Improved Robustness and Hyperparameter Selection in the Modern Hopfield Network

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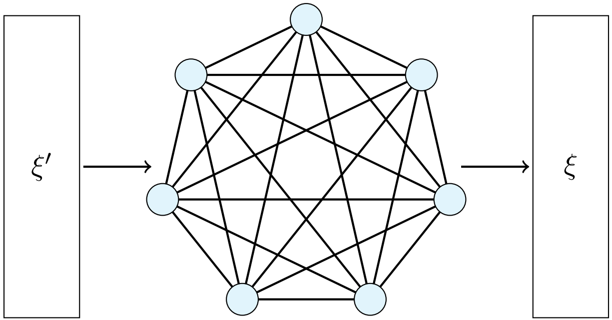
Autoassociative Memories

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

Classical Hopfield Network



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).

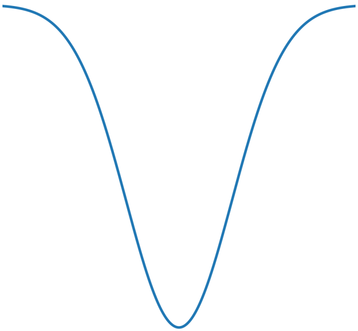
$$W = \sum_k \xi_k \otimes \xi_k \tag{1}$$

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

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

Modern Hopfield Network

- Classical energy wells are too shallow.



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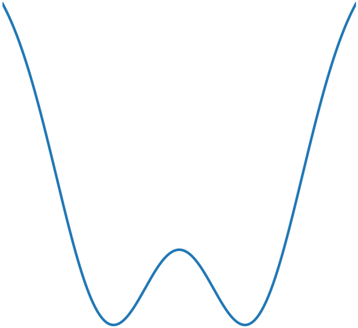


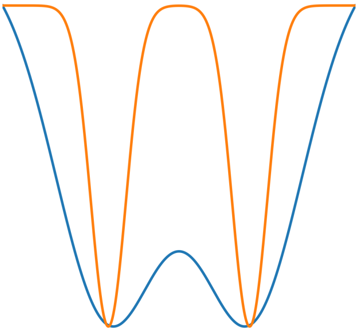
Modern Hopfield Network

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

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

$$f_n(x) = \begin{cases} x^n \text{ if } x \geq 0 \\ 0 \text{ if } x < 0 \end{cases}$$

$$f_n(x) = \begin{cases} x^n \text{ if } x \geq 0 \\ -\epsilon x \text{ if } x < 0 \end{cases}$$

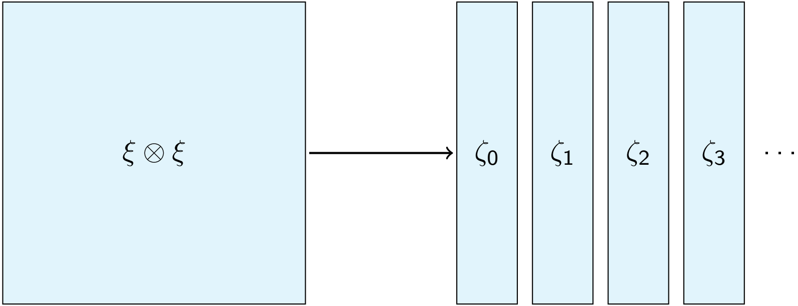


Modern Hopfield Network

n – The Interaction Vertex

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

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



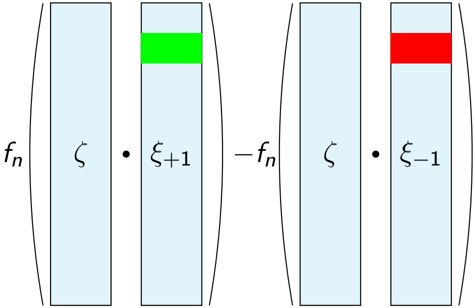
Modern Hopfield Network

n – The Interaction Vertex

- 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

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

Learning no longer supports Hebbian – now requires gradient descent.

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

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

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:

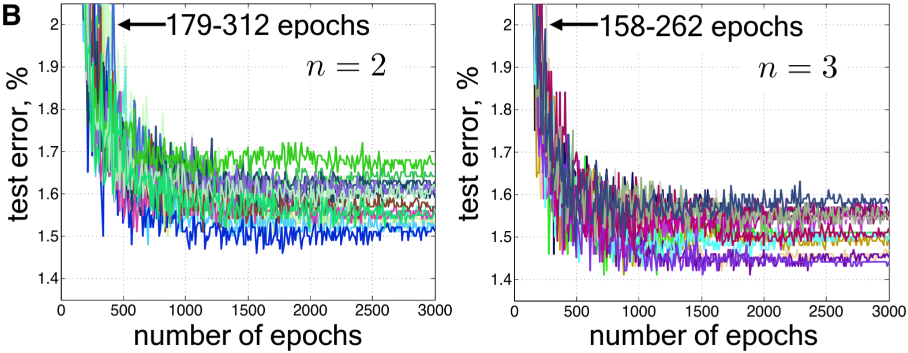


Figure: Krotov and Hopfield 2016, Figure 01

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:

