Improved Robustness and Hyperparameter Selection in the Modern Hopfield Network

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Overview

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- Learn to associate a state with itself.
- Relax probe towards a learned state.

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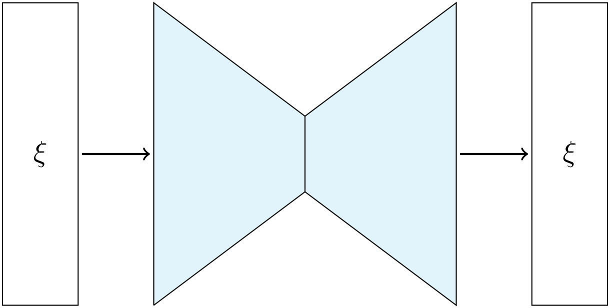

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Classical Hopfield Network

- Association by Hebbian learning.
  - Biological inspiration.
  - Easy to analyze.
- Relax by matrix multiplication.
  - Mean field approximation.
  - Nonlinearity keeps states in bipolar domain.
  - Energy guaranteed to achieve a minima (under sensible conditions).

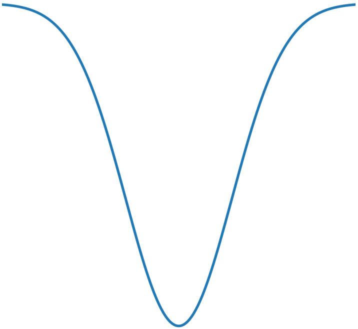
$$W = \sum_k \xi_k \otimes \xi_k \tag{1}$$

$$\xi_{t+1} = \text{Sign}\left(W \cdot \xi_t\right) \tag{2}$$

$$E\left(\xi\right) = -\frac{1}{2}\xi^T W \xi \tag{3}$$

Modern Hopfield Network

- Classical energy wells are too shallow.



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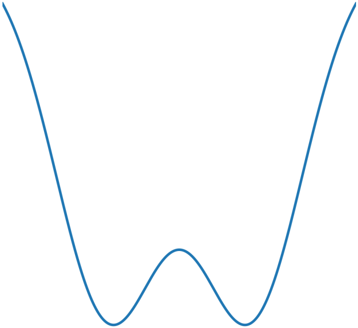

Modern Hopfield Network

- Key trick: Replace quadratic energy with general polynomial.
  - Heck, anything with a vaguely polynomial shape.

$$f_n(x) = x^n$$

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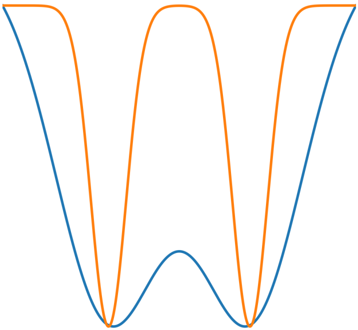

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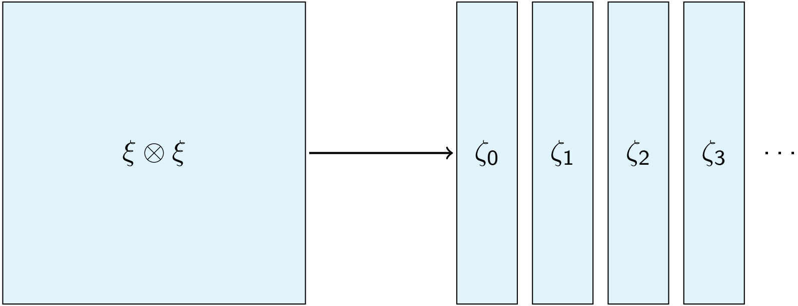
Memory matrix replaced by list of memory states – vectors of same dimension as data.



