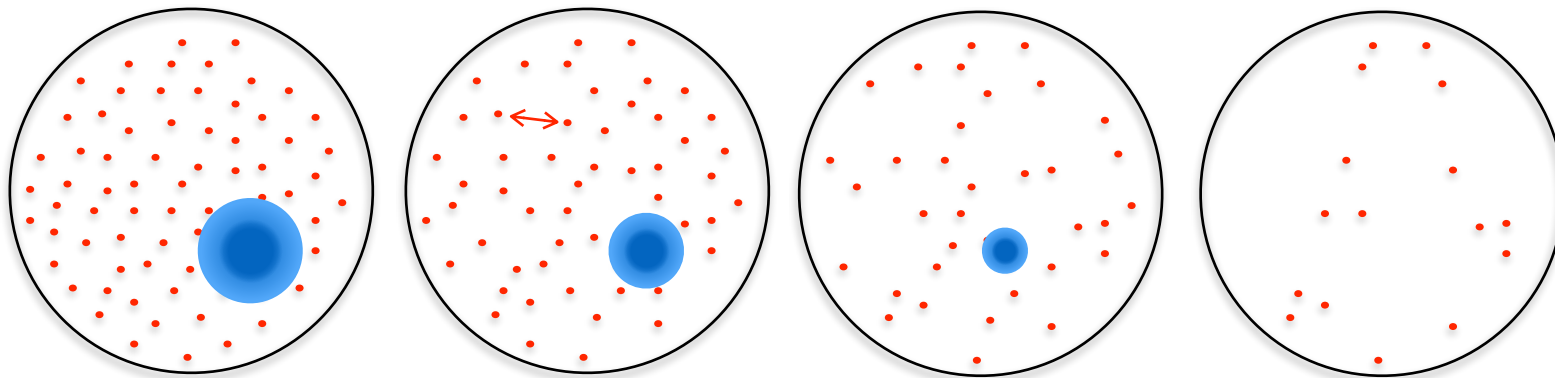
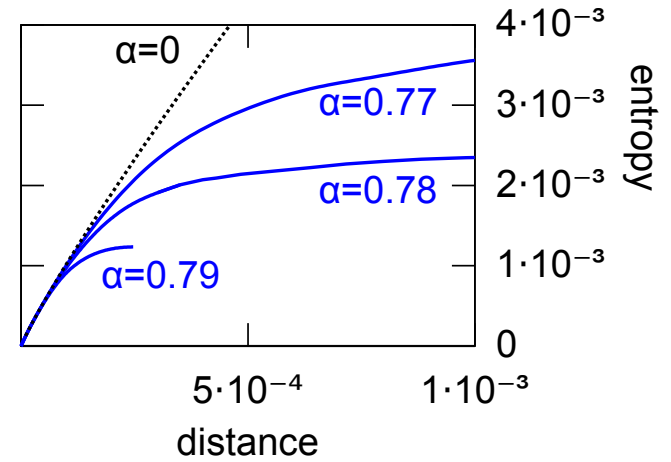
$$\mathcal{S}_E(d, y) = -y (\mathcal{F}(d, y) + \mathcal{S}_I(d, y))$$

external entropy

Large deviation analysis



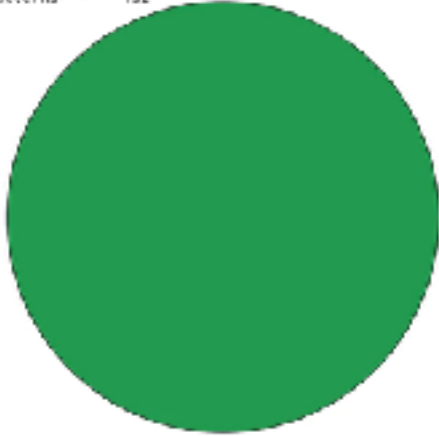
ultra-dense cluster



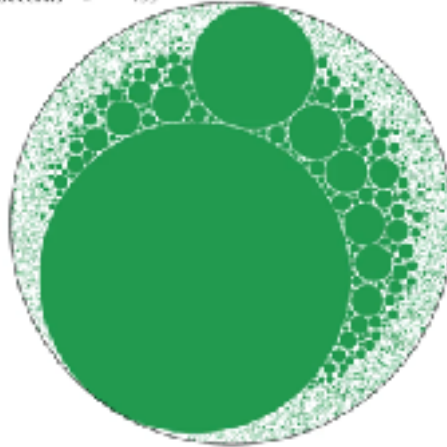
in the 90s we were not aware of this fundamental structural property

close to capacity the dense clusters breaks up

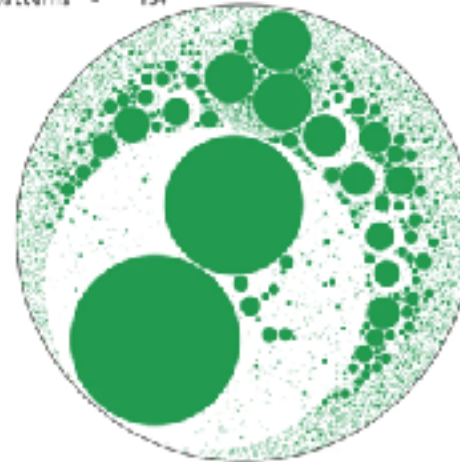
SOLUTIONS = 9908
 CLUSTERS = 1
 LARGEST = 9908
 α = 0.256
 patterns = 152



SOLUTIONS = 79371
 CLUSTERS = 4640
 LARGEST = 47613
 α = 0.761
 patterns = 153



SOLUTIONS = 69058
 CLUSTERS = 4888
 LARGEST = 25158
 α = 0.765
 patterns = 154

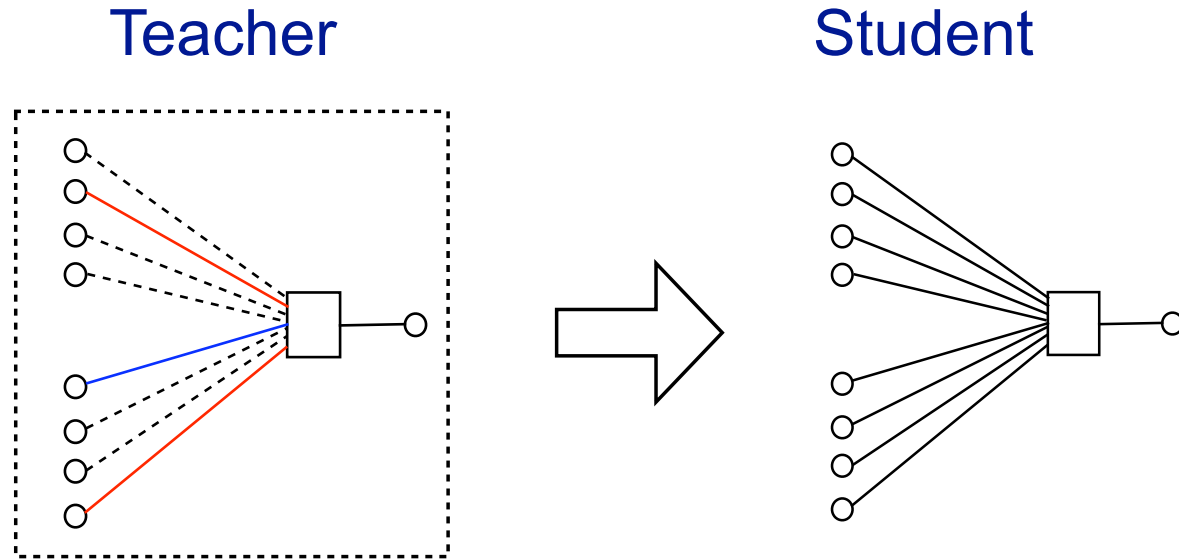


SOLUTIONS = 14199
 CLUSTERS = 3044
 LARGEST = 3149
 α = 0.771
 patterns = 155



the shape is not spherical ...

