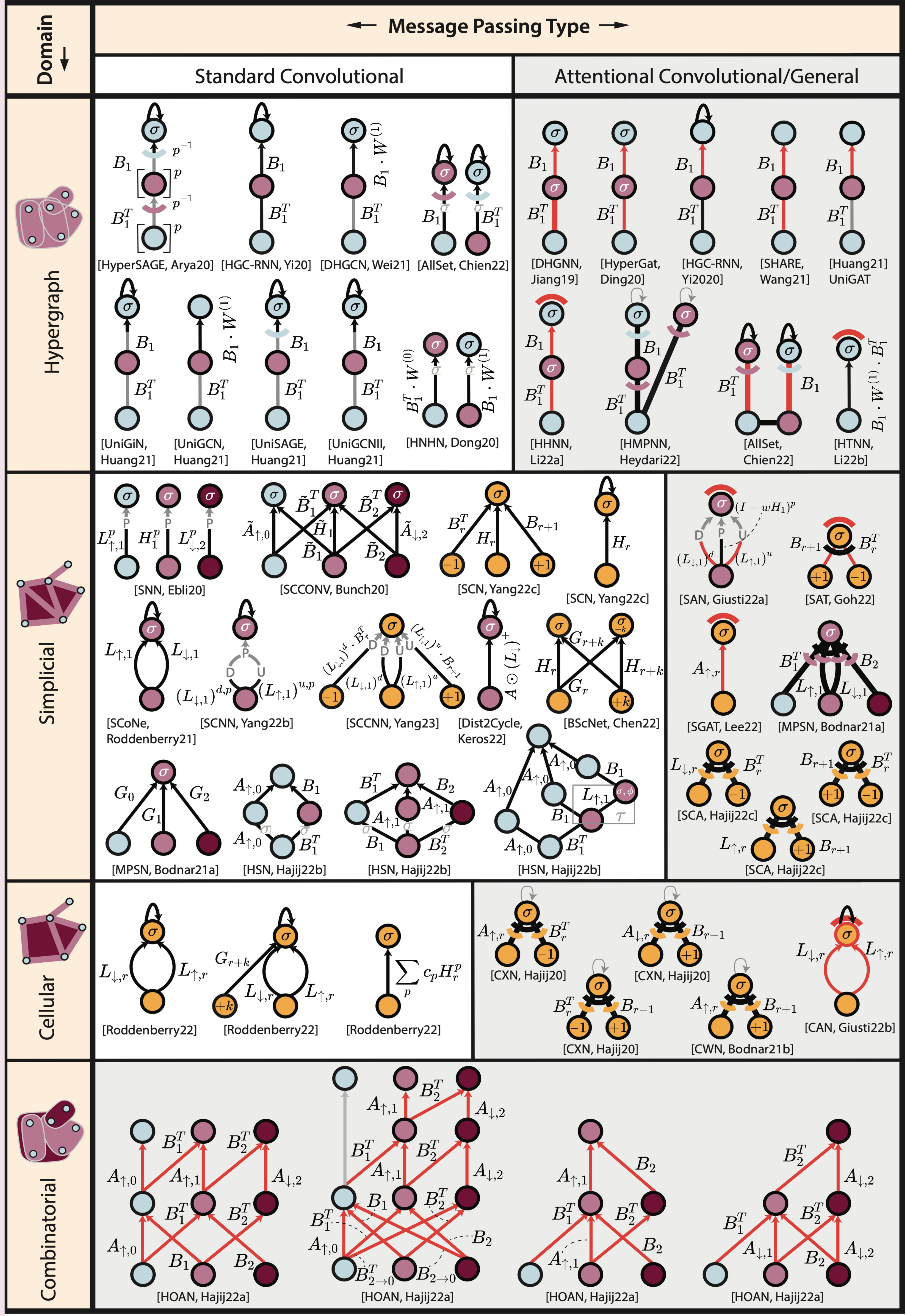
A Survey of Message Passing Topological Neural Networks

Nina Miolane, UC Santa Barbara

Joint work with Mathilde Papillon, Sophia Sanborn & Mustafa Hajij

CoSyNe 2025 @ It's All Connected!



