Statistical mechanics of autoregressive models: towards a theory of Self-Attention

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Outline of the talk

1. Introduction
   - Associative memories (Hopfield networks)
   - Self-Attention and LLMs
2. Our results
   - Self-Attention as pseudolikelihood optimization
   - Pseudolikelihood produces associative memories
   - Vector-spin associative memories
3. Last step: work in progress

Introduction

- Associative memories (Hopfield networks)
- Self-Attention and LLMs

Associative memories (Hopfield networks)

- Network of N binary neurons, $\vec{\sigma} \in \{-1,+1\}^N$
- $$H = -\sum_{(i,j)}^{N} J_{ij}\sigma_i\sigma_j \quad , \quad J_{ij} := \frac{1}{N}\sum_{\mu}^{P} \xi_i^{\mu}\xi_j^{\mu} \quad \leftarrow \textbf{Hebb's rule}$$

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- T=0 dynamical rule:

$$\sigma_i(t+\Delta t) = \text{sign}\left[\sum_{j(\neq i)} J_{ij}\sigma_j(t)\right]$$

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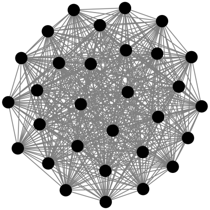

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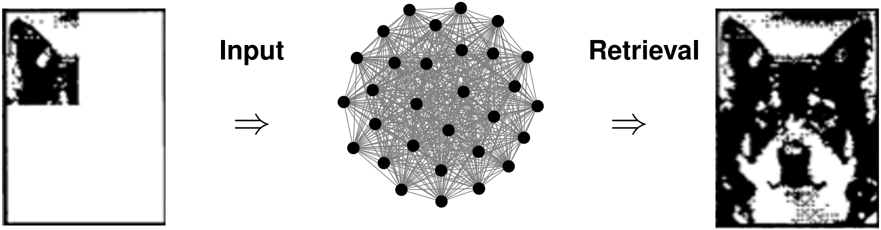

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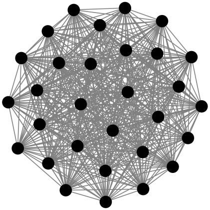
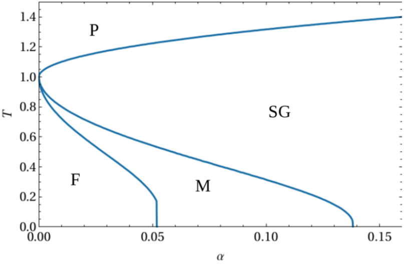


Retrieval

$\Rightarrow$

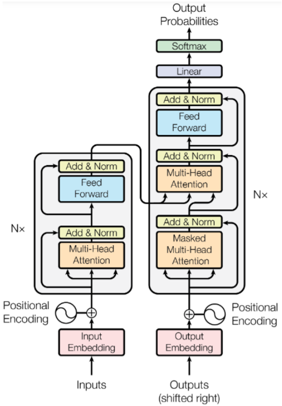
Phase diagram of retrieval

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



Self-Attention and LLMs

- Transformer architecture:
  Vaswani et al. (2017) Attention Is All You Need



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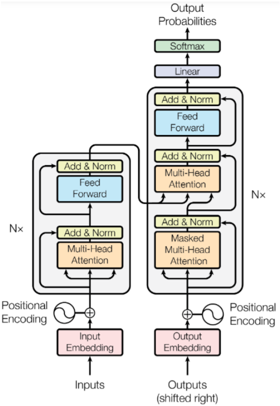

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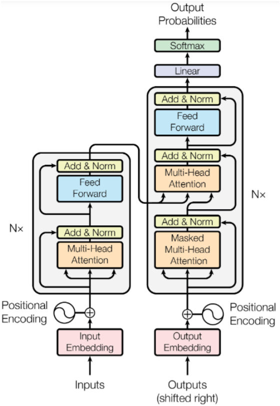
- Building block: Self-Attention layer

$$\vec{X}_i^{\text{out}} = \sum_{j=1}^{N} \text{softmax}_j \left[\left(\mathbf{K}\vec{X}_i \right)^T \left(\mathbf{Q}\vec{X}_j \right) \right] \mathbf{V}\vec{X}_j$$

