Pseudo-likelihood produces associative memories able to generalize, even for asymmetric couplings

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What is pseudo-likelihood? *Generative framework*

- Energy-based generative models:

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- P random training data $\xi^\mu \in \{\pm 1\}^N$ i.i.d. are the *memories*

- $\alpha = \frac{P}{N}$ is the control parameter

Hopfield associative memory

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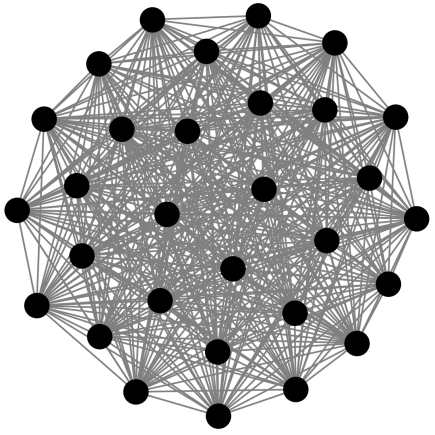
Input

$\Rightarrow$



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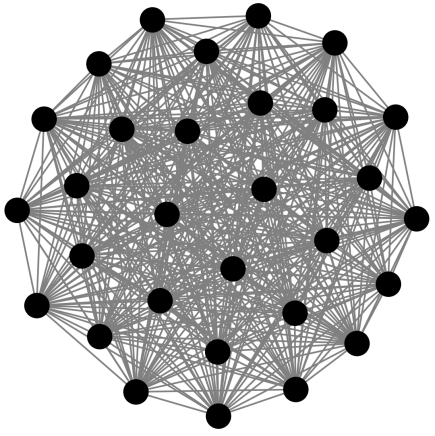

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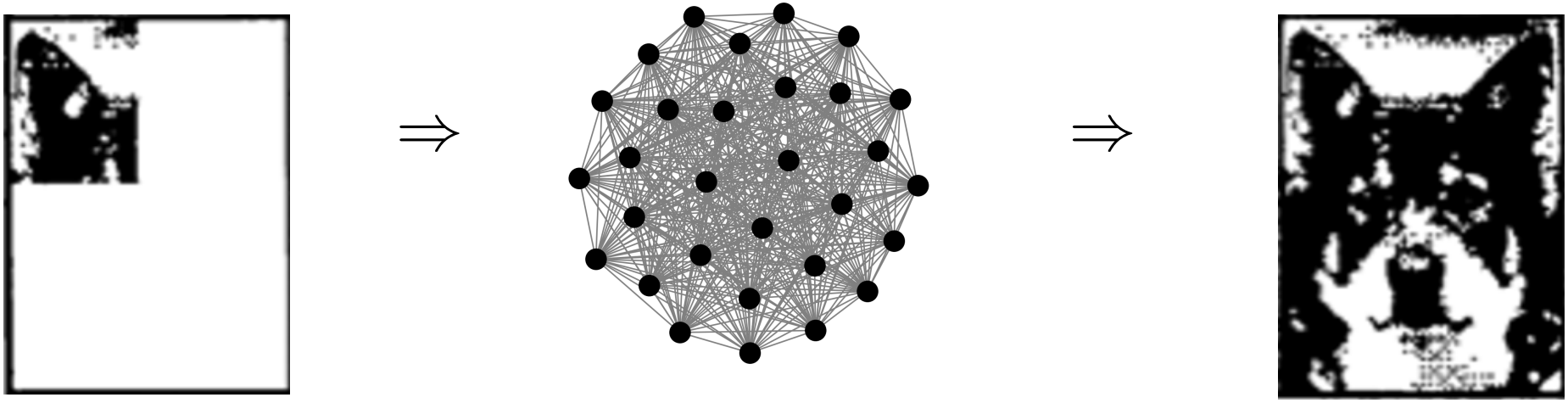
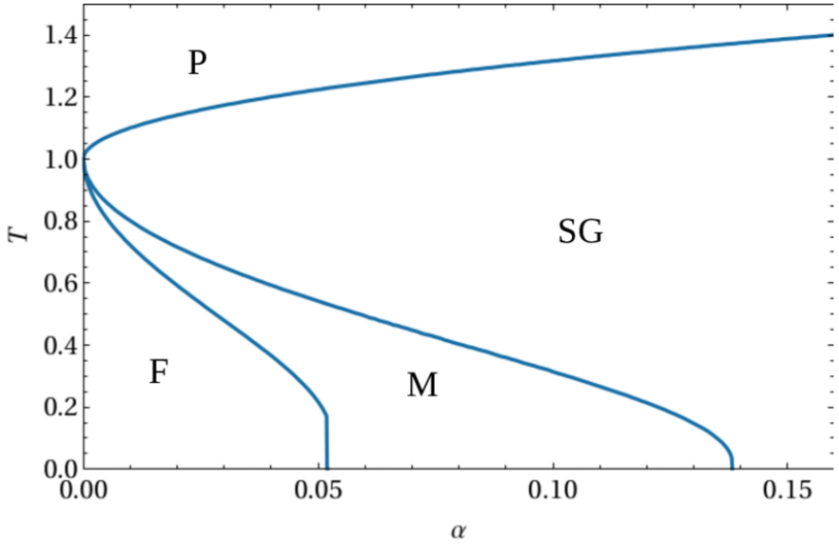