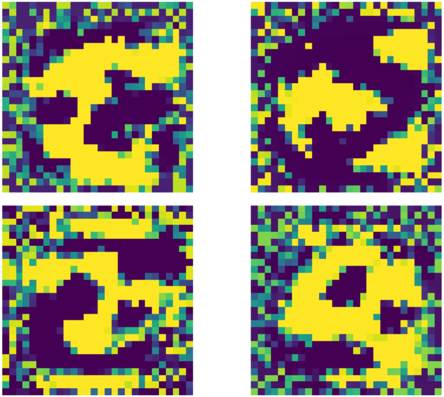


Figure: Feature-like Memories, $n = 2$

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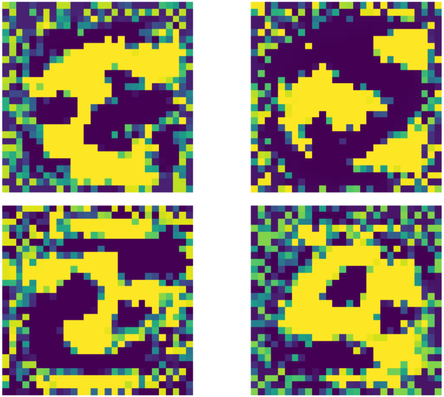

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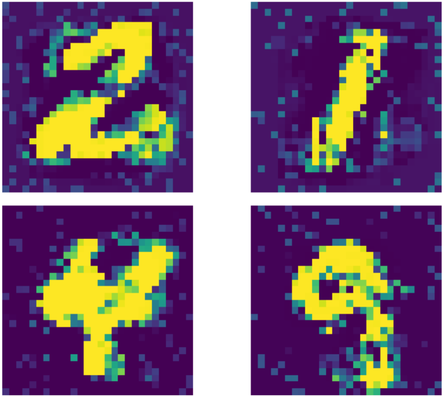

Figure: Prototype-like Memories, $n = 20$

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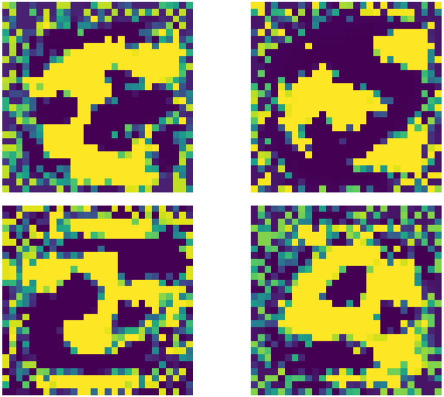

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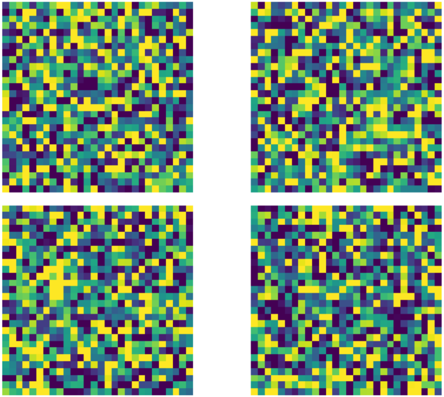

Figure: Prototype-like Memories, $n = 20$

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
5. Pass through activation function (e.g. Sign or tanh)

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$$\zeta,\xi\in[-1,1]^N \implies \zeta\cdot\xi\in[-N,N]$$

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$$\zeta, \xi \in [-1,1]^N \implies \zeta \cdot \xi \in [-N, N]$$
$$f_n(\zeta \cdot \xi) = (\zeta \cdot \xi)^n$$

Network Dynamics Step by Step

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$$\begin{aligned}\zeta,\xi\in[-1,1]^N &\implies \zeta\cdot\xi\in[-N,N]\\ f_n(\zeta\cdot\xi) &= (\zeta\cdot\xi)^n\\ &= N^n\end{aligned}$$

How large is too large?

Network parameters	Interaction function value
$N = 100, n = 2$	10^4
$N = 100, n = 5$	10^{10}
$N = 100, n = 10$	$10^{18.89}$
$N = 100, n = 20$	10^{40}

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Maximum value of a float32 is $\approx 3.4 \cdot 10^{38}$.
Maximum value of a float64 is $\approx 1.8 \cdot 10^{304}$.

Fixing the Problem

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

Fixing the Problem

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If f_n is homogenous: $f(\alpha x)=\alpha^k f(x)$.