Modern Hopfield Network

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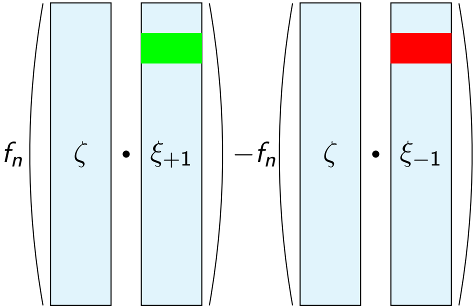
- Controls the range of influence that memories have.
- However, also radically alters the network architecture.

Relaxation no longer uses mean field – now a contrastive difference.

- Negative energy no longer means "stable" – the energy *difference* between a neuron clamped on and off indicates stability.



Modern Hopfield Network

n – The Interaction Vertex

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- However, also radically alters the network architecture.

Learning no longer supports Hebbian – now requires gradient descent.

$$W = \sum_k \xi_k \otimes \xi_k$$

$$\text{Loss}\left(\xi\right) = \tanh\left[\beta \sum_\mu \left(f_n\left(\zeta_{\mu,i} + \sum_{j\neq i} \zeta_{\mu,j}\xi_j\right) - f_n\left(-\zeta_{\mu,i} + \sum_{j\neq i} \zeta_{\mu,j}\xi_j\right)\right)\right]$$

Properties – Network Capacity

Larger network capacities with higher interaction vertices:

$$K_{\max} = \frac{1}{2\,(2n-3)!!}\frac{N^{n-1}}{\ln(N)} \tag{4}$$

Notably, super-linear for $n > 2$.

Properties – Training Times

Faster training times with higher interaction vertices:

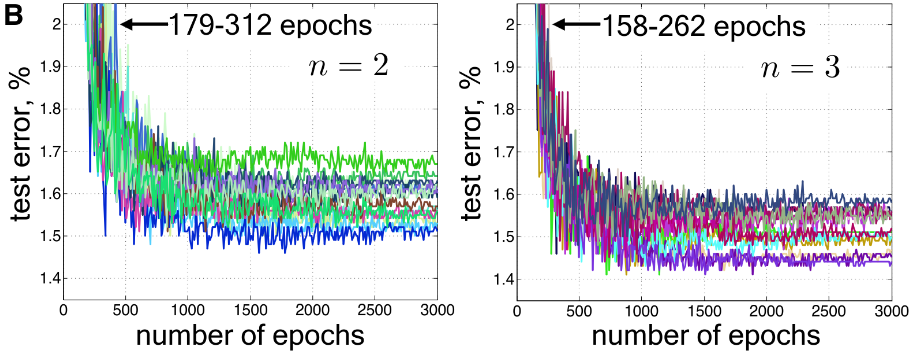

Figure: Krotov and Hopfield 2016, Figure 01

Properties – Feature to Prototype Transition

Low interaction vertices result in memories that look like features, while higher interaction vertices result in memories that look like prototypes:

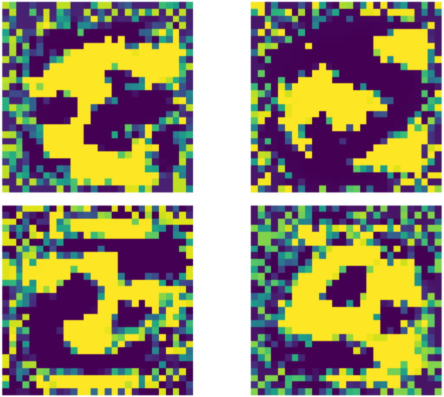

Figure: Feature-like Memories, $n = 2$

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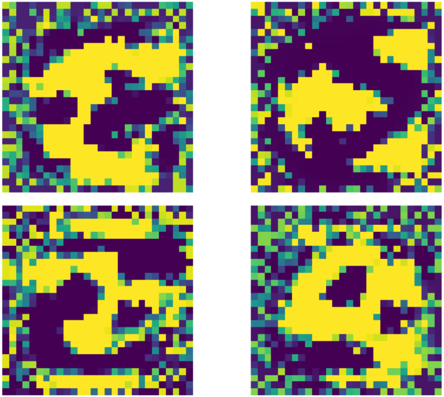