Phase diagram of retrieval

Amit et al. (1987)
Statistical Mechanics of Neural Networks Near Saturation



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$$\Delta_i^{\mu} := \xi_i^{\mu}\sum_{j(\neq i)}J_{ij}\xi_j^{\mu}$$

If $\Delta_i^{\mu} > 0 \quad \forall i \quad \Rightarrow \quad \xi^{\mu}$ is a fixed point of dynamics

Technical contribution (1) - fixed $||J||$

- Equivalent to N independent perceptrons, each one with loss

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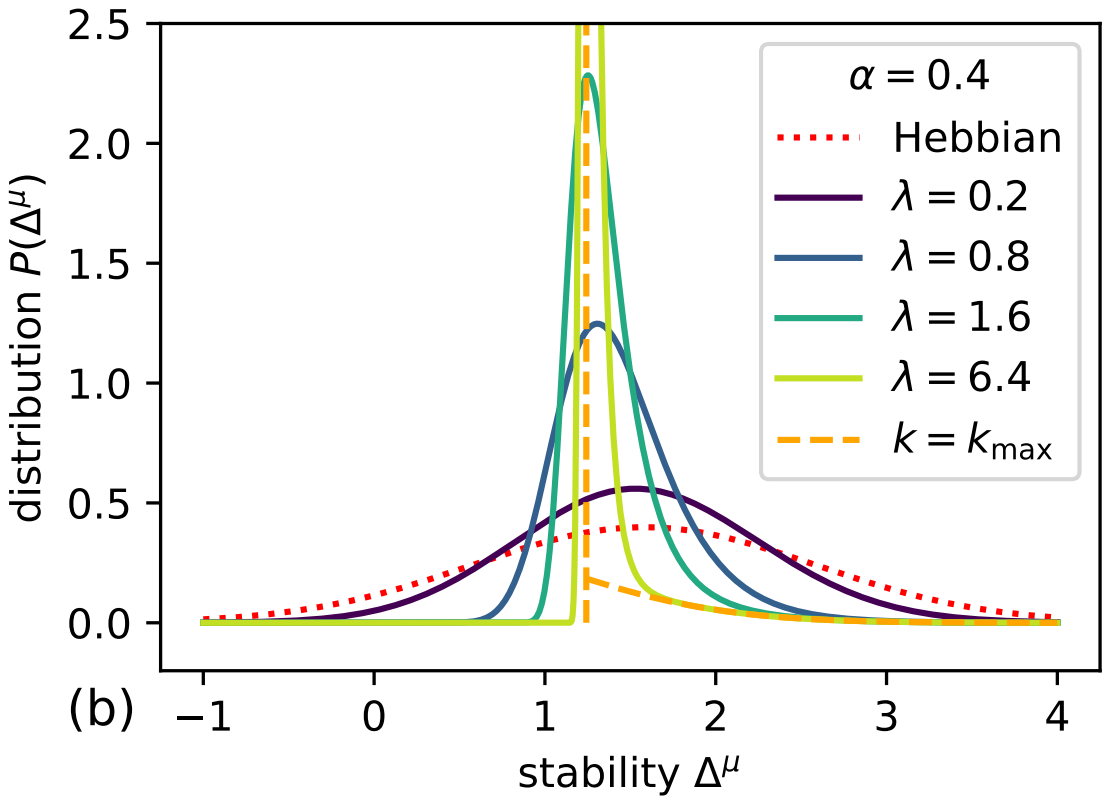