Weaker than linear – includes Polynomial and Rectified Polynomial.

Fixing the Problem

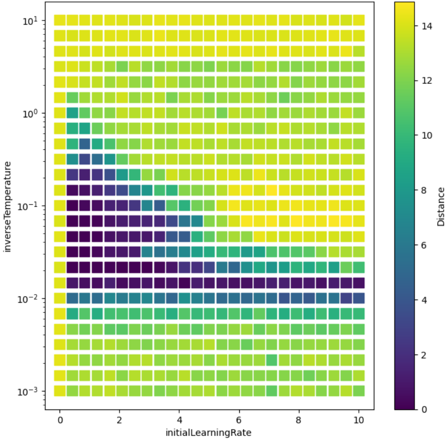
$$\tanh\left[\sum_{\mu}\left(f_n\left(\frac{\boldsymbol{\beta}}{N}\left(\zeta_{\mu,i}+\sum_{j\neq i}\zeta_{\mu,j}\xi_j\right)\right)-f_n\left(\frac{\boldsymbol{\beta}}{N}\left(-\zeta_{\mu,i}+\sum_{j\neq i}\zeta_{\mu,j}\xi_j\right)\right)\right)\right]$$

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

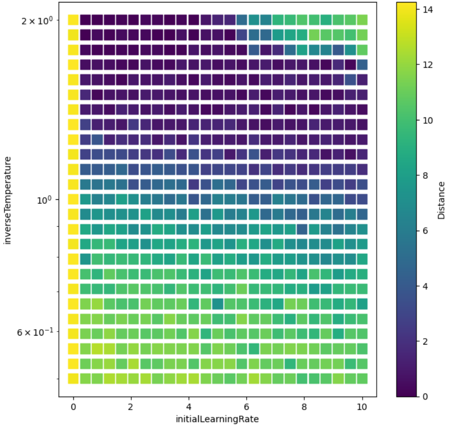
Provably doesn't alter network properties (e.g. capacity)

Results of Modifications – Autoassociative Memory

$n = 2$



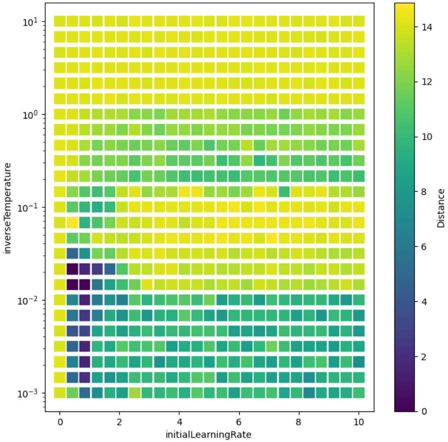
Original



Modified

Results of Modifications – Autoassociative Memory

$n = 10$



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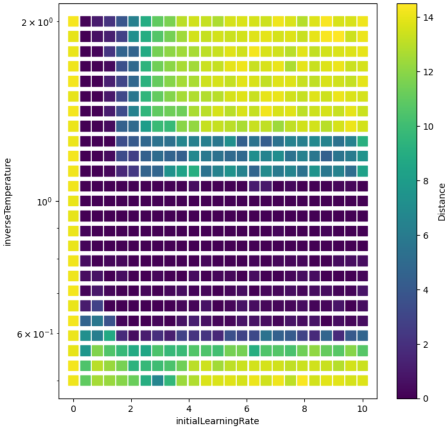
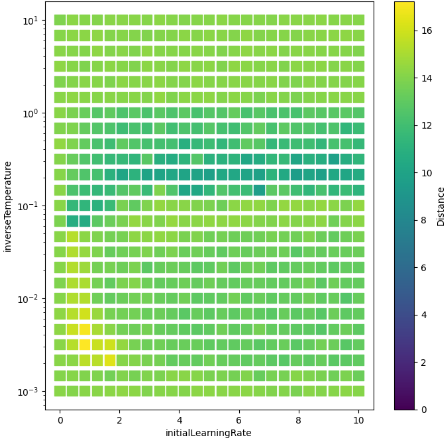


Modified

$n = 20$



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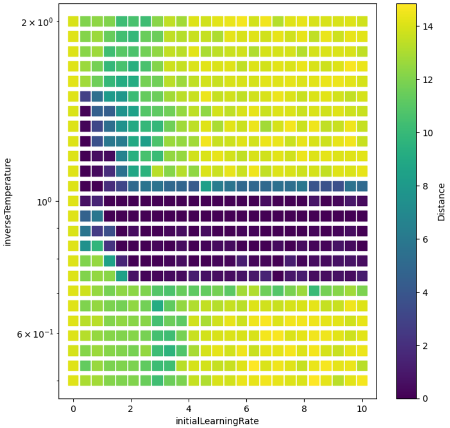

Modified

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.