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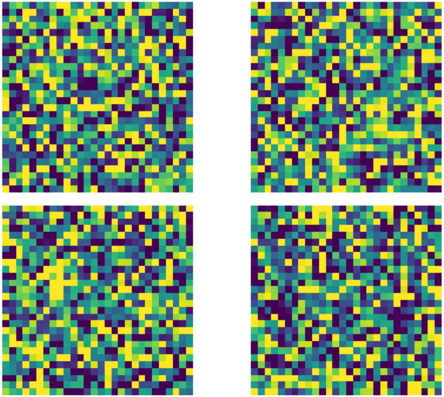

Figure: Prototype-like Memories, $n = 20$

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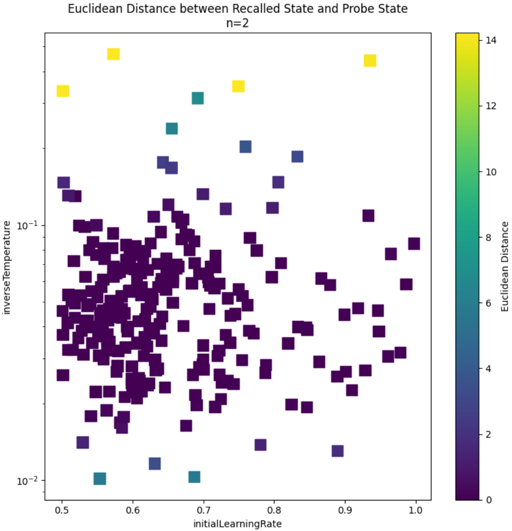
- Other implementations online...
  - Most use a feed-forward architecture that isn't as general.
  - An example of the autoassociative memory exists, and works!
  - When translated line by line to PyTorch, still broken...
- Hyperparameters are numerous and "magic".

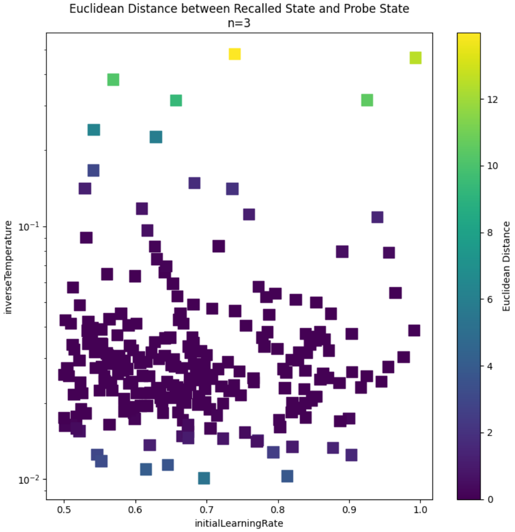
Hyperparameter Search

Training our network on autoassociative tasks of dimension 100.
We measure the Euclidean distance between learned state and recalled state. Lower is better, as this corresponds to a well recalled memory.