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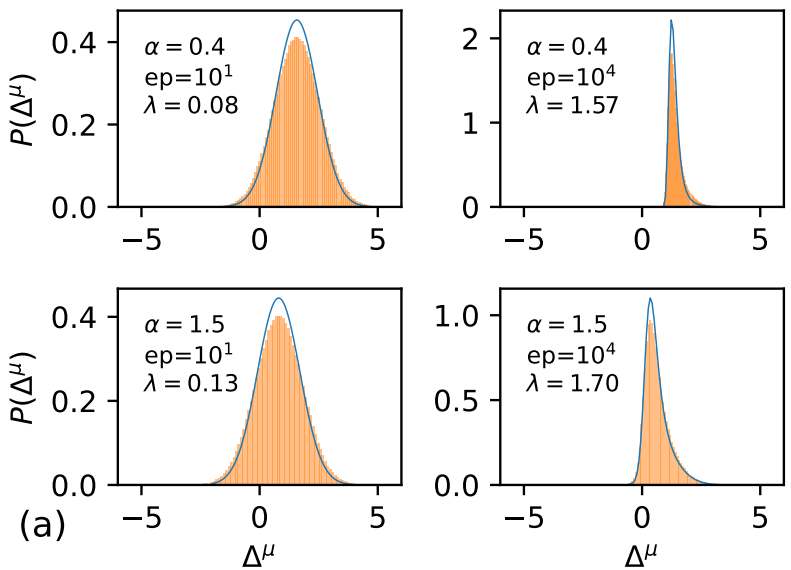

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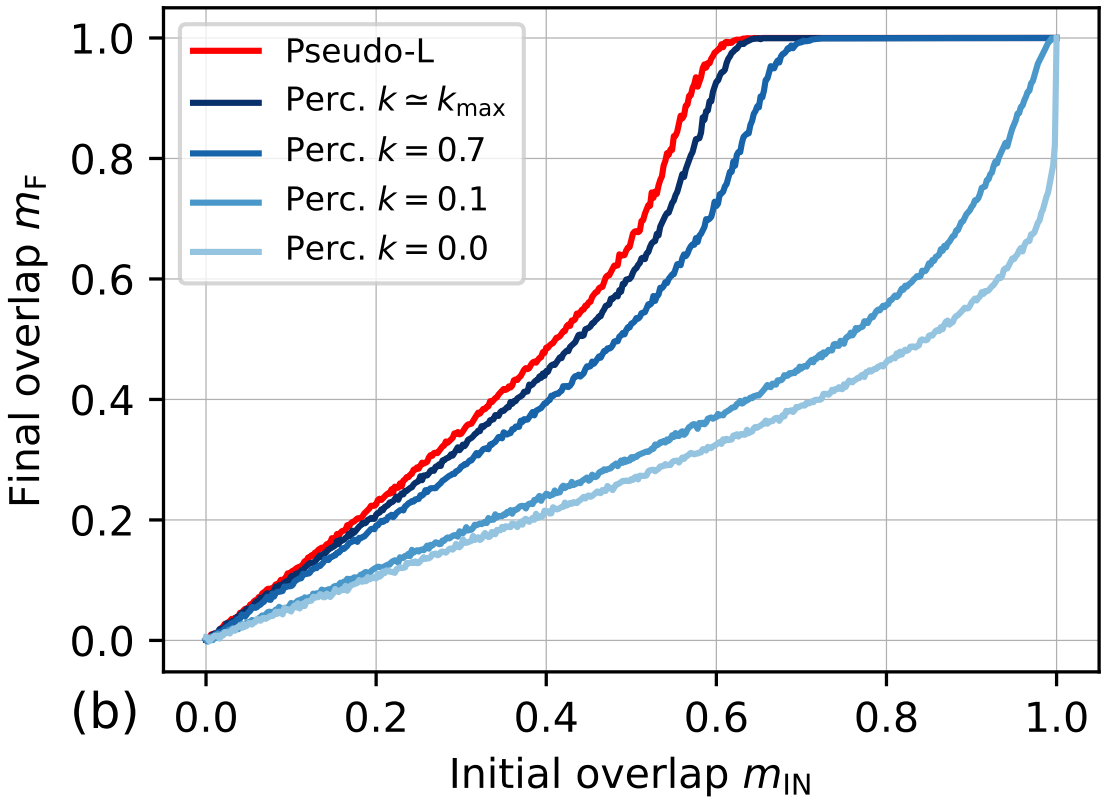
(1) *Random data*