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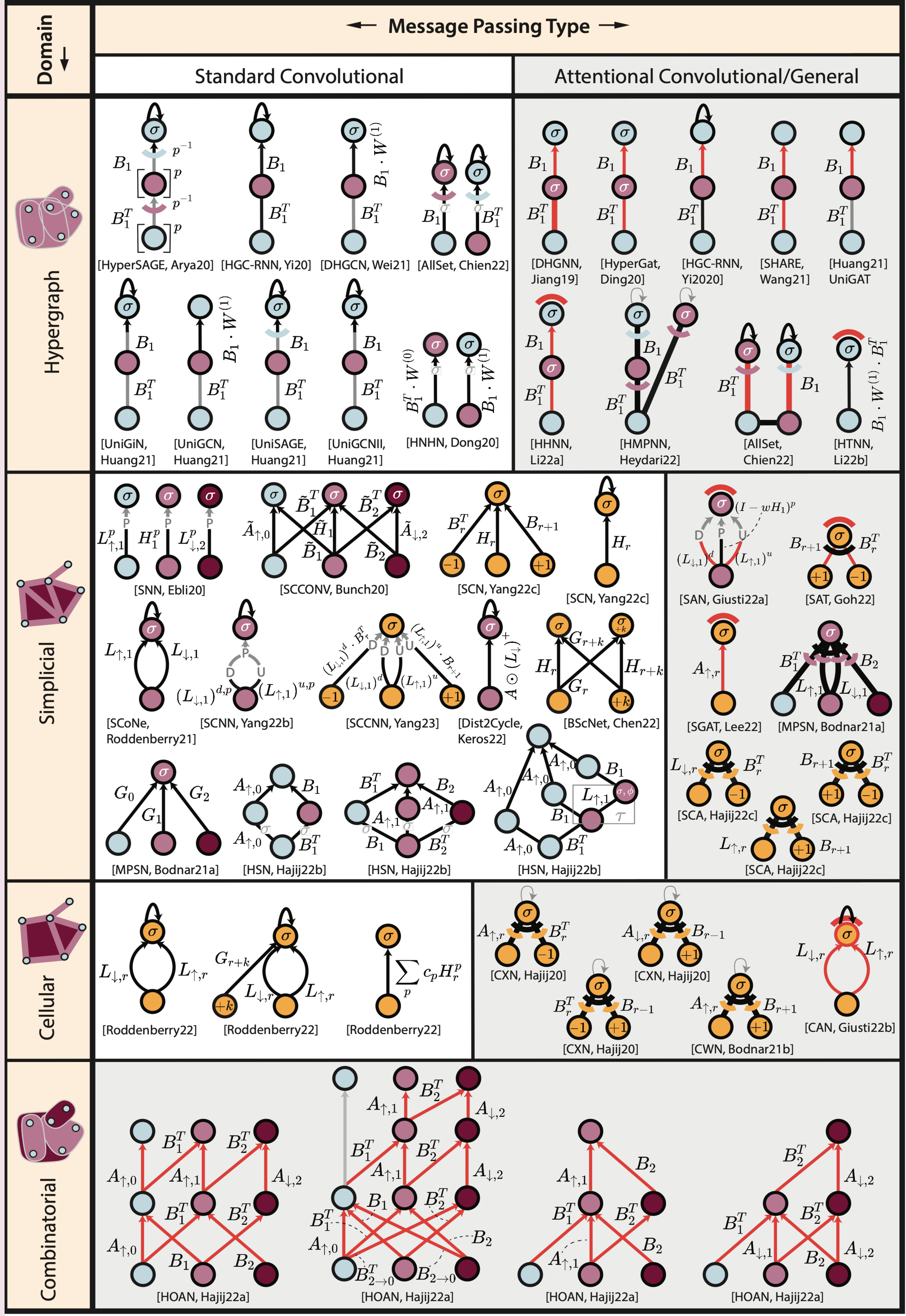
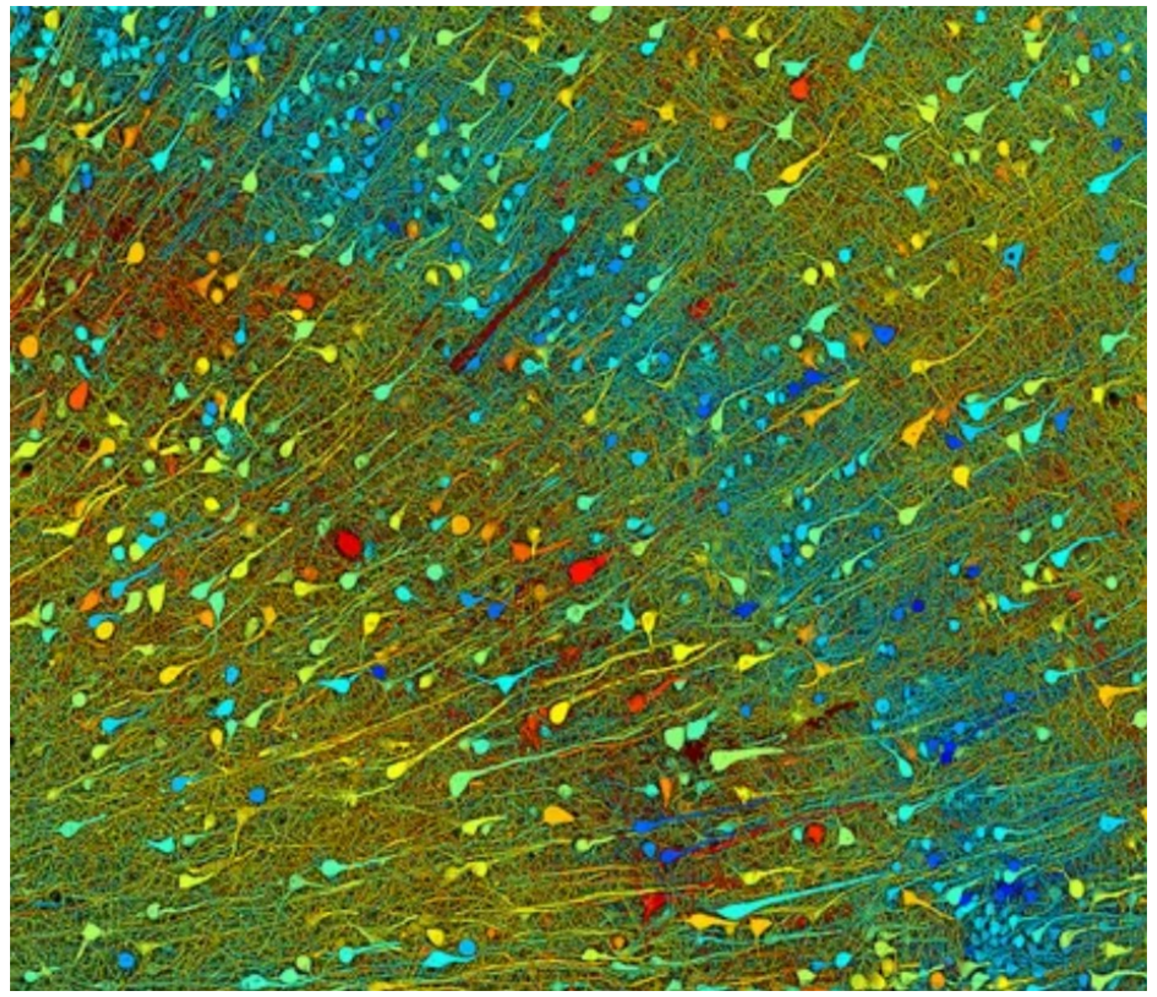