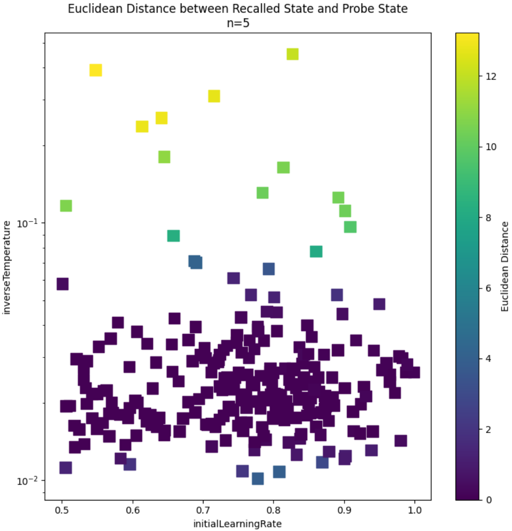
Hyperparameter Search: $n = 2$



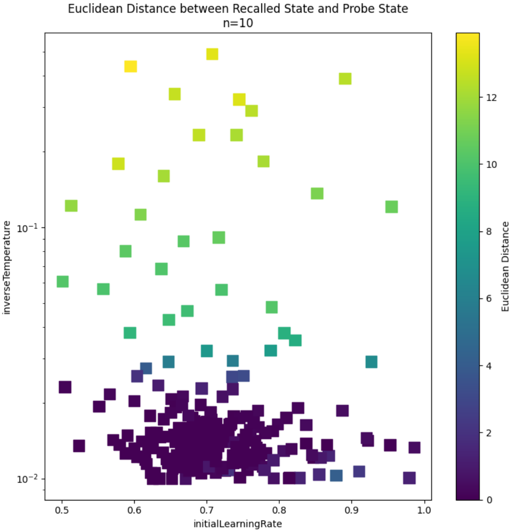
Hyperparameter Search: $n = 3$



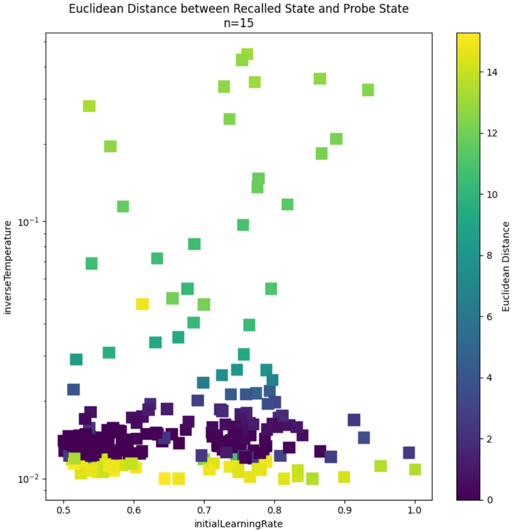
Hyperparameter Search: $n = 5$



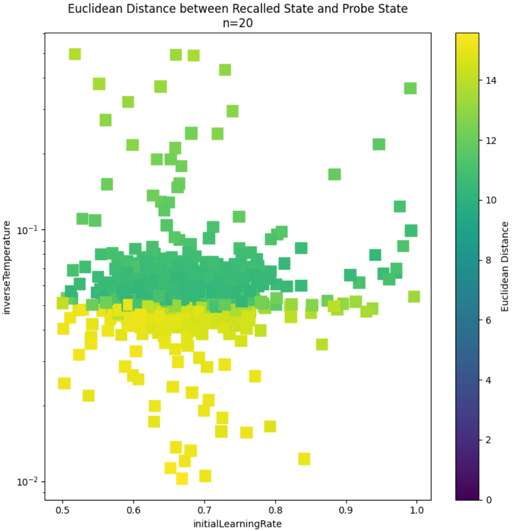
Hyperparameter Search: $n = 10$



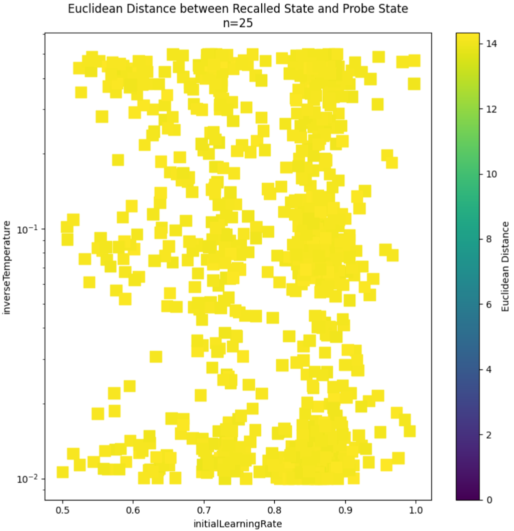
Hyperparameter Search: $n = 15$



Hyperparameter Search: $n = 20$



Hyperparameter Search: $n = 25$



Network Dynamics Step by Step

$$\tanh\left[\beta\sum_{\mu}\left(f_n\left(\zeta_{\mu,i}+\sum_{j\neq i}\zeta_{\mu,j}\xi_j\right)-f_n\left(-\zeta_{\mu,i}+\sum_{j\neq i}\zeta_{\mu,j}\xi_j\right)\right)\right]$$

1. Calculate similarities $\zeta\cdot\xi_{+1},\ \zeta\cdot\xi_{-1}$
2. Pass similarities through interaction function f_n
3. Sum the result over all memories $\sum_\mu$
4. Multiply by a scaling factor β
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How large is too large?