Pseudo-likelihood produces optimal basins of attraction



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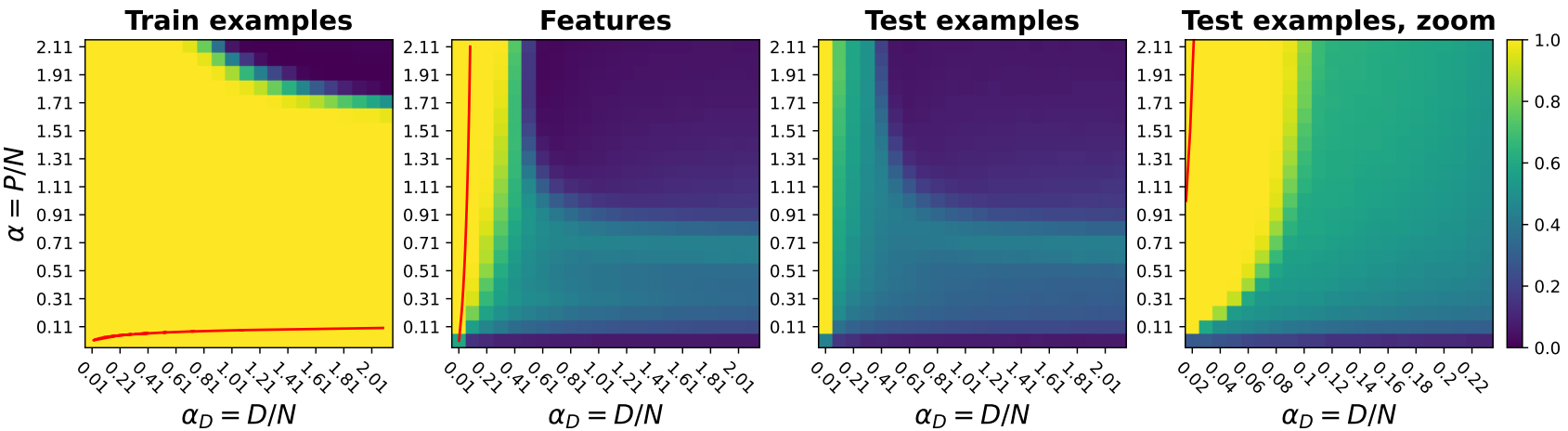
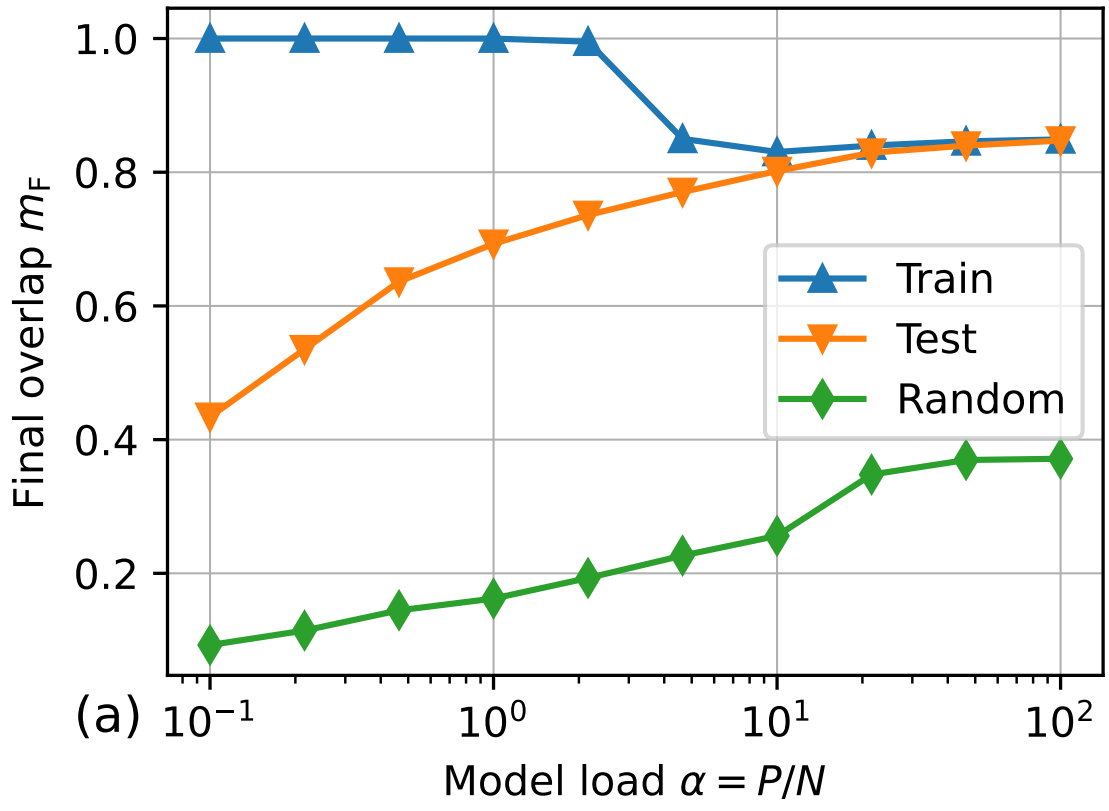
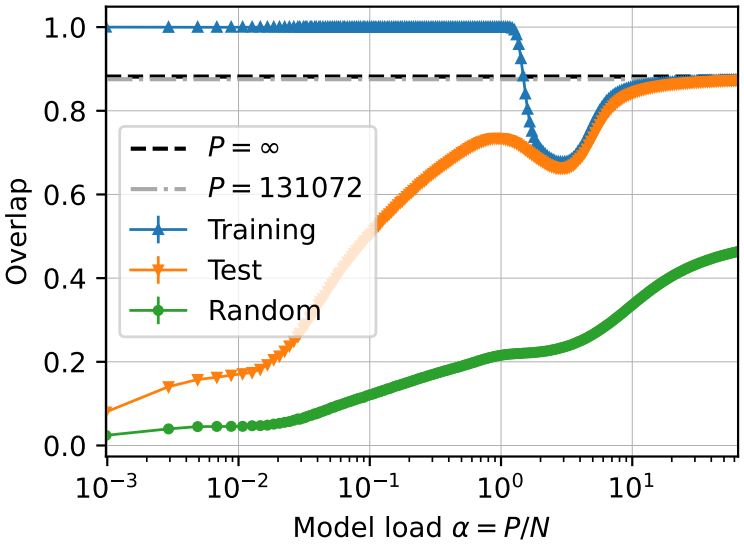


