Minimal Filling Architectures of Polynomial Neural Networks: Counterexamples, Frontier Search, and Defects

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Polynomial Neural Networks (PNNs)

Definition. A (feedforward) **polynomial neural network** with activation σ is

$$p_\theta : \mathbb{R}^{d_0} \to \mathbb{R}^{d_L}, \quad p_\theta(x) = W_L\, \sigma(W_{L-1} \cdots \sigma(W_1 x)),$$

where

$$W_i \in \mathbb{R}^{d_{i+1} \times d_i}, \qquad \sigma(z)_j = z_j^r, \quad r \in \mathbb{N}.$$

Terminology.
Architecture: $(d_0, \ldots, d_L)$.
Parameters: $\theta = (W_1, \ldots, W_L)$.
Depth: L.

Polynomial Structure.
p_θ is homogeneous of degree r^{L-1}
$p_\theta \in \mathrm{Sym}_{r^{L-1}}(\mathbb{R}^{d_0})^{\oplus d_L}$.

Functional Space and neurovariety.
The **parameter map**

$$\Psi_{\mathbf{d},r} : \prod_{i=1}^{L} \mathrm{Mat}_{d_i \times d_{i-1}}(\mathbb{R}) \to \mathrm{Sym}_{r^{L-1}}(\mathbb{R}^{d_0})^{\oplus d_L}$$

sends weight matrices to the **functional space** $\mathcal{F}_{\mathbf{d},r}$ contained in the **ambient space** $\mathrm{Sym}_{r^{L-1}}(\mathbb{R}^{d_0})^{\oplus d_L}$. The (Zariski) closure of $\mathcal{F}_{\mathbf{d},r}$ is an algebraic set (solution set of polynomials) and called a neurovariety

$$\mathcal{V}_{\mathbf{d},r} = \overline{\mathcal{F}_{\mathbf{d},r}}$$

In some cases the closure is the entire ambient space. When this happens we say $\mathcal{V}_{\mathbf{d},r}$ is **filling**. It is **minimal filling** if shrinking intermediate width leads to a nonfilling architecture.

Open problem: Characterize when $\mathcal{V}_{\mathbf{d},r}$ is filling.

Neuroalgebraic Geometry: Key Lemmas

Lemma 1 (Kubjas–Li–Wiesmann, 2024). Fix $r \geq 1$. If $\mathbf{d}'$ is a subarchitecture of $\mathbf{d}$ (same endpoints, every hidden width $\leq$ that of $\mathbf{d}$), then $\mathcal{V}_{\mathbf{d}'} \subseteq \mathcal{V}_{\mathbf{d}}$.

Lemma 2 (Kileel–Trager–Bruna, 2019). Fix $r \geq 1$. For any $k \in \{1, \ldots, L-1\}$,

$$\dim \mathcal{V}_{(d_0,\ldots,d_L)} \;\leq\; \dim \mathcal{V}_{(d_0,\ldots,d_k)} + \dim \mathcal{V}_{(d_k,\ldots,d_L)} - d_k.$$

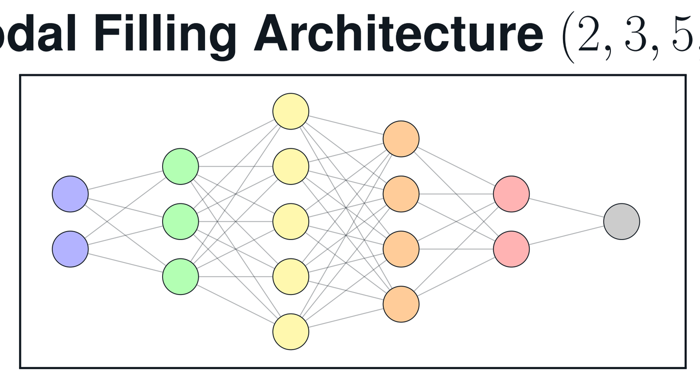
Unimodal Minimal Filling Architecture Conjecture