Making predictions

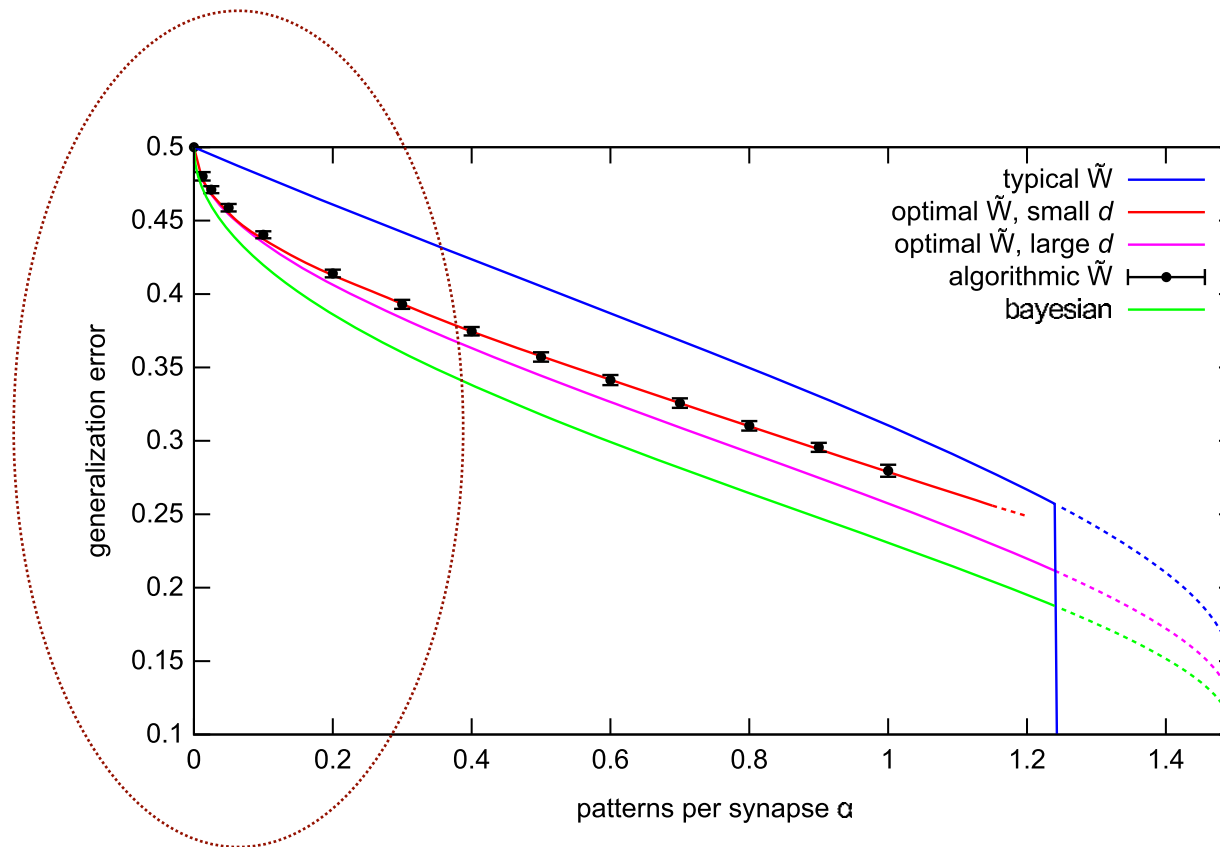


Probability to give the same answer of the teacher on a new input

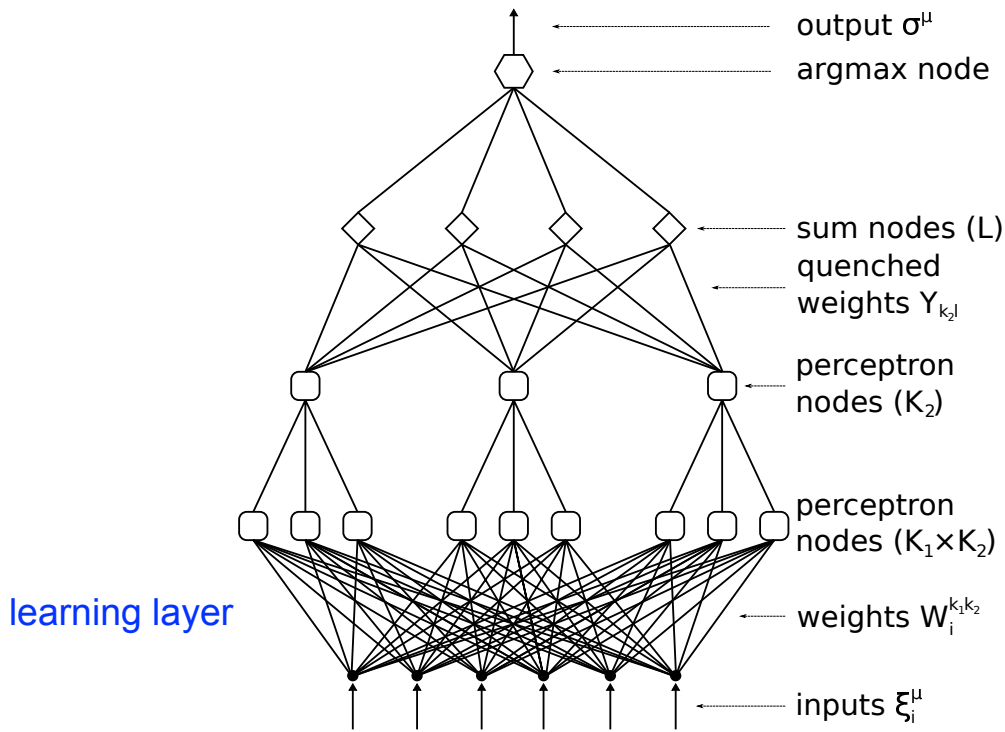
Optimal Bayesian prediction:

$$P(\sigma|\xi^{new}, \{\xi^\mu, \sigma_\mu\}) = \int dW P(\sigma|W, \xi^{new},)P(W, \{\xi^\mu, \sigma_\mu\})$$