(3) binary MNIST

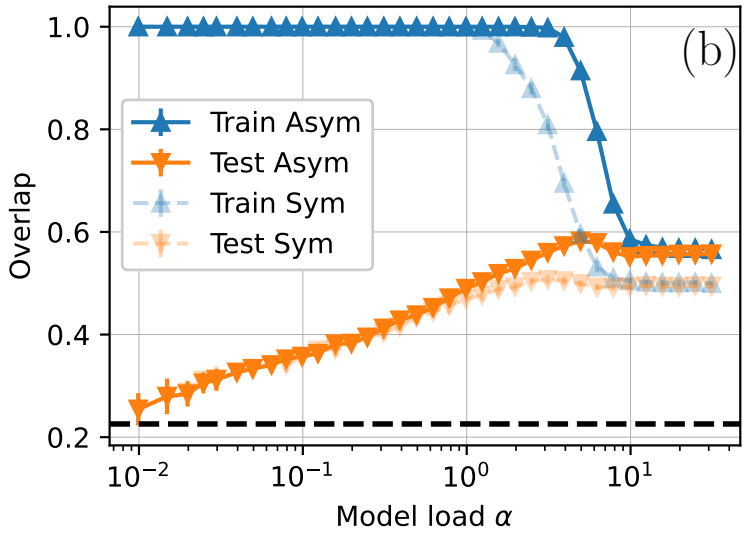
Memorization-to-generalization transition at increasing dataset size α



(3) other datasets



(a) Edwards-Anderson in two dimensions



(b) Potts model of protein family Beta Lactamase

Conclusions

- Local + max entropy learning rule:

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- Structured data:

  Memorization-to-generalization transition

Thank you for your attention!

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Formulae

Pseudo-likelihood cost:

$$p - \mathscr{L} = -\sum_{\mu}\sum_{i}\left[\lambda \mathscr{H}(\xi_i^{\mu}|\{\xi_j^{\mu}\}_{j\neq i}) - \log\int dx_i e^{-\lambda \mathscr{H}(\xi_i^{\mu}|\{\xi_j^{\mu}\}_{j\neq i})}\right]$$

Self-Attention is pseudolikelihood optimization

- Layer of simplified Self-Attention: weights tensor $\mathbb{J} \in \mathbb{R}^{N \times N \times d \times d}$

$$\vec{X}_i^{t+1} = \sum_{j(\neq i)} \alpha_{i \leftarrow j} \mathbf{J}_{ij} \vec{X}_j^t \tag{1}$$

$$\alpha_{i \leftarrow j} = \text{softmax}_j \left[\lambda \vec{X}_i^t \cdot \mathbf{J}_{ij} \vec{X}_j^t \right] \tag{2}$$

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- Eq. 1: minimization dynamics of cost

$$F(\{\vec{X}_i\}; J) = -\frac{1}{\lambda} \sum_i \log \Big[\sum_{j(\neq i)} \exp\big(\lambda \vec{X}_i \cdot \mathbf{J}_{ij} \vec{X}_j\big) \Big] = \sum_i e_i(\{\vec{X}_i\}; \mathbb{J}) \tag{3}$$

$$\vec{X}_i^{t+1} = -\nabla_{\vec{X}} F(\{\vec{X}_i\}; J) \tag{4}$$

Vector-spin associative memories

Vector spins: towards Self-Attention

Statistical mechanics of vector Hopfield network near and above saturation

Flavio Nicoletti,[1,2,*] Francesco D'Amico,[2,3,†] and Matteo Negri[2,3,‡]