Network parameters	Interaction function value
$N = 100, n = 2$	10^4
$N = 100, n = 5$	10^{10}
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Maximum value of a float64 is $\approx 1.8 \cdot 10^{304}$. Default data type of NumPy.

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- The optimal hyperparameter region shrinks as n grows.
- The optimal region also shifts considerably as n grows.
- When n reaches some critical threshold, the optimal region is disrupted and the network does not learn at all.
  - Large n makes prototype memories.
  - Prototype memories have high similarities.
  - High similarities and large n causes overflow.

Fixing the Problem

$$\tanh\left[\beta\sum_{\mu}\left(f_n\left(\zeta_{\mu,i}+\sum_{j\neq i}\zeta_{\mu,j}\xi_j\right)-f_n\left(-\zeta_{\mu,i}+\sum_{j\neq i}\zeta_{\mu,j}\xi_j\right)\right)\right]$$

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If f_n is homogenous: $f(\alpha x)=\alpha^k f(x)$.
Weaker than linear – includes Polynomial and Rectified Polynomial.

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Results of Modifications – Autoassociative Memory

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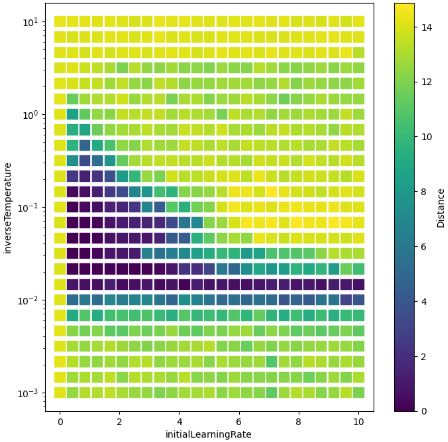

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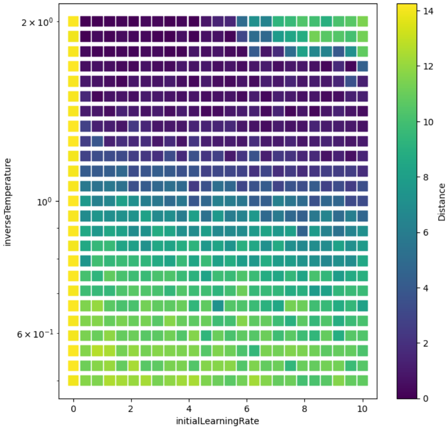

Modified

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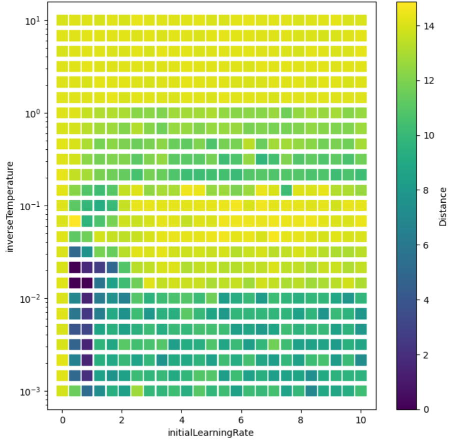

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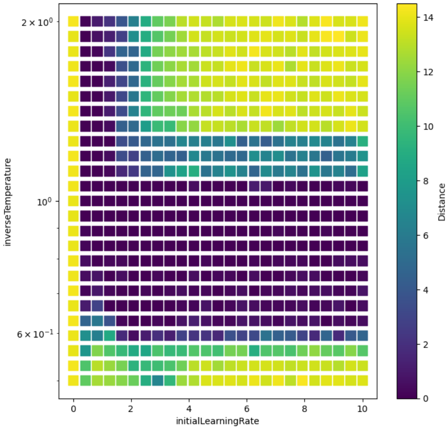