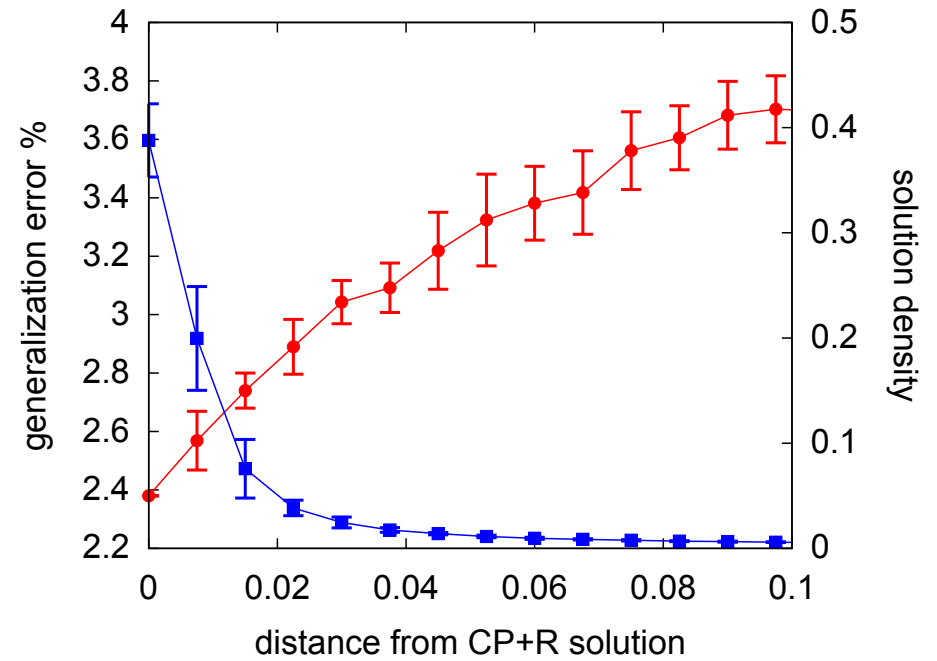
Dense states have the propensity to generalise



- contribution to the Bayesian integral from the dense cluster
- the Teacher is an isolated weight vector

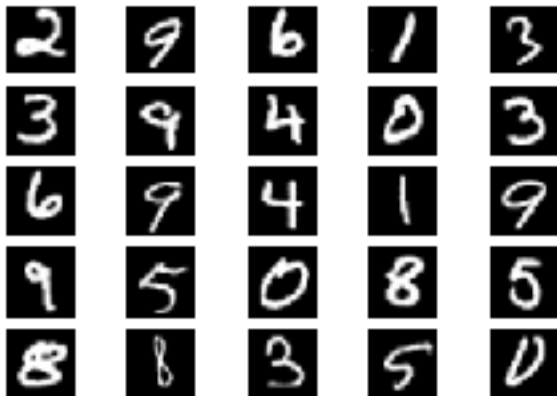


Smallest architecture with zero errors on the training set



(70000 patterns)

Random sampling of MNIST



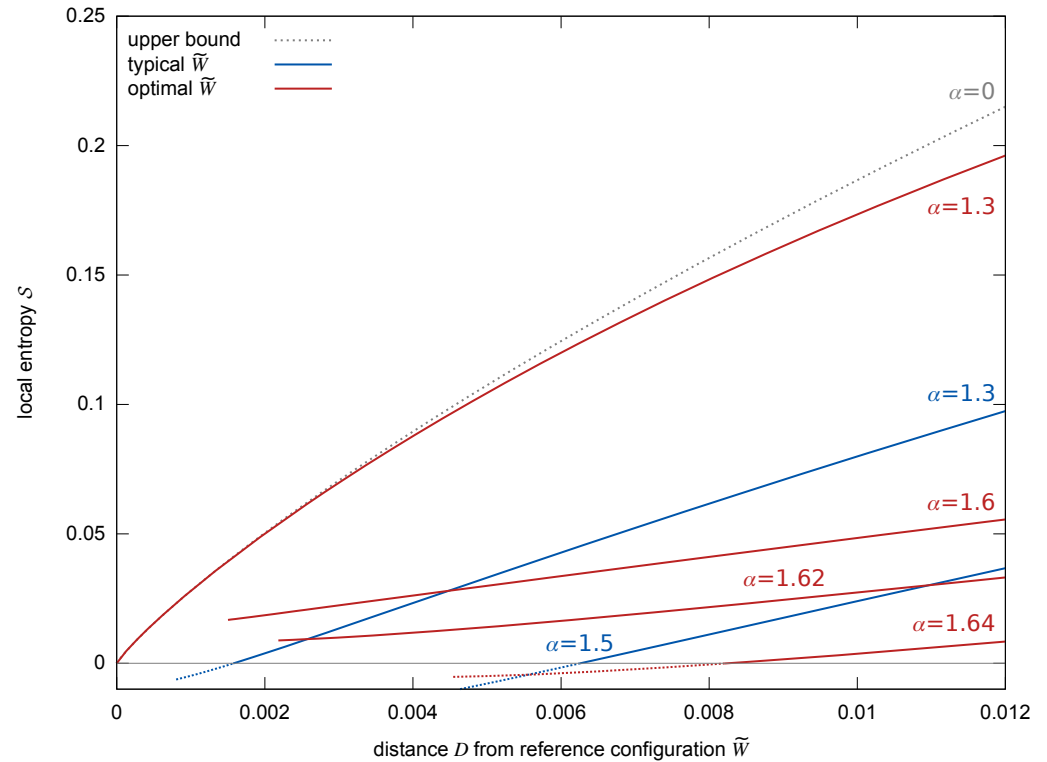
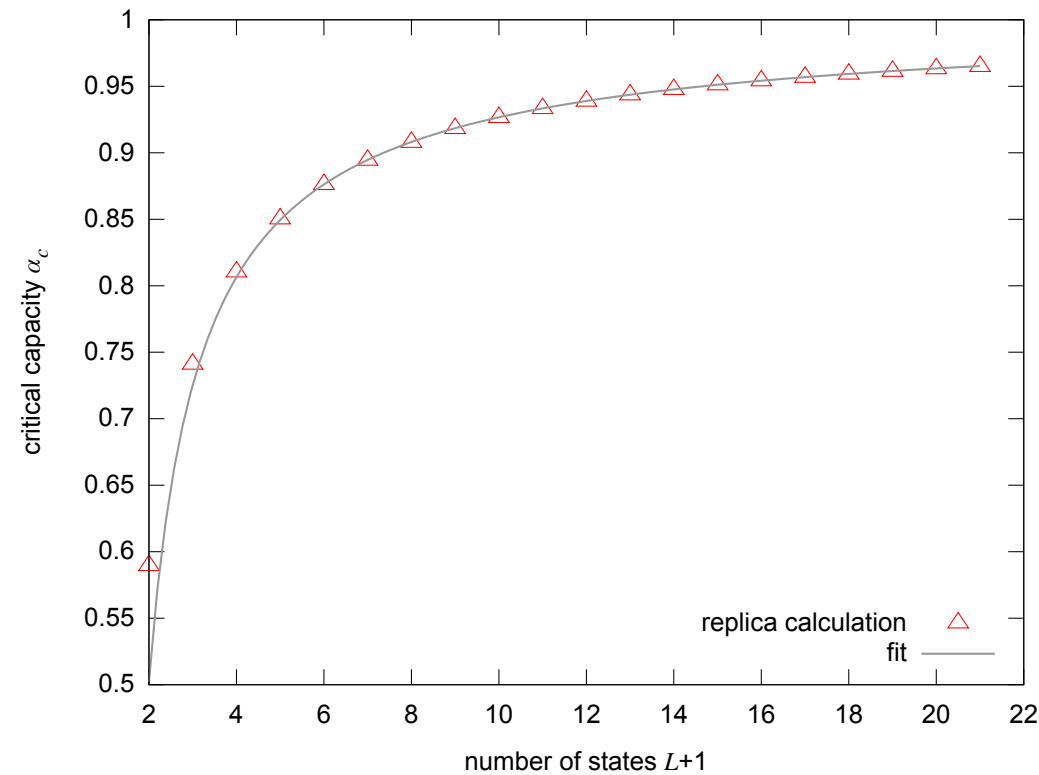
Prediction error ~ 1.2 % with binary weights