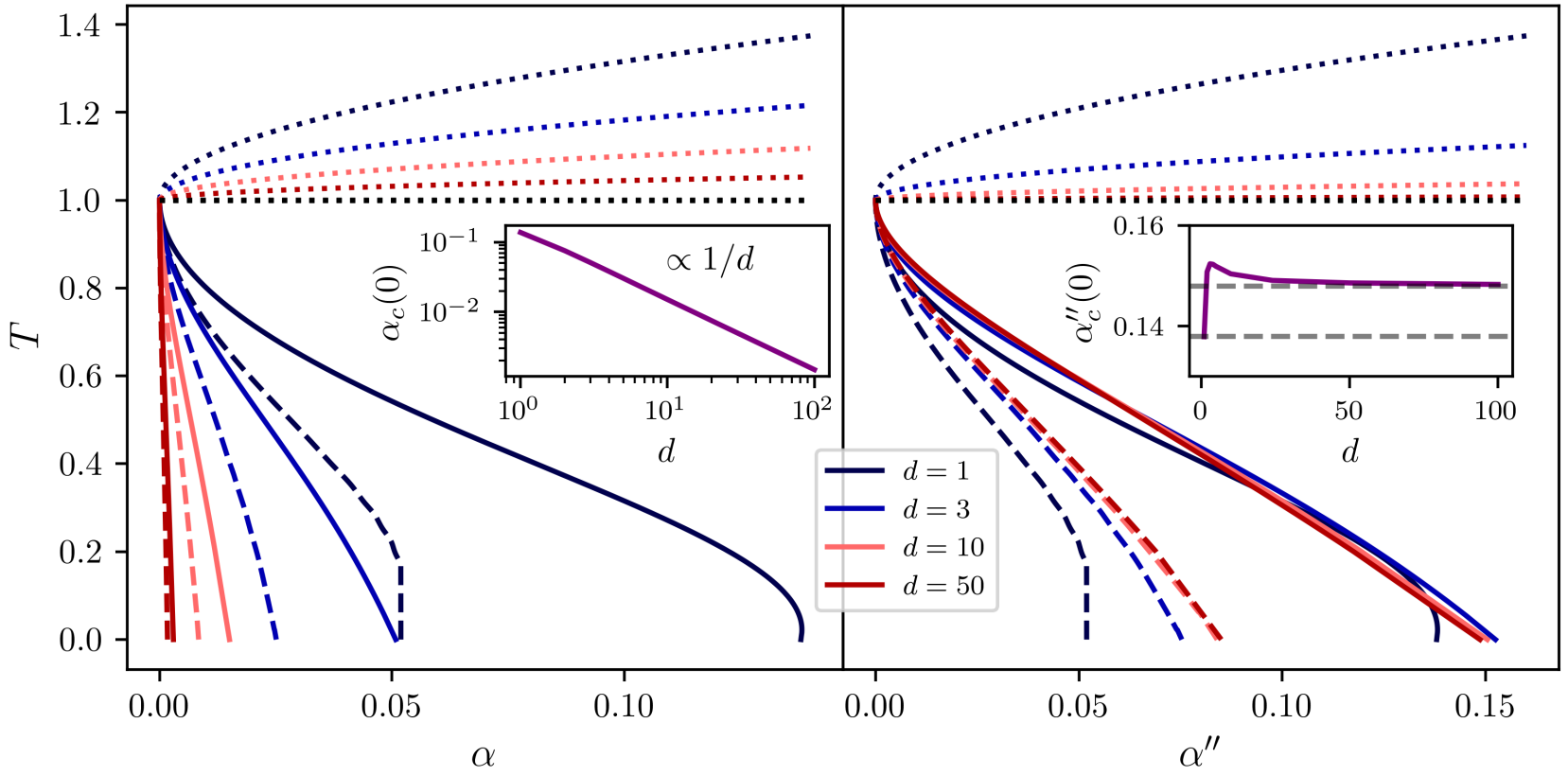
[1] *Department of Computer Science and Engineering Chalmers University of Technology and University of Gothenburg SE-41296 Gothenburg, Sweden*
[2] *Dipartimento di Fisica, Sapienza Università di Roma, 00185 Rome, Italy*
[3] *Institute of Nanotechnology, National Research Council of Italy, CNR-NANOTEC, Rome Unit*