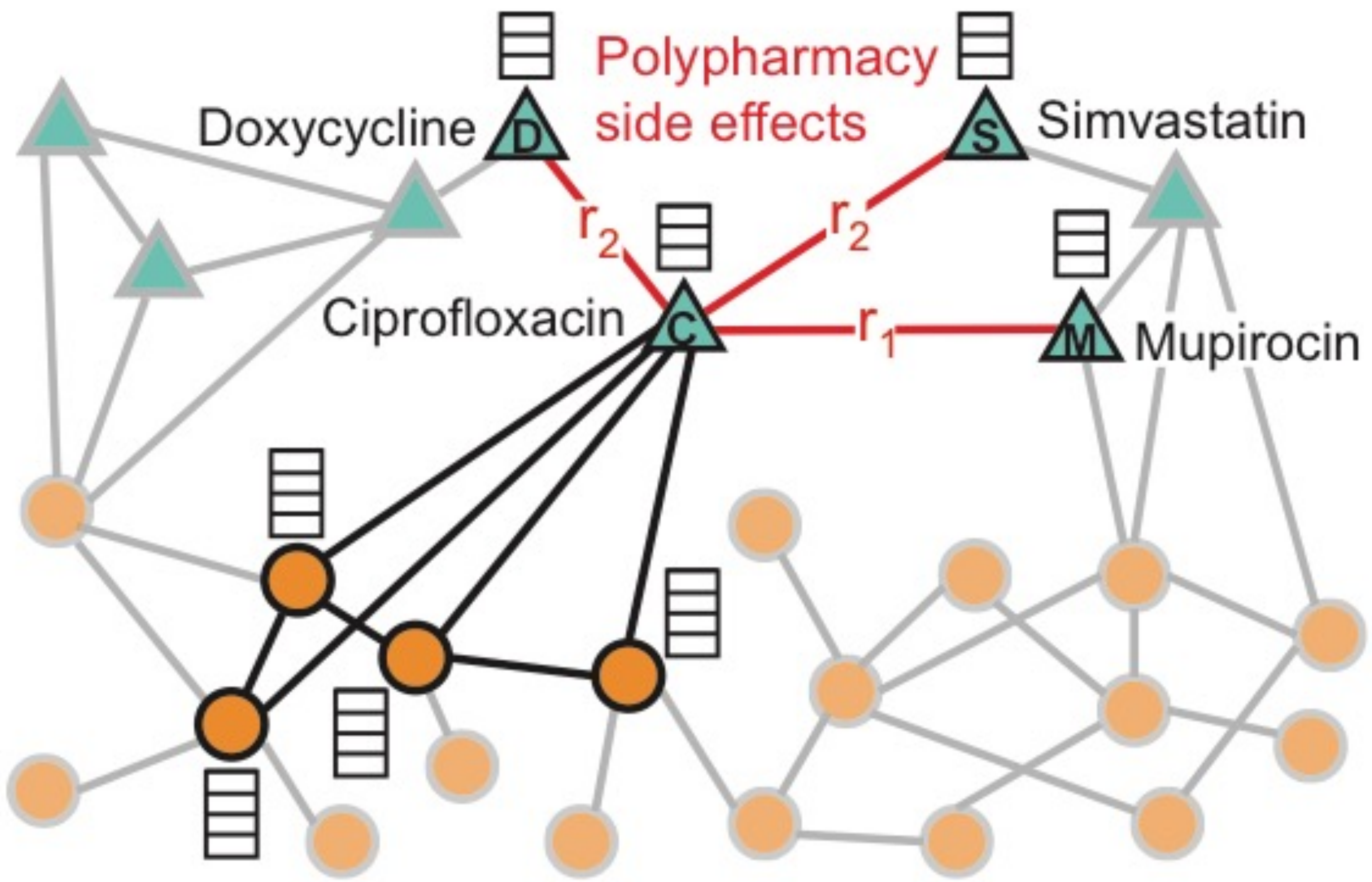
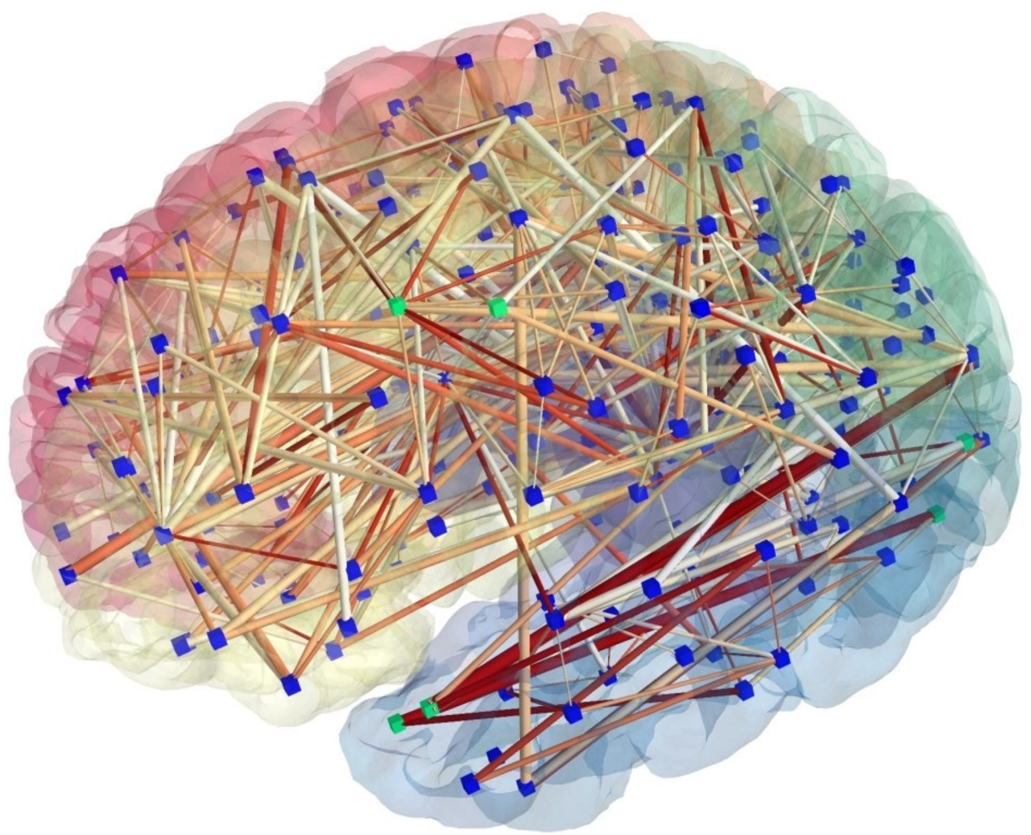