no overfitting with size

Generalisation to multiple state variables

Few levels almost saturate performance

$L+1=5$



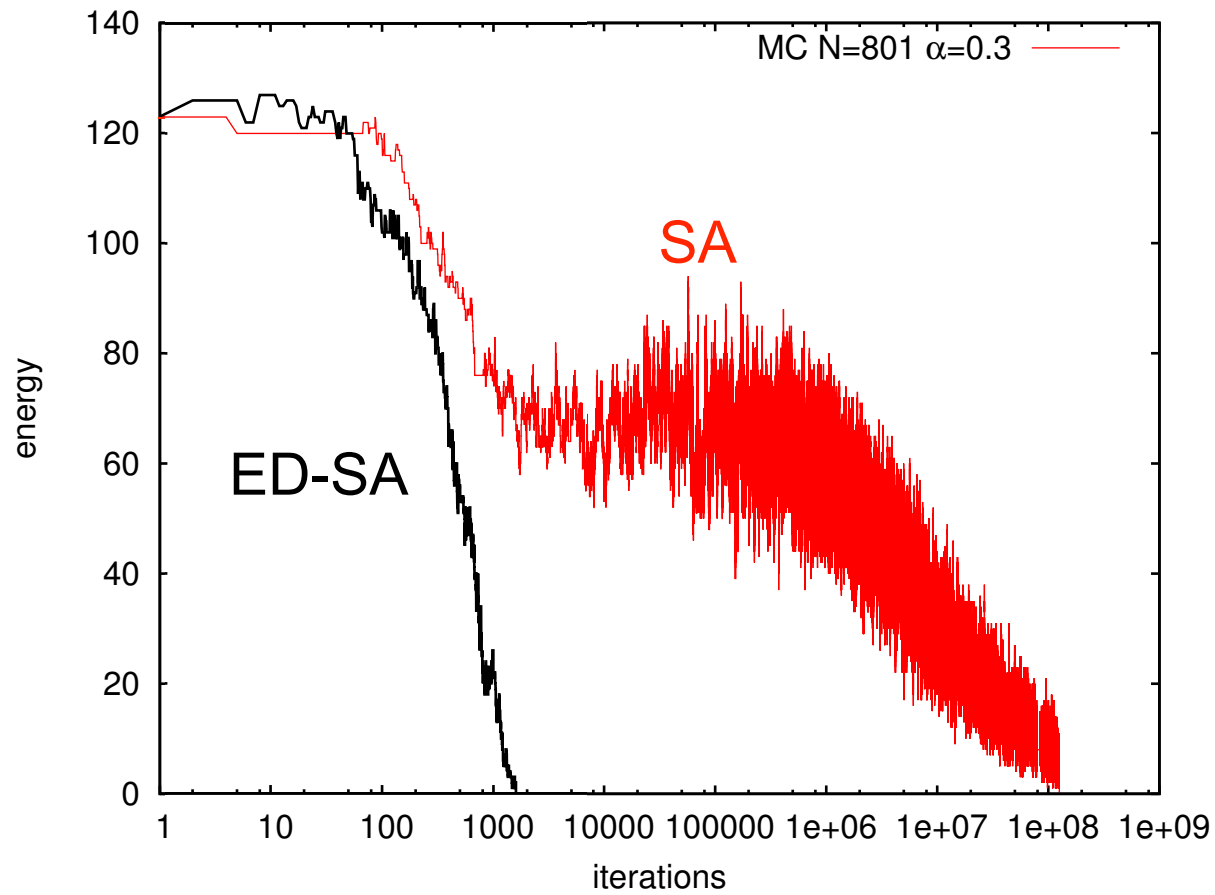
Principled algorithm: Local Entropy driven Simulated Annealing

Objective Function:

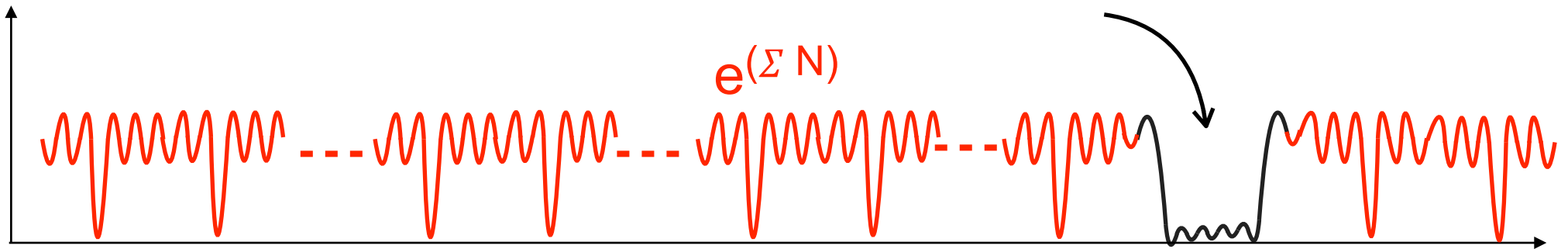
search for configurations which maximize the local entropy
(minimize the “energy”)

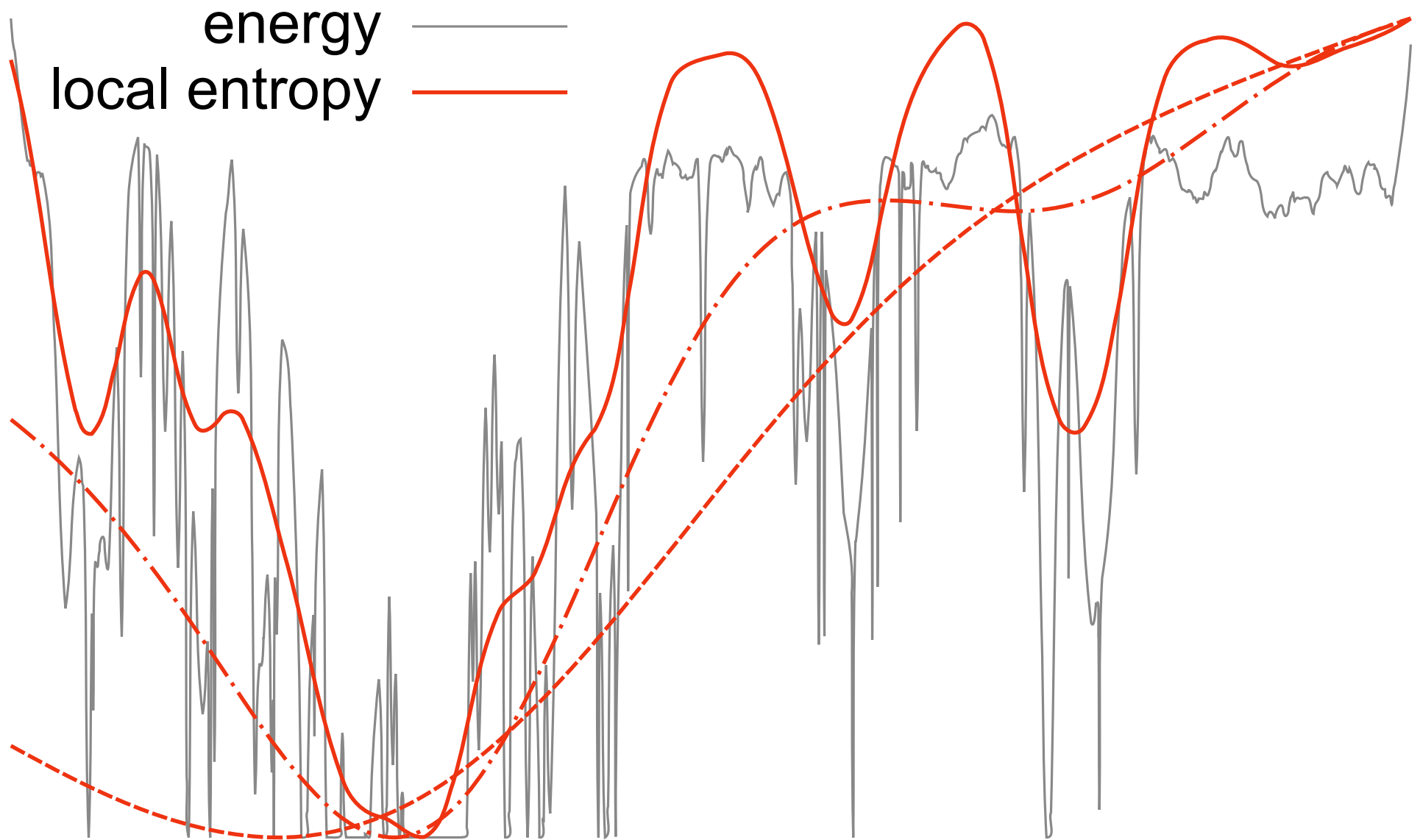
$$\mathcal{E} \left(\tilde{W} \right) = - \log \mathcal{N} \left(\tilde{W}, d \right)$$

