What do Graph Neural Networks learn?
Insights from Tropical Geometry

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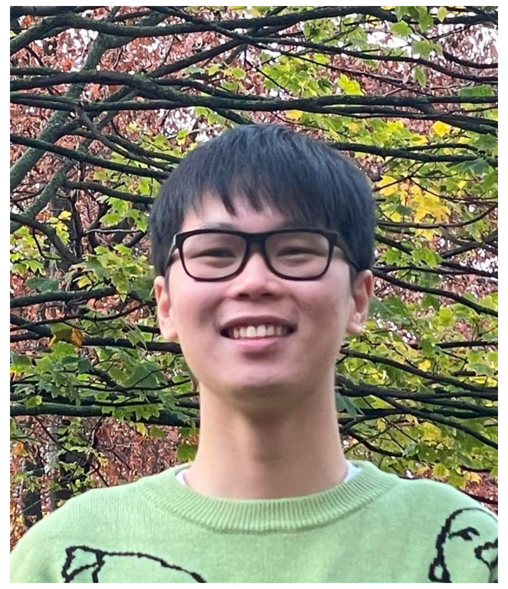

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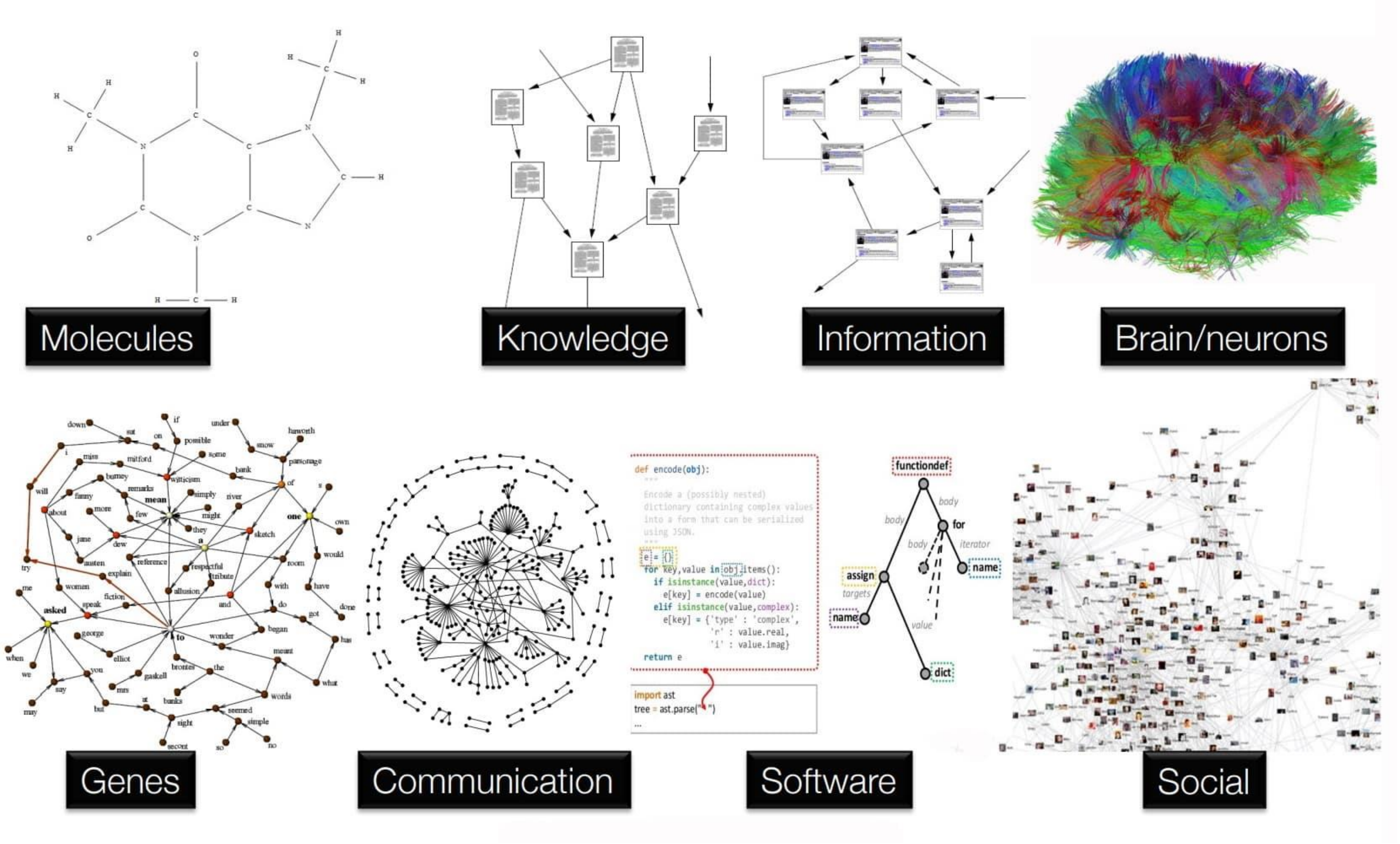
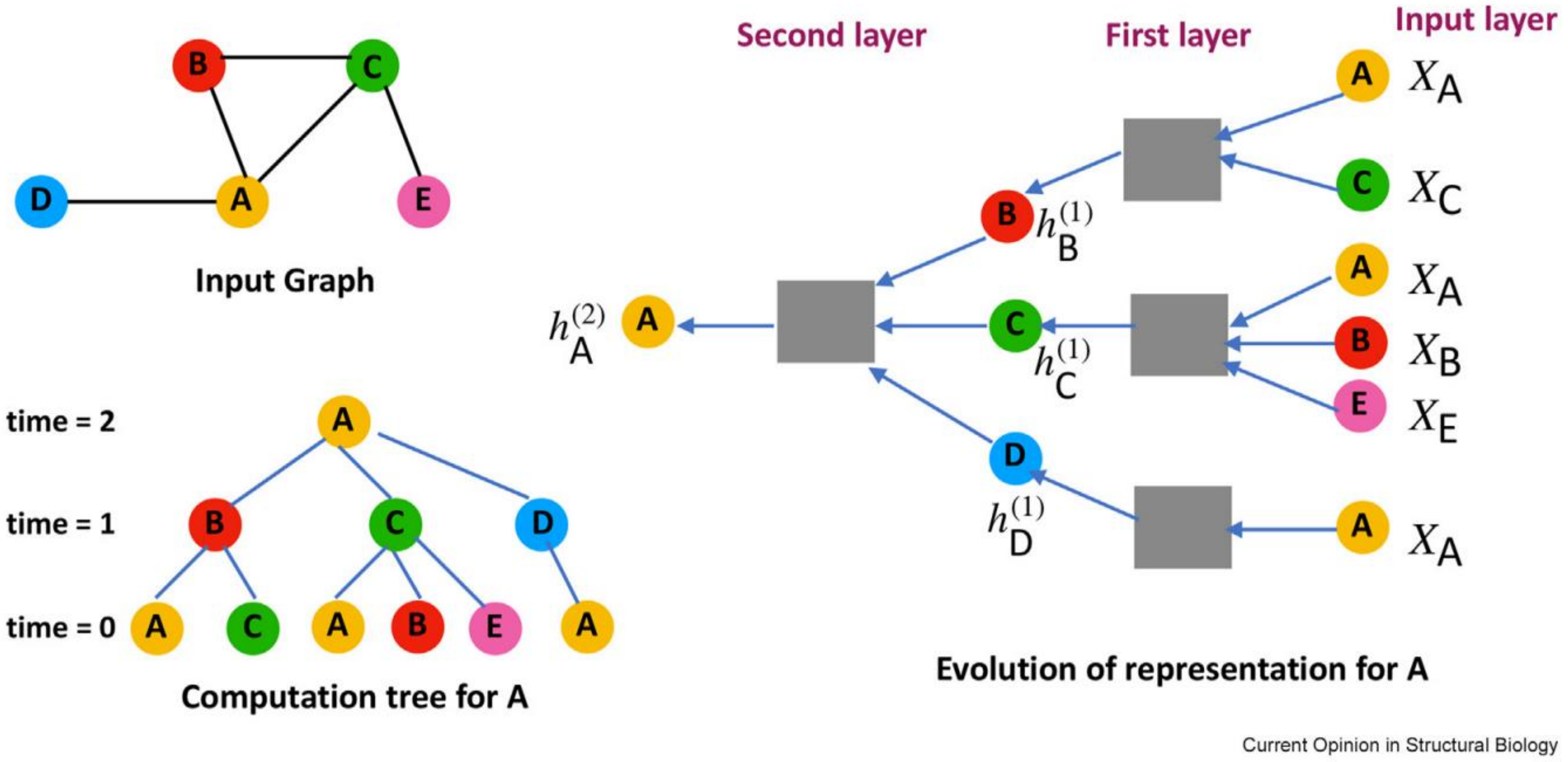
Thirty-Eighth Annual Conference on Neural Information Processing Systems (NeurIPS 2024)

Graph Neural Network



NVIDIA

ReLU Message Passing Neural Network (Gilmer et al 2017)



Garg V. (2024): Generative AI for graph-based drug design: Recent advances and the way forward

- Unlike the WL test that strives to expose what GNNs cannot do, we aim to understand **what they can**.
- WL formalism relies on <u>injective hash functions</u>; in contrast, several successful GNNs employ ReLU activations that violate injectivity.