Topological Neural Networks

extract knowledge from data by exploiting **relations** between **components** of a system.

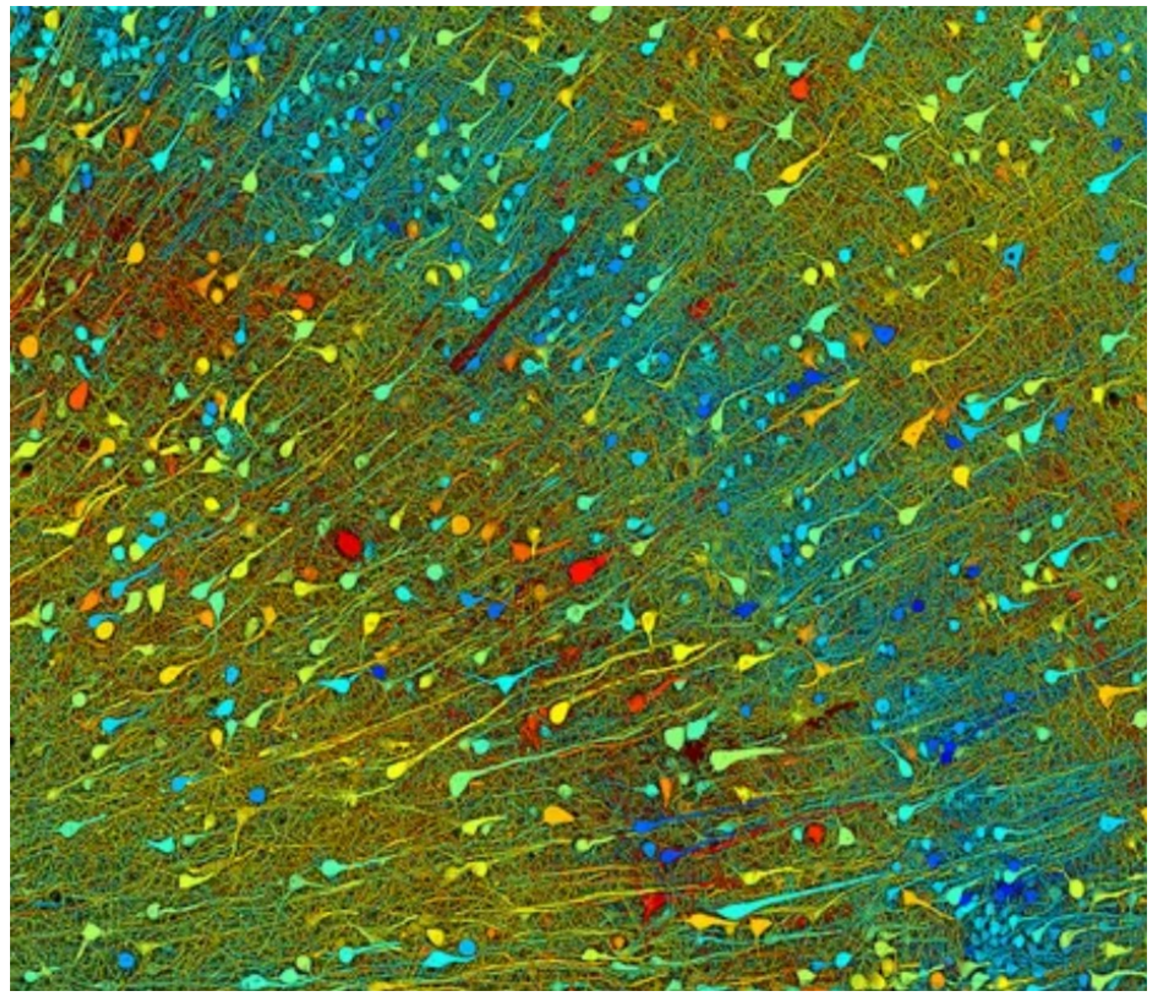