1. SA moves
2. Belief Propagation method to estimate the local entropy



$N = 801, \alpha = 0.3$



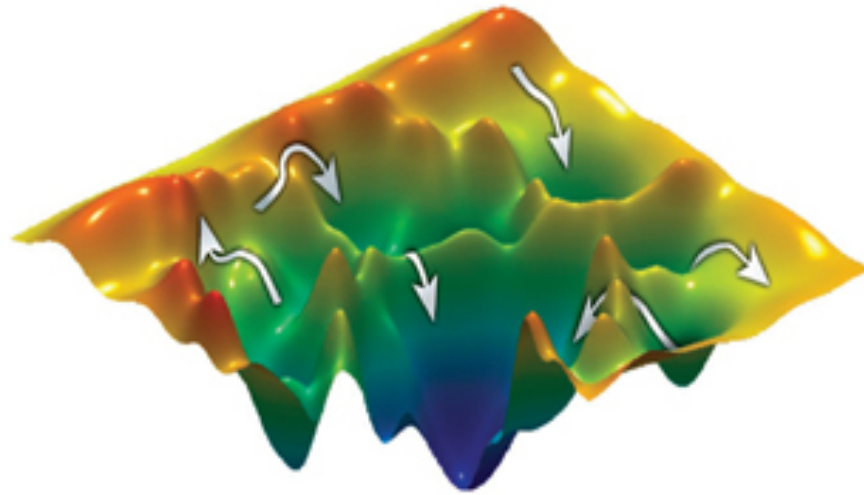


Local should not be interpreted as *infinitesimal*: the local entropy is the log of the number of optimal configuration within a hyper-sphere of radius $O(N)$ or fractional volume $O(1)$.

What we have learned from non-convex 1-2 layer NN learning random patterns?

- ✓ The loss function presents an exponential proliferation of metastable states which trap SA or full batch Langevin dynamics
- ✓ HOWEVER, there exist rare dense regions (small but still of extensive size) which are accessible to simple non-detailed-balance stochastic algorithms. These regions have good generalisation capabilities.
- ✓ Accessibility and generalization are not in conflict
- ✓ The Local Entropy Measure amplifies the weight of these regions (from exponentially small to dominant!)
- ✓ shape of dense regions depends on the data, difficult to study analytically even for random patterns

back to question:



Successful algorithms never “simply” minimize the loss.

Why?

Because the stationary measure of the stochastic learning process should not be the equilibrium Gibbs measure of the loss function. Many (simple!) out-of-equilibrium processes are attracted by the rare dense states (wide minima).

From Local entropy measure to the Robust Ensemble

$$\mathcal{P}(\tilde{W}) \propto e^{-y\mathcal{E}_d(\tilde{W})} \quad \mathcal{E}_d(\tilde{W}) \doteq -\log \mathcal{N}(\tilde{W}, d)$$

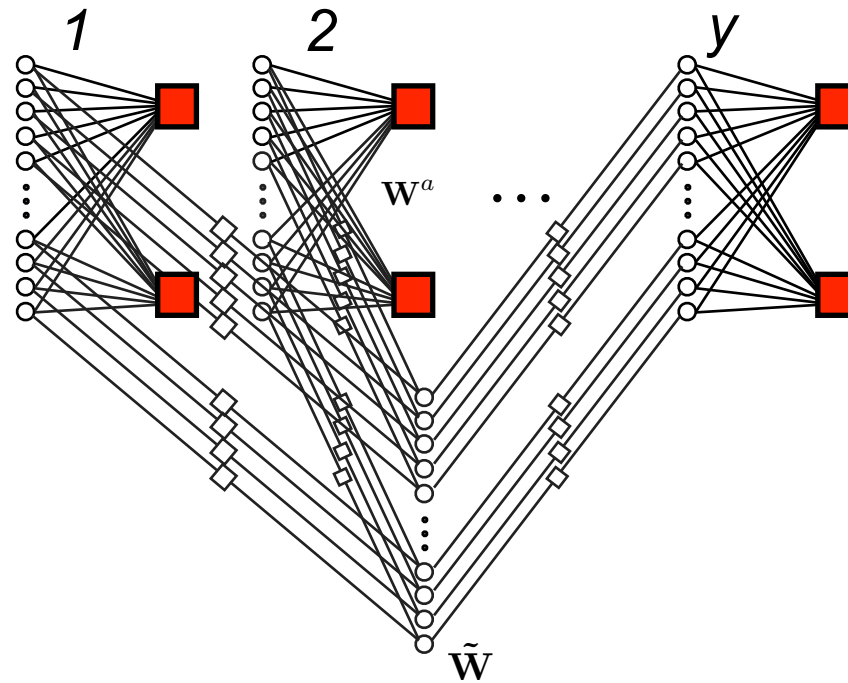
We may write
$$\mathcal{P}(\tilde{W}) \propto \lim_{\beta \rightarrow \infty} \left(\sum_{\{W\}} (e^{-\beta E(W) + \gamma W \cdot \tilde{W}})^y$$

where γ is a Lagrange multiplier controlling the distance

y integer \Rightarrow multiple real replicas

$$\begin{aligned} \mathcal{P}(\tilde{W}) &\propto \lim_{\beta \rightarrow \infty} \left(\sum_{\{W\}} e^{-\beta E(W) + \gamma W \cdot \tilde{W}} \right)^y = \lim_{\beta \rightarrow \infty} \prod_{a=1}^y \sum_{\{W^a\}} e^{-\beta E(W^a) + \gamma W^a \cdot \tilde{W}} = \\ &= \lim_{\beta \rightarrow \infty} \sum_{\{W^1, W^2, \dots, W^y\}} e^{-\beta \sum_{a=1}^y E(W^a) + \gamma \sum_{a=1}^y W^a \cdot \tilde{W}} \\ &= \lim_{\beta \rightarrow \infty} \sum_{\{W^1, W^2, \dots, W^y\}} e^{-\beta \sum_{a=1}^y E(W^a) + \gamma \sum_{a=1}^y \sum_{j=1}^N W_j^a \tilde{W}_j} \end{aligned}$$

Robust Ensemble



$$\mathcal{P}_{RE}(\tilde{W}, \{W^a\}) \propto e^{-\beta \sum_{a=1}^y E(W^a) + \gamma \sum_{a=1}^y \sum_{j=1}^N W_j^a \tilde{W}_j}$$