- N spherical vector spins $\{\vec{S}_i\}_{i=1,..,N} \in \mathbb{R}^d$, $\|\vec{S}_i\| = 1$
- P memories $\{\vec{\xi}_i\}^\mu$
- $H = -\frac{1}{2}\sum_{i\neq j}^{1,N} \vec{S}_i \cdot \mathbb{J}_{ij}\vec{S}_j$
- Hebb's couplings $\mathbb{J}_{ij} = \frac{1}{N}\sum_{\mu=1}^{P} \vec{\xi}_i^{\,\mu} \times \vec{\xi}_j^{\,\mu} \Rightarrow \mathbb{J}_{ij} \in \mathbb{R}^{d\times d}$

Vector-spin associative memories

Phase diagram of retrieval at equilibrium

Two order parameters: $\alpha = \frac{P}{N}$, $\alpha'' = \frac{Pd}{N}$



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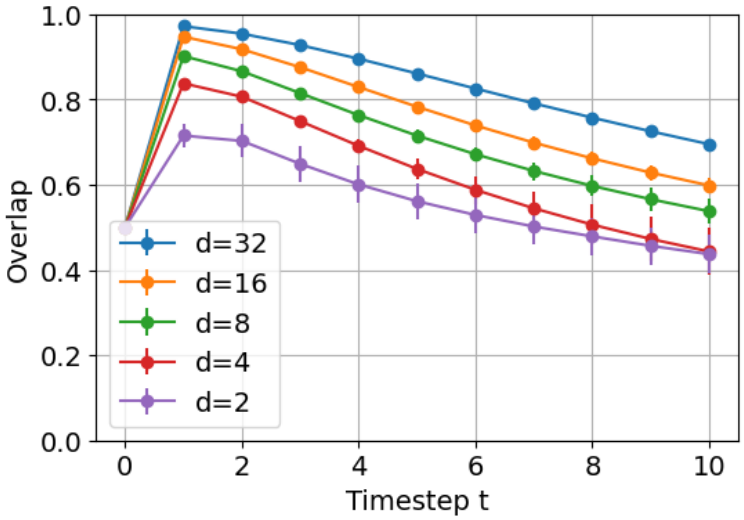
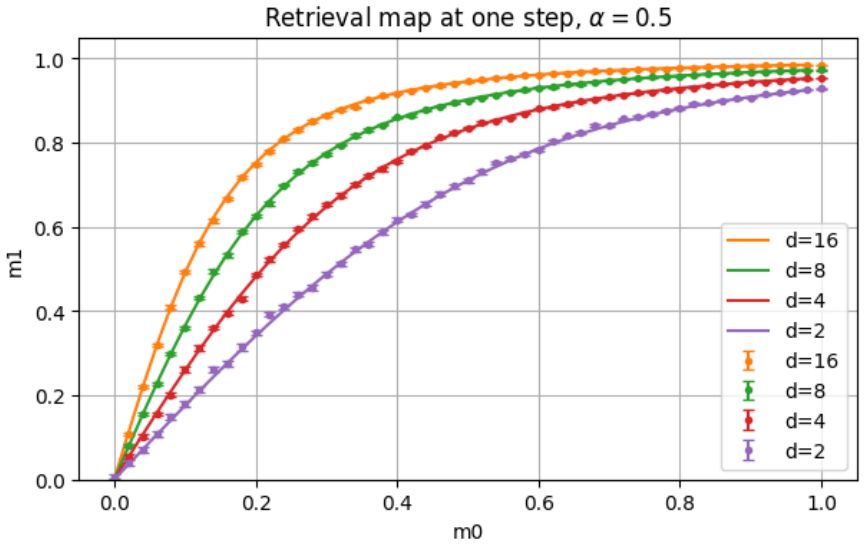
First step denoising





$$\Rightarrow P = \alpha' N d$$