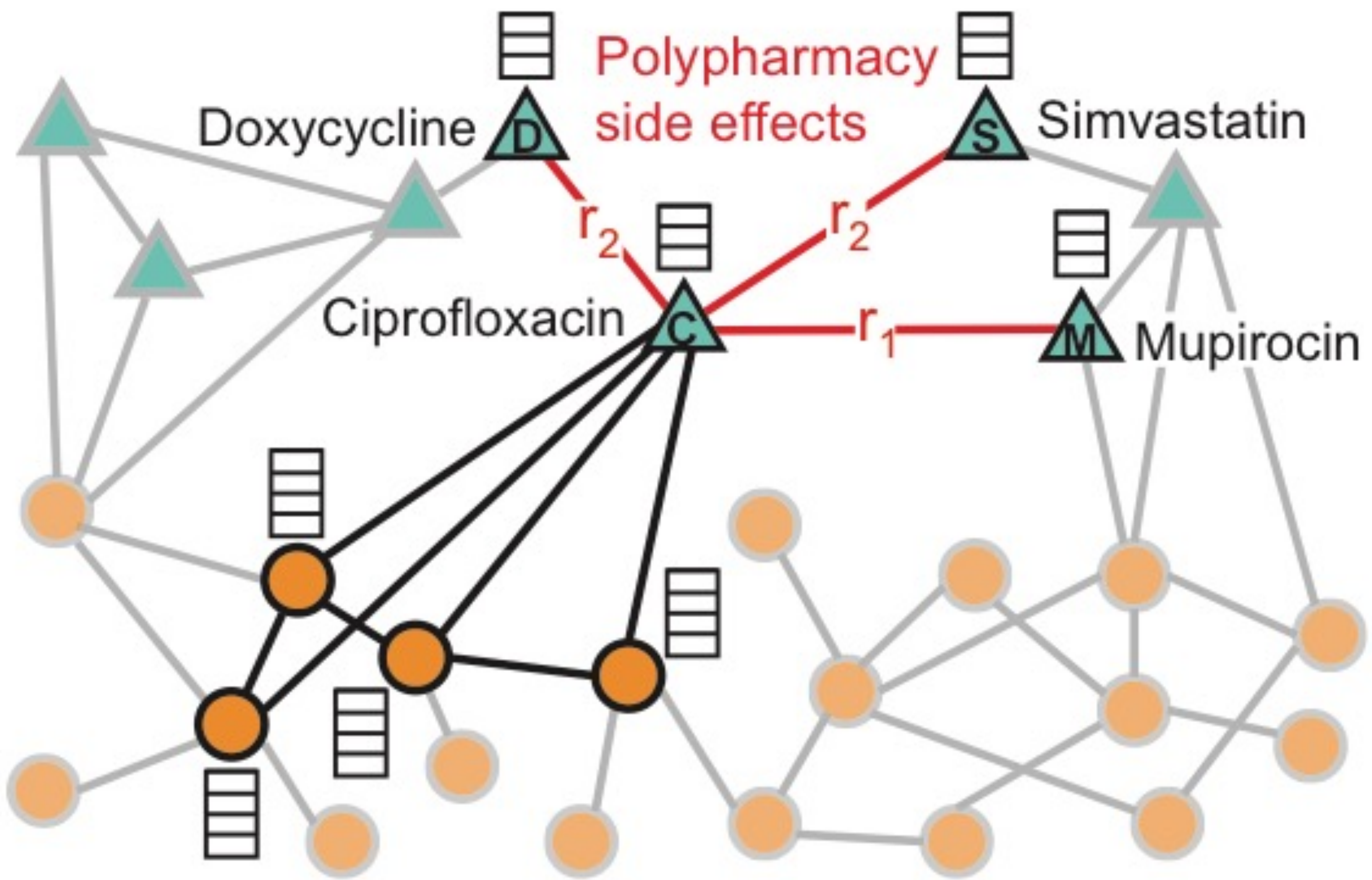
Topological Neural Networks answer questions such as:

Is this neuron inhibitory or excitatory?