Marginalizing the center

$$\hat{\mathcal{P}}_{RE}(\{W^a\}) \propto e^{-\beta(\sum_{a=1}^y E(W^a) - \frac{1}{\beta} \sum_j \log(2 \cosh(\gamma \sum_{a=1}^y W_j^a)))}$$

Expectations of observables: $E[f(\tilde{W})] = \sum_{\tilde{W}} \sum_{\{W^a\}} f(\tilde{W}) \mathcal{P}_{RE}(\tilde{W}, \{W^a\})$

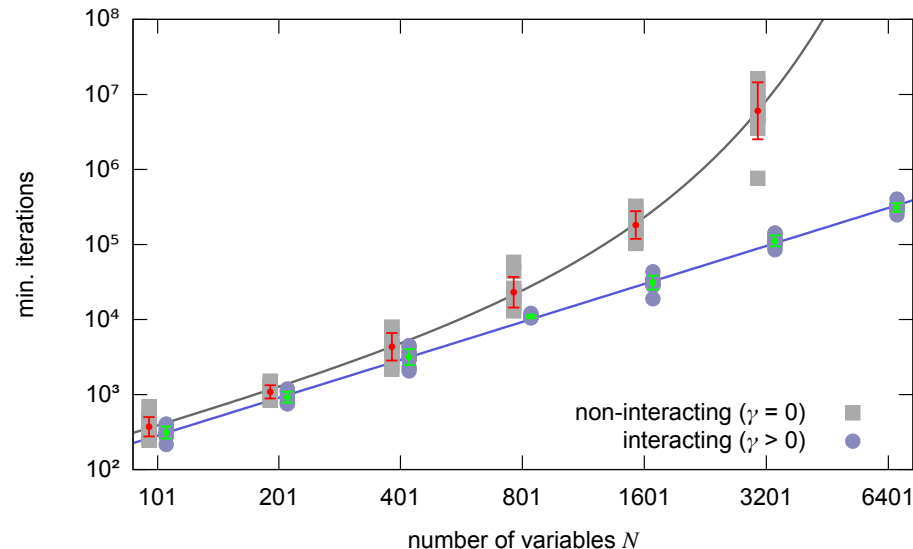
Replicated MC

$$E(\mathbf{W}) = \sum_{a=1}^y E(W^a) - \frac{1}{\beta} \sum_j \log(2 \cosh(\gamma \sum_{a=1}^y W_j^a))$$

- 1) $\Delta E = E(\mathbf{W}') - E(\mathbf{W})$ can be computed efficiently when \mathbf{W}' and \mathbf{W} differ in one weight
- 2) efficient MC sampling for rejection rate reduction (non trivial)
- 3) most probable of the centroid value: $\tilde{W}_j = \text{sign} \sum_{a=1}^y W_j^a$ (typically $E(\tilde{W}) \leq \langle E(W^a) \rangle_a$)

$\alpha = 0.3$

$y = 3$



Notice: landscape of local minima could be different from the MC using BP

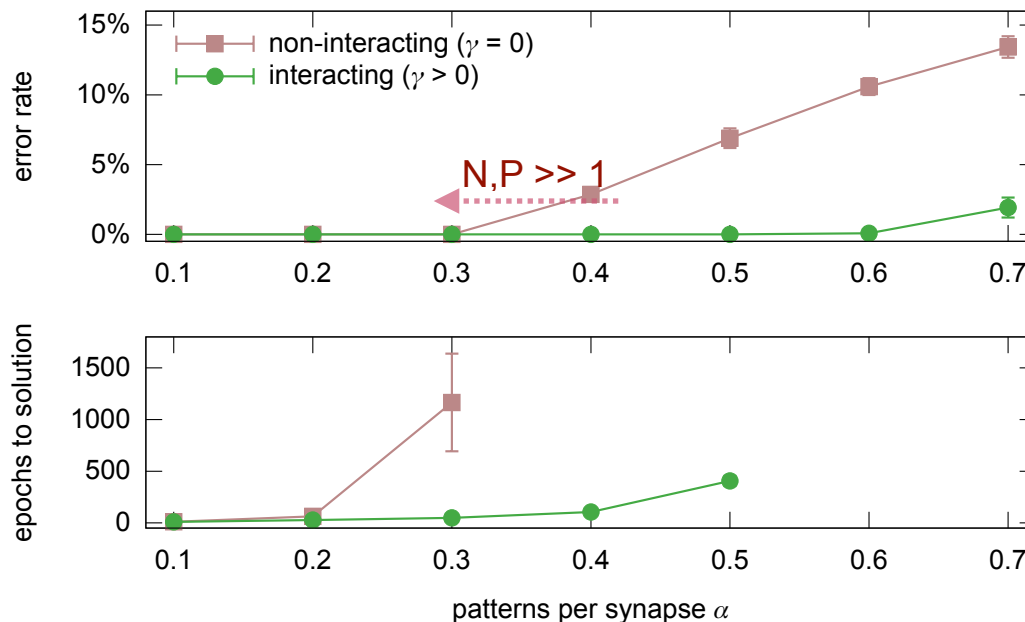
Replicated Stochastic Gradient Descent

$$H(\{W^a\}) = \sum_{a=1}^y E(W^a) + \frac{1}{\beta} \sum_{j=1}^N \log \left(e^{-\frac{\gamma}{2} \sum_{a=1}^y (W_j^a - 1)^2} + e^{-\frac{\gamma}{2} \sum_{a=1}^y (W_j^a + 1)^2} \right)$$

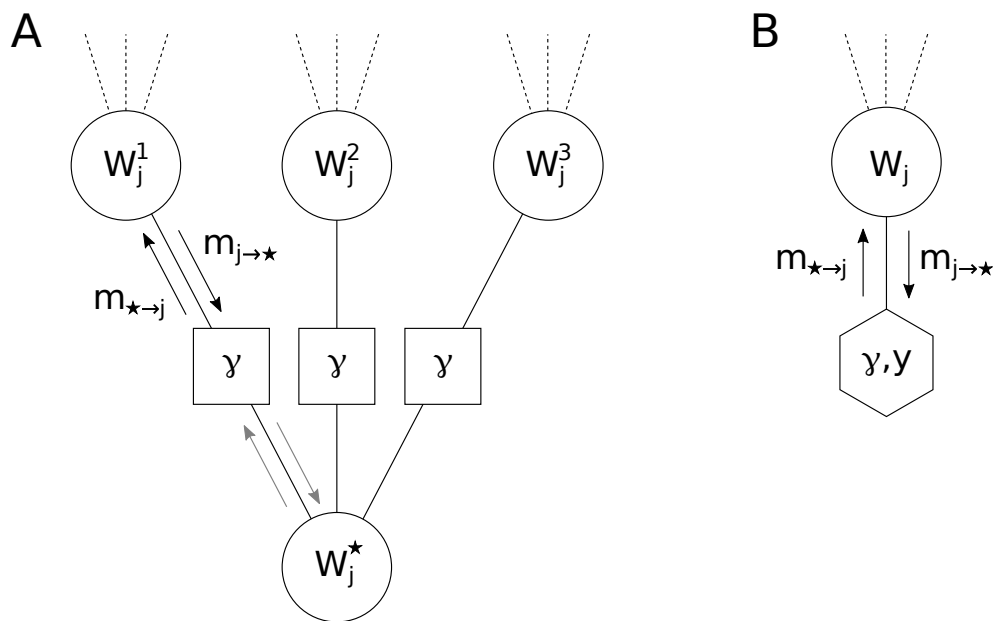
$$\frac{\partial H}{\partial W_i^a}(\{W^b\}) = \frac{\partial E}{\partial W_i}(W) \Big|_{W=W^a} + \frac{\gamma}{\beta} \left(\tanh \left(\gamma \sum_{b=1}^y W_i^b \right) - W_i^a \right)$$

$$(\mathcal{W}_i^a)^{t+1} = (\mathcal{W}_i^a)^t - \eta \frac{1}{|m(t)|} \sum_{\mu \in m(t)} \frac{\partial E^\mu}{\partial W_i}(W) \Big|_{W=(W^a)^t} + \eta' \left(\tanh \left(\gamma \sum_{b=1}^y (\mathcal{W}_i^b)^t \right) - (\mathcal{W}_i^a)^t \right) \quad \eta' = \frac{\gamma}{\beta \eta}$$