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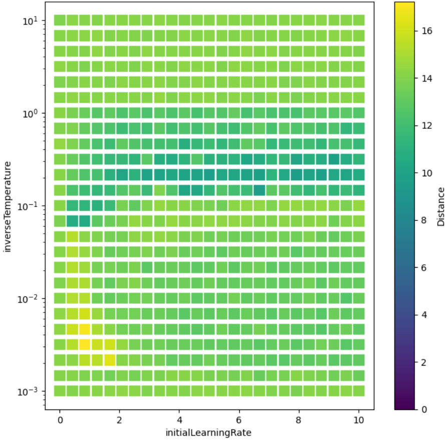

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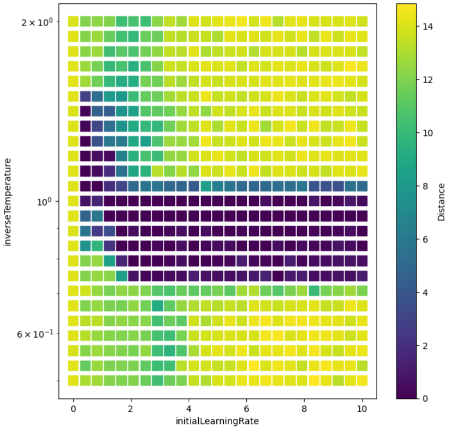

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Results of Modifications – MNIST Classification

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Original

Modified

Results of Modifications – MNIST Classification

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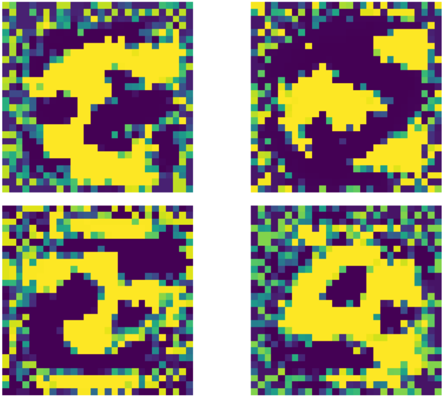

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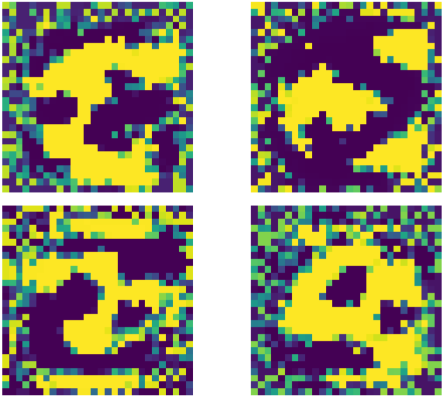

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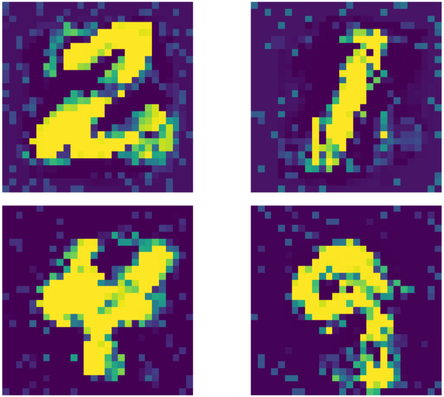

Figure: Prototype-like Memories, $n = 20$

Conclusion

- Modern Hopfield Network generalizes Classical Hopfield Network.
- Network capacity increases with the interaction vertex, even super-linearly.
- The original network (Krotov and Hopfield, 2016) has very unstable behavior for larger interaction vertices.
- The original network also has wildly shifting optimal hyperparameter regions.
- Our modifications solve both the instability and shifting hyperparameter regions at no additional cost.