$\mathbf{K}, \mathbf{Q} \in \mathbb{R}^{r \times d}$, $\mathbf{V} \in \mathbf{R}^{d \times d}$ are learnable matrices



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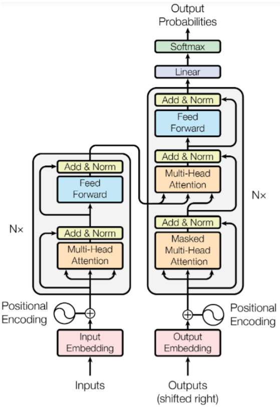
- Simplified version: $\mathbf{K}^T \cdot \mathbf{Q} = \mathbf{V} = J$

$$\vec{X}_i^{\text{out}} = \sum_{j=1}^{N} \text{softmax}_j \left[\vec{X}_i^T \mathbf{J} \vec{X}_j \right] \mathbf{J}\vec{X}_j$$



Our work

- Self-Attention as pseudolikelihood optimization
- Pseudolikelihood produces associative memories
- Vector-spin associative memories

Self-Attention as pseudolikelihood optimization

Self-attention as an attractor network: transient memories without backpropagation

1st Francesco D'Amico 2nd Matteo Negri

- 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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- t layer index $\rightarrow$ promoted to time index
- Eq. 1: minimization dynamics of cost

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

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

Pseudolikelihood method

- Model with two-bodies interaction: $E(x) = -\sum_{i \neq j} J_{ij} x_i x_j$
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- Pseudo-likelihood approximation: $\mathscr{L} = -\sum_{\mu=1}^{P} \sum_{i=1}^{N} \log p_i(\xi_i^\mu | \xi^\mu{}_{\setminus i})$

Pseudolikelihood produces associative memories

Step back:

What happens for the simplest possible model trained with pseudolikelihood?

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$\Downarrow$

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

Francesco D'Amico,[1,2] Dario Bocchi,[1,2] Luca Maria Del Bono,[1,2] Saverio Rossi,[1] and Matteo Negri[1,2]

[1] *Physics Department, Sapienza University of Rome, Piazzale Aldo Moro 5, 00185 Rome, Italy*
[2] *Institute of Nanotechnology, National Research Council of Italy, CNR-NANOTEC, Rome Unit*

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$$NLP = \sum_{i=1}^{N} \ell_i(J_i) = \sum_{i=1}^{N}\sum_{\mu=1}^{P} \log\left(1 + e^{-\xi_i^\mu \sum_{j\neq i} J_{ij}\xi_j^\mu}\right)$$

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- Quantity of interest: stabilities

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Pseudolikelihood on random data: Gardner computation

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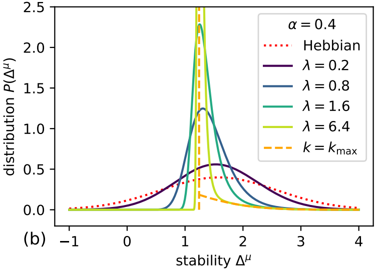

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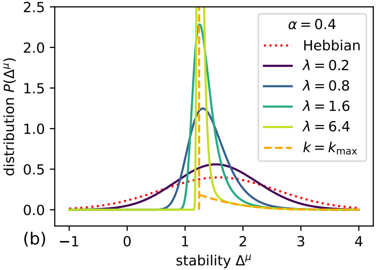