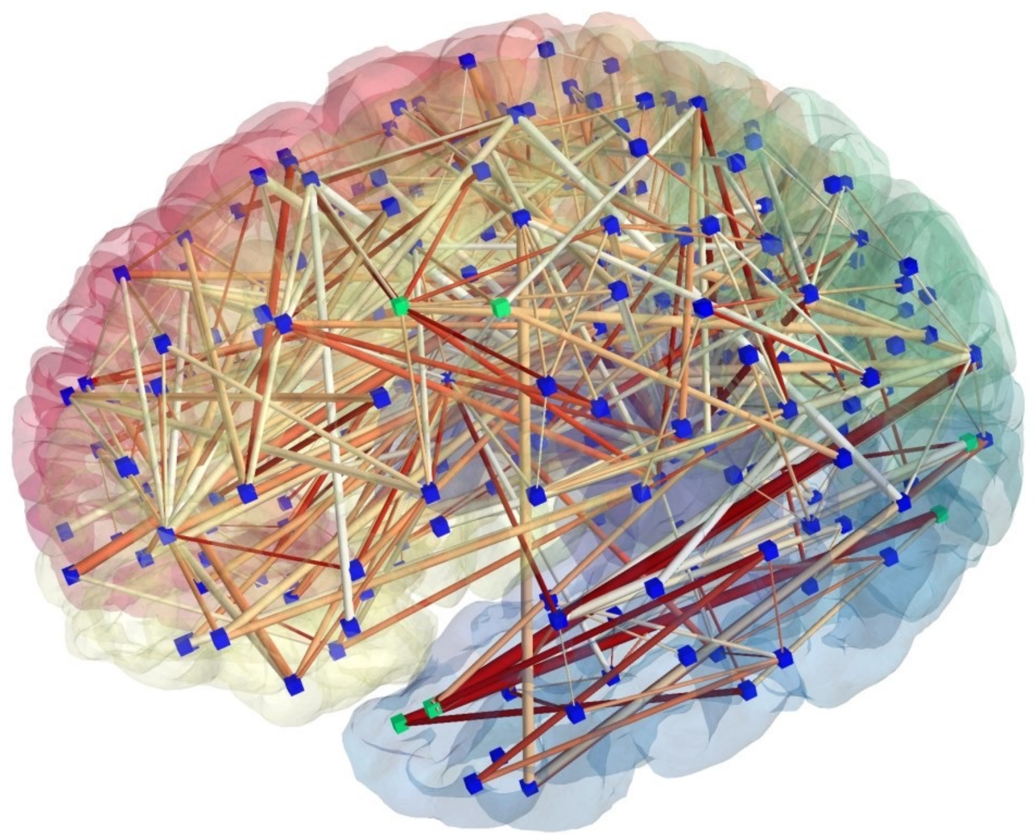
Node-level prediction

Does Fluoxetine interact with Venlafaxine?



Edge-level prediction

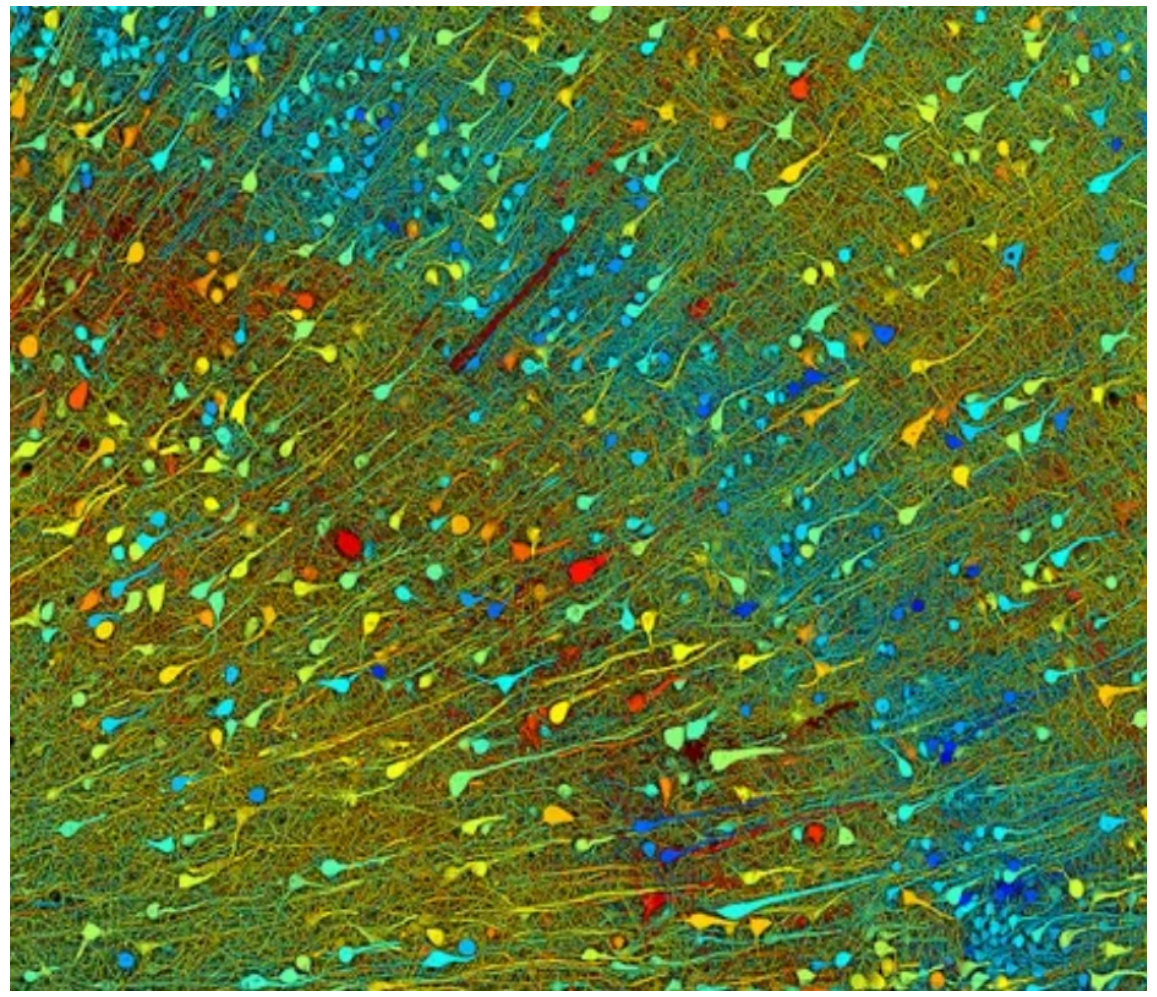
What is the brain state associated with this connectome?