Motivating questions

1. What class of functions can be represented by ReLU GNNs?
2. How does the number of linear region (geometric complexity) vary with choice of aggregation and update functions?
3. What complexity tradeoffs exist for models of comparable expressivity?
4. What decision boundary emerges for node and graph classification tasks?

Tropical Algebra and Geometry

A powerful tool to study the algebraic geometry and combinatorics of continuous piecewise linear functions

Basic idea:

- Form a semi-ring $\mathbb{T} = \mathbb{R} \cup \{-\infty\}$ with 2 operator: tropical sum $a \oplus b = \max(a, b)$ and tropical multiplication $a \odot b = a + b$.
- We can then define polynomials and rational functions on $\mathbb{T}$ and study their algebraic geometry and combinatorics.

Zhang et al. 2018 used tropical algebra to show that ReLU FNNs are equivalent to continuous piecewise linear map (CPLM), establishing the link between tropical geometry and deep learning.

This has motivated related works and provided further understanding of ReLU FNNs. We want to extend the link to GNNs.

Liwen Zhang, Gregory Naitzat, and Lek-Heng Lim. Tropical geometry of deep neural networks. (2018)

Key results

Theorem 1: *The set of functions represented by ReLU MPNNs and ReLU FNNs are the* ***same****: they can learn any continuous piecewise linear function.*

But there is a discrepancy in practice: often ReLU MPNNs outperform ReLU FNNs in learning.

Previously	**Message layers**	**Feedforward layers**	**Learnable parameters**
Deep NN in [19]	None	$\lceil \log_2(r) \rceil + 1$	$\mathcal{O}(rm)$
Deep NN in [83]	None	$\lceil \log_2(m) \rceil + 1$	$\mathcal{O}(rm)$
New (in this work)			
Local (Algorithm 6)	2	$\lceil \log_2(r/m) \rceil + 5$	$\mathcal{O}(rm)$
Global (Algorithm 7)	$\lceil \log_2(r) \rceil + 1$	$3 \lceil \log_m(r) \rceil + 2$	$\mathcal{O}(rm)$
Constant (Algorithm 8)	2	7	$\mathcal{O}(mr^{m+2})$
Hybrid (Algorithm 9)	1	1	$\mathcal{O}(rm)$