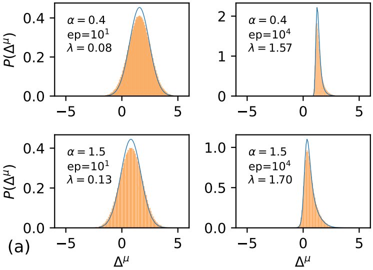

At fixed norm $\|\mathbf{J}\| = \lambda$

GD at free norm

Vector spins: towards Self-Attention

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Statistical mechanics of vector Hopfield network near and above saturation

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- Hebb's couplings $\mathbb{J}_{ij} = \frac{1}{N}\sum_{\mu=1}^{P} \vec{\xi}_i^{\,\mu} \times \vec{\xi}_j^{\,\mu} \Rightarrow \mathbb{J}_{ij} \in \mathbb{R}^{d\times d}$

Phase diagram of retrieval at equilibrium

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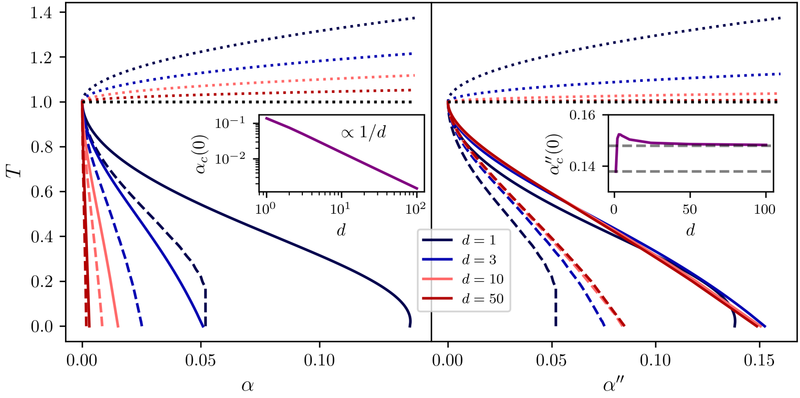
Two order parameters: $\alpha = \frac{P}{N}$, $\alpha'' = \frac{Pd}{N}$



First step denoising

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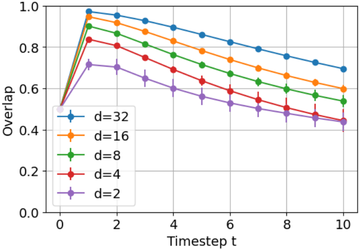

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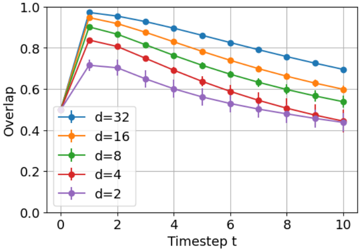

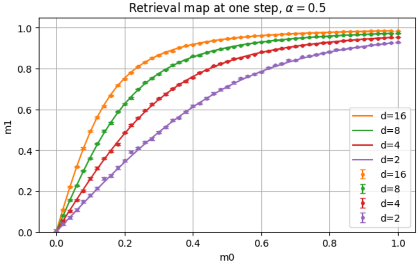

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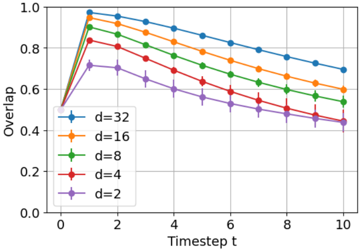

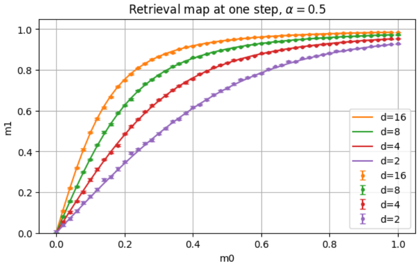

$$\Rightarrow P = \alpha' N d$$

Last step

$J_{ij} = \sum_\mu \xi_i^\mu \xi_j^\mu$

Pseudolikelihood

$\boldsymbol{s}_i \in \{\pm 1\}$

✓ *Amit et al. (1987)*

$\boldsymbol{s}_i \in \boldsymbol{s}_{d-1}$

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