N = 1605 weights K = 5



Replicated Belief Propagation: focusing BP (fBP) ~ BP with reinforcement



$$\{W_j^a\}_{a=1}^y$$

$$P_j(\{W_j^a\}_{a=1}^y) = P_j(\sum_{a=1}^y W_j^a)$$

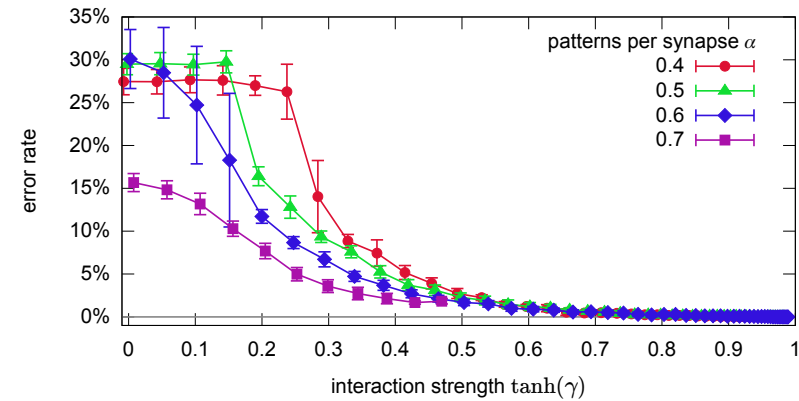
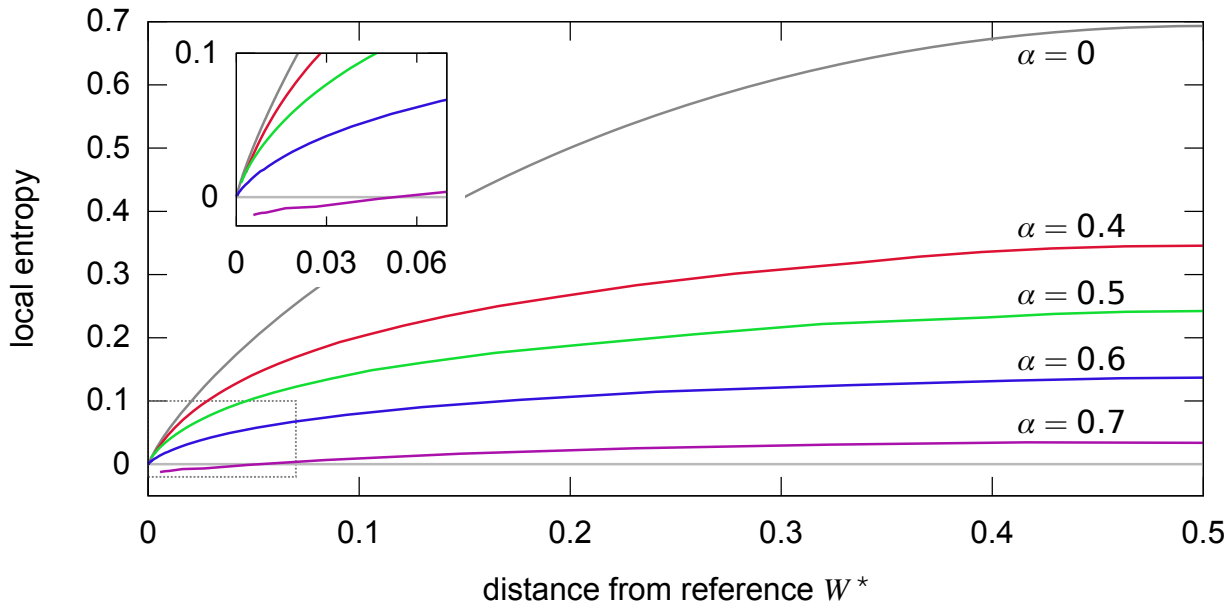
assume that each replica of the system behaves in exactly the same way, and therefore that the same messages are exchanged along the edges of the graph regardless of the replica index. ...single system, which is identical to the original one except that each variable now also exchanges messages with $y - 1$ identical copies of itself through an auxiliary variable (which we can just trace away at this point).

extra message at time t:

$$m_{\star \rightarrow j}^{t+1} = \tanh \left((y - 1) \tanh^{-1} \left(m_{j \rightarrow \star}^t \tanh \gamma \right) \right) \tanh \gamma \quad \text{focusing BP}$$

fBP becomes a solver looking for high density regions of solution. Interesting convergence properties (to be further studied).

Replicated BP is also an analytical tool: phase diagram on NN with one hidden layer



committee machine with $N = 1605$, $K = 5$, $y = 7$, increasing γ from 0 to 2.5, averages on 10 samples. Top: local entropy versus distance to the reference W^* for various α (error bars not shown for clarity). The topmost grey curve ($\alpha = 0$) is an upper bound, representing the case where all configurations within some distance are solutions.

Unreasonable effectiveness of learning neural networks: From accessible states and robust ensembles to basic algorithmic schemes, C. Baldassi, C. Borgs, J.T. Chayes, A. Ingrosso, C. Lucibello, L. Saglietti and Riccardo Zecchina, PNAS 113, E7655-E7662 (2016)

The case of Deep Networks

Modified sampling measure: $P(x') \propto e^{y\Phi(x')}$

Local free entropy:

$$\Phi(x') = \log \int_x e^{-\beta f(x)} e^{-\lambda \|x - x'\|^2} dx$$

where: x are the continuous weights, and $f(x)$ is the loss/energy function

Langevin dynamics:

Algorithm 1: Entropy-SGD algorithm

Input : current weights x , Langevin iterations L
Hyper-parameters: scope γ , learning rate η , SGLD step size η'

// SGLD iterations;

```
1  $x', \mu \leftarrow x$ ;  
2 for  $\ell \leq L$  do  
3    $\Xi^\ell \leftarrow$  sample mini-batch;  
4    $dx' \leftarrow \frac{1}{m} \sum_{i=1}^m \nabla_{x'} f(x'; \xi_{\ell_i}) - \gamma (x - x')$ ;  
5    $x' \leftarrow x' - \eta' dx' + \sqrt{\eta'} \varepsilon \mathcal{N}(0, I)$ ;  
6    $\mu \leftarrow (1 - \alpha)\mu + \alpha x'$ ;
```

// Update weights;

```
7  $x \leftarrow x - \eta \gamma (x - \mu)$ 
```

ENTROPY-SGD: BIASING GRADIENT DESCENT INTO WIDE VALLEYS

Pratik Chaudhari, A. Choromanska, S. Soatto, Y. LeCun, C. Baldassi, C. Borgs, J. Chayes, L. Sagun, R. Zecchina, ICLR 2017

Local Entropy & Robust Ensemble



Elastic Averaging SGD with momentum

$\beta \rightarrow \infty$ sampling from

$$\mathcal{P}_{RE}(\tilde{x}) \propto \int dx^1 \dots dx^y e^{-\beta \phi(\tilde{x}, \{x^a\})}$$

$$\phi(\tilde{x}, \{x^a\}) = \sum_{a=1}^y E(x^a) + \frac{\lambda}{\beta} \sum_{a=1}^y \|x^a - \tilde{x}\|^2$$

$$\min_{x^1, \dots, x^p, \tilde{x}} \sum_{i=1}^p \left(\mathbb{E}[f(x^i, \xi^i)] + \frac{\rho}{2} \|x^i - \tilde{x}\|^2 \right)$$

Work in progress with [L. Bottou](#), L. Sagun, J. Chayes, C. Borgs, C. Baldassi, ...