Conjecture (Kileel–Trager–Bruna). *Fix r, L, d_0, d_L. If $\mathbf{d} = (d_0, d_1, \ldots, d_L)$ is an minimal filling architecture (MFA), then $\mathbf{d}$ is **unimodal**: there exists i such that*

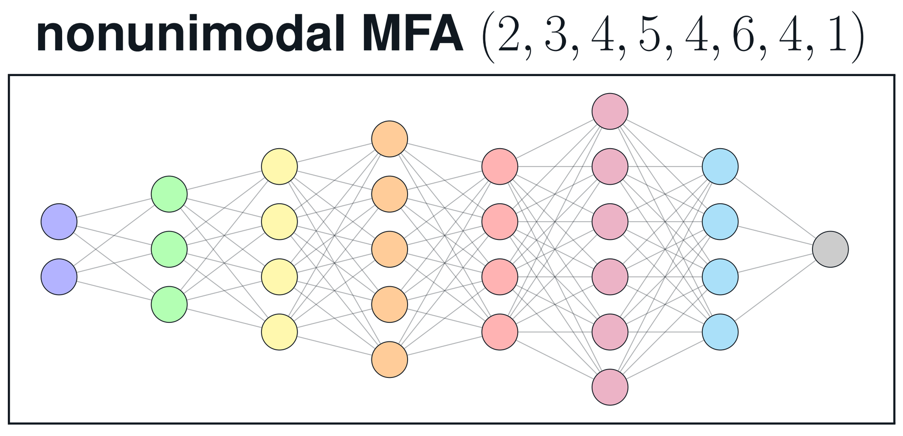
$$d_0 \leq d_1 \leq \cdots \leq d_i \qquad \& \qquad d_i \geq d_{i+1} \geq \cdots \geq d_L.$$

Motivation. The conjecture formalises the conventional ML wisdom that a network first expands its representational capacity and then narrows for prediction.

Unimodal Filling Architecture $(2, 3, 5, 4, 2, 1)$



nonunimodal MFA $(2, 3, 4, 5, 4, 6, 4, 1)$



Result: The Counterexample

Theorem. *For $r = 2$, $\mathbf{d} = (2, 3, 4, 5, 4, 6, 4, 1)$ is a nonunimodal MFA.*
Filling. The ambient space is $\mathrm{Sym}_{64}(\mathbb{R}^2) \cong \mathbb{R}^{65}$. A finite field computation easily finds a prime p and parameter θ with $\mathrm{rank}\,\mathrm{Jac}(\Psi_{\mathbf{d},2}(\theta \bmod p)) = 65$.
Minimality. Decreasing any hidden layer by one gives a subarchitecture $\mathbf{d}_i$. Lemma 1 & 2 together with the filling status of auxiliary subarchitectures (verified by computer computation) provide $\dim(\mathcal{V}_{\mathbf{d}_i,2}) < 65$ for each i.

Subarchitecture	Reported Dim	Proven bound	Reported Codimension
$(2, 2, 4, 5, 4, 6, 4, 1)$	35	≤ 53	30
$(2, 3, 3, 5, 4, 6, 4, 1)$	60	≤ 61	5
$(2, 3, 4, 4, 4, 6, 4, 1)$	62	≤ 63	3
$(2, 3, 4, 5, 3, 6, 4, 1)$	39	$= 39$	26
$(2, 3, 4, 5, 4, 5, 4, 1)$	61	≤ 62	4
$(2, 3, 4, 5, 4, 6, 3, 1)$	59	≤ 62	6

Losing Expressive Power: Measuring Architecture Defect

Definition. The **expected dimension** of $\mathcal{V}_{\mathbf{d},r}$ is

$$\mathrm{expdim}(\mathcal{V}_{\mathbf{d},r}) = \min\left(\dim(\mathrm{Sym}_{r^{L-1}}(\mathbb{R}^{d_0})^{\oplus d_L}),\; \sum_{i=1}^{L} d_i d_{i-1} - \sum_{i=1}^{L-1} d_i\right).$$