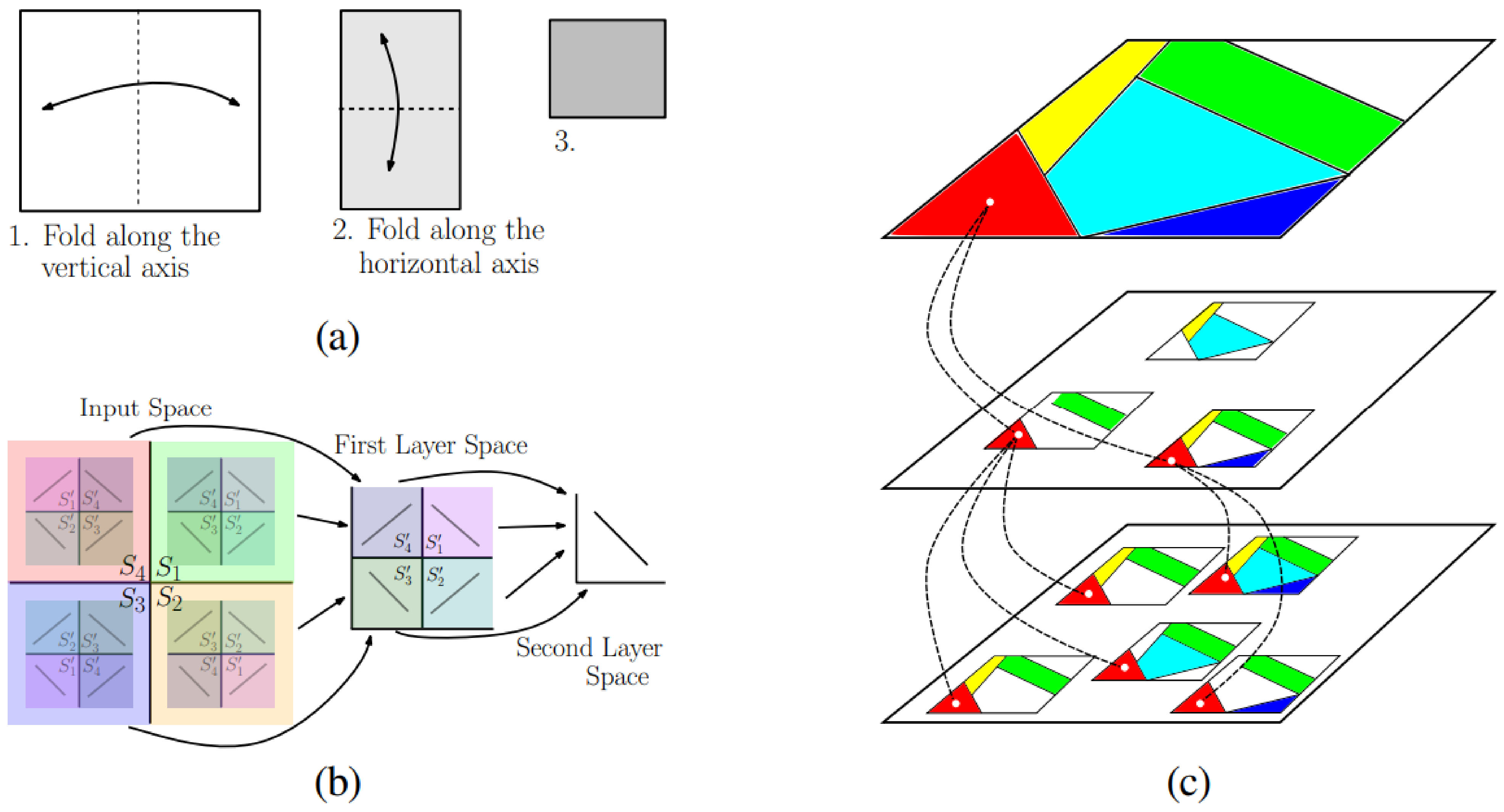
Table 1: Complexity of representing any tropical signomial function (TSFs) $f : \mathbb{R}^m \to \mathbb{R}$ consisting of r tropical monomials with different architectures. One more layer is required to compute any tropical rational signomial map (TRSM). The four new methods introduced here construct a graph (based on m and r) and leverage message passing to efficiently compare these monomials.

Key results (cont.)

For a CPLM f, we define its **linear degree** to be the least number of connected regions such that f restricted to this region is affine. This can be used to measure the **geometric complexity** of a deep learning model.

Theorem 2: *We obtain the **lower bound** for the **maximum** number of linear degree of a ReLU MPNN architecture .*

We use the idea of space folding and hyperplane arrangement introduced in Montufar et al. 2014



Montufar et al. 2014

Guido F Montufar, Razvan Pascanu, Kyunghyun Cho, and Yoshua Bengio. On the number of linear regions of deep neural networks. (2014)

Key results (cont.)

We use tools from tropical geometry and results from Zhang et al. 2018 to analyze the upper bound for the linear degree, thus completing the story.

Theorem 3: *We obtain a general **upper bound** for the linear degree of ReLU MPNN .*

- This is a first general bound for geometric complexity of ReLU MPNNs under some mild assumptions.
- Recover existing upper bound for ReLU FNNs and GCNs
- New bounds for popular GNNs: e.g. GraphSAGE and GIN.

New insight: Coordinate-wise max is more "expressive" than sum.

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Theoretical contributions of this work	
Characterizing the class of functions learned by ReLU MPNNs:	
Equivalence with ReLU FNNs, TRSMs and CPLMs	Proposition 1
Estimating the number of linear regions, and complexity tradeoffs:	
First general lower bound for ReLU MPNNs	Theorem 3
First general upper bound for ReLU MPNNs	Theorem 4
Max aggregation has greater geometric complexity than sum	Proposition 5
Recovery of existing upper bounds for FNN and GCN	Corollary 1, 2
New upper bounds for GraphSAGE and GIN	Corollary 3, 4
New ReLU MPNNs and complexity tradeoffs:	
New architectures that can all learn CPLMs, and their tradeoffs	Proposition 6
Characterizing the decision boundary:	
Decision boundary of ReLU MPNNs for graph classification	Proposition 7
Decision boundary of ReLU MPNNs for node classification	Proposition 8

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