Deep learning with Elastic Averaging SGD

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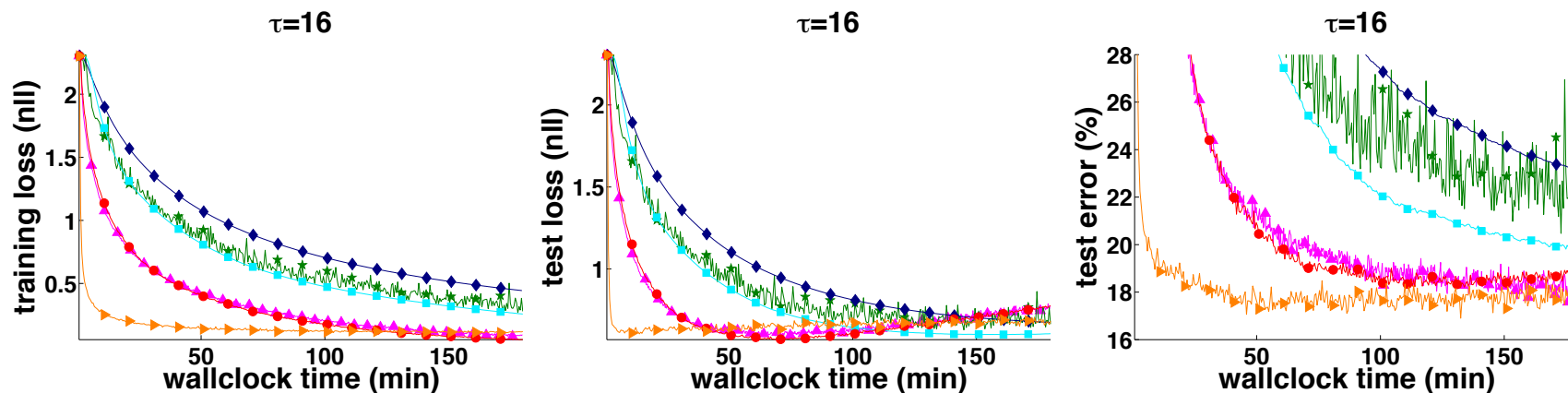
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Loss function:

$$\min_{x^1, \dots, x^p, \tilde{x}} \sum_{i=1}^p \mathbb{E}[f(x^i, \xi^i)] + \frac{\rho}{2} \|x^i - \tilde{x}\|^2,$$

with Momentum SGD.



CIFAR dataset with the 7-layer convolutional neural network.

The idea of Flat Minima is not new:

Hochreiter, Sepp and Schmidhuber, Jürgen. Flat minima. *Neural Computation*, 9(1):1–42, 1997

and many others ...

ON LARGE-BATCH TRAINING FOR DEEP LEARNING: GENERALIZATION GAP AND SHARP MINIMA

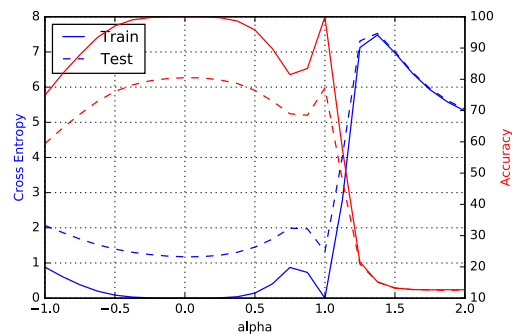
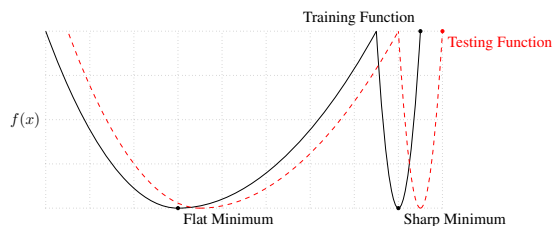
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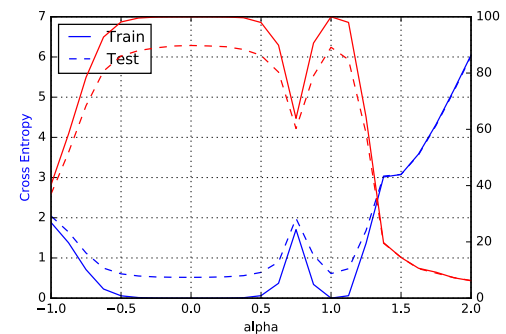
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(c) C_1



(d) C_2

C_1	(Shallow) Convolutional	Section B.3	CIFAR-10 (Krizhevsky & Hinton, 2009)
C_2	(Deep) Convolutional	Section B.4	CIFAR-10

Binarized Neural Networks: Training Neural Networks with Weights and Activations Constrained to +1 or -1

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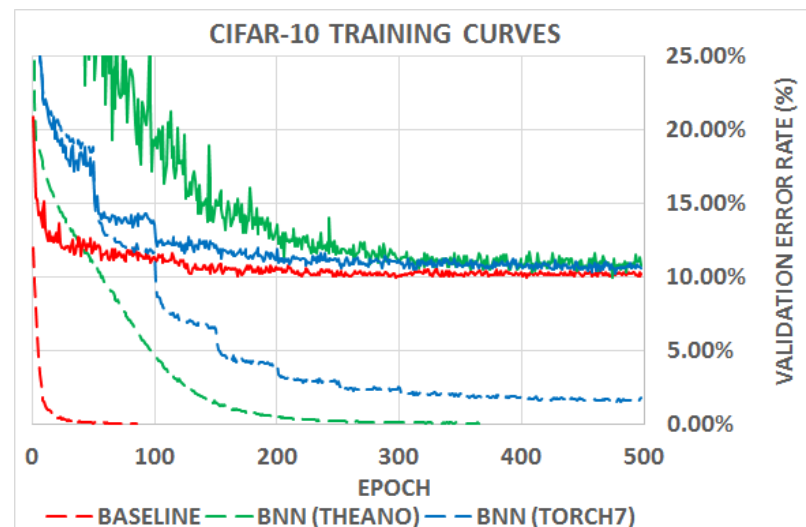
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*Indicates equal contribution. Ordering determined by coin flip.



“Although BNNs are slower to train, they are nearly as accurate as 32-bit float DNNs.”

Conclusion and what next

Theoretical framework:

out-of-equilibrium statistical physics and large deviations studies are a key framework for understanding learning phenomena

Next algorithmic developments:

- Accessible dense states in DNN, connections with regularization techniques (dropout), temporal version of local entropy
- An opportunity for acceleration?
- Simple forms of stochastic learning process
- Learning with low precision weights: can we design new neural hardware?
- Generalization to unsupervised learning
- ...