The **defect** is $\mathrm{expdim}(\mathcal{V}_{\mathbf{d},r}) - \dim(\mathcal{V}_{\mathbf{d},r}) \geq 0$. Often defect equals codimension (this is the case in all our examples). Positive defect implies the neurovariety loses predicted expressive power. The subarchitectures of the counterexample exhibit **unusually large defects**, among the first nontrivial examples in the literature.

Approach: Frontier Search Algorithm

To find MFAs $(d_0, \mathbf{a}, d_L)$, perform a **frontier search** over $\mathbf{a} \in \mathbb{N}^{L-1}$.
Pruning rules:

- If $\mathbf{a}' \geq \mathbf{a}$ and $\mathbf{a}$ is filling $\Rightarrow$ skip $\mathbf{a}'$ (already filling).
- If $\mathbf{a}' \leq \mathbf{a}$ and $\mathbf{a}$ is non-filling $\Rightarrow$ skip $\mathbf{a}'$ (still non-filling).

Each candidate $\mathbf{a}$ is tested by a finite-field Jacobian rank computation (implementation of Kubjas et al. 2024). **Dickson's Lemma** guarantees that the set of MFAs is *finite* for fixed r, L, d_0, d_L.

Result. For $d_0 = 2, d_L = 1, r = 2$ we found:

- $L = 7$: **13 MFAs**, of which **1 is non-unimodal**.
- $L = 8$: **82 MFAs**, of which **20 are non-unimodal**.

For $d_0 = 2, d_L = 1$, we found the proved the complete list of MFAs is:

L	Minimal Filling Architecture
$L = 2$	$(2, 2, 1)$
$L = 3$	$(2, 2, 2, 1)$
$L = 4$	$(2, 3, 3, 2, 1)$
$L = 5$	$(2, 3, 3, 3, 2, 1)$
$L = 6$	$(2, 3, 3, 4, 4, 2, 1)$
$L = 7$	$(2, 3, 4, 5, 4, 6, 4, 1), (2, 3, 4, 5, 6, 4, 2, 1)$ $(2, 3, 3, 5, 6, 4, 4, 1), (2, 3, 3, 5, 7, 4, 2, 1)$ $(2, 3, 3, 4, 6, 5, 2, 1), (2, 3, 4, 5, 5, 4, 4, 1)$ $(2, 3, 4, 4, 5, 5, 4, 1), (2, 3, 3, 6, 6, 4, 3, 1)$ $(2, 3, 3, 5, 5, 5, 4, 1), (2, 3, 4, 6, 5, 4, 3, 1)$ $(2, 3, 5, 5, 5, 4, 3, 1)$

The search time scales with the complexity of the neural network since we need to compute the dimension of each candidate $\mathbf{a}$.

Discussion & Next Steps

Practical relevance. Polynomial activations trade expressivity for stability (lower degree activation & less layers). Understanding MFAs informs architecture selection when low-degree power activations are preferred.

Future directions.

- Extend neuroalgebraic geometry to other PNNs (Chebyshev, Π-nets).
- Compare training dynamics on MFAs v.s. nonMFAs.
- Develop a systematic theory of defective architectures.
- Prove completeness of MFA lists for large L without exhaustive search.

References and Acknowledgments

[1] Joe Kileel, Matthew Trager, and Joan Bruna. "On the Expressive Power of Deep Polynomial Neural Networks". In: *Advances in Neural Information Processing Systems*. Vol. 32. 2019.

[2] Kaie Kubjas, Jiayi Li, and Maximilian Wiesmann. "Geometry of polynomial neural networks". In: *Algebraic Statistics* 15.2 (Dec. 2024), pp. 295–328. ISSN: 2693-2997.

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