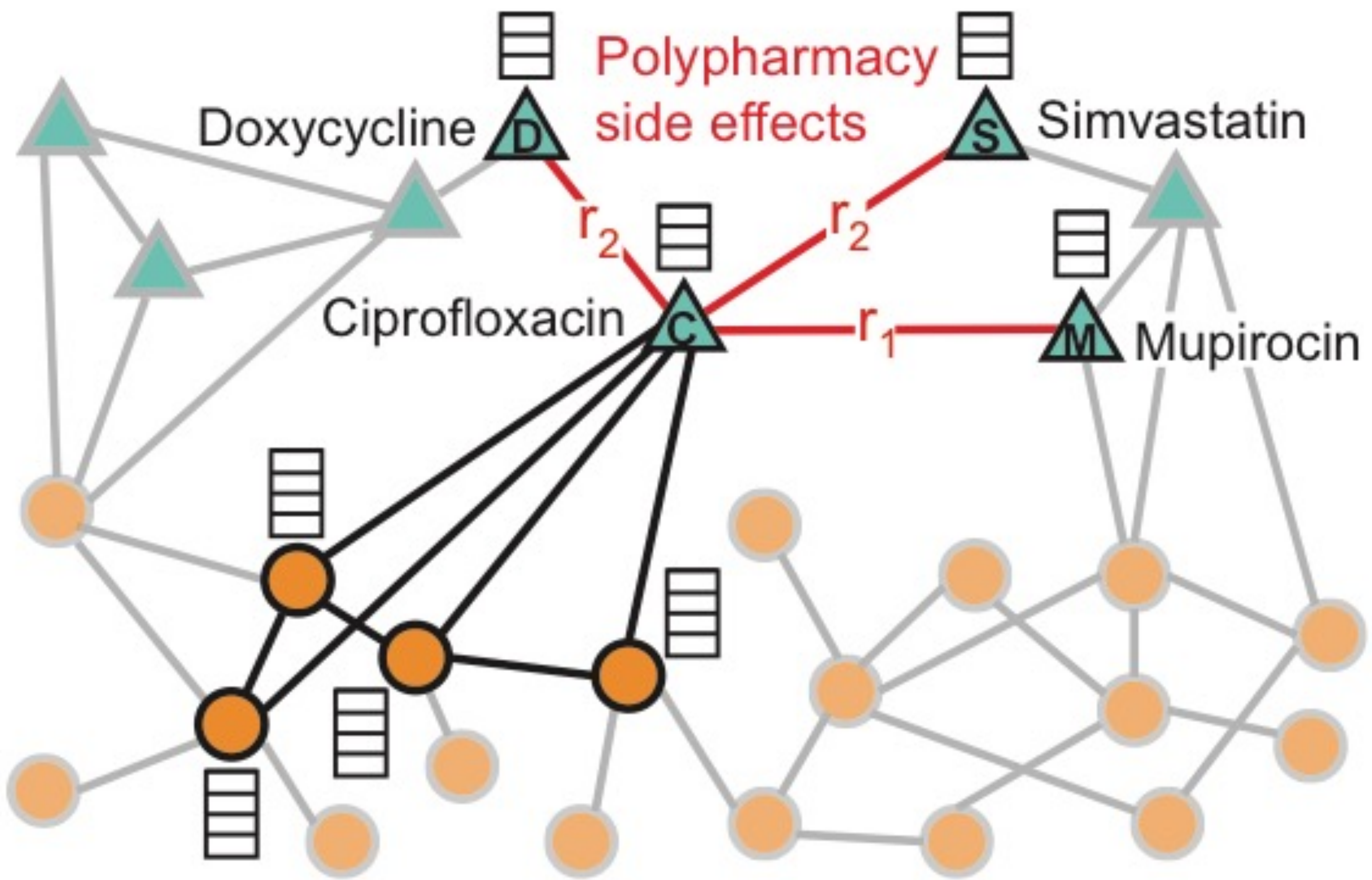
System-level prediction

Topological Neural Networks extend Graph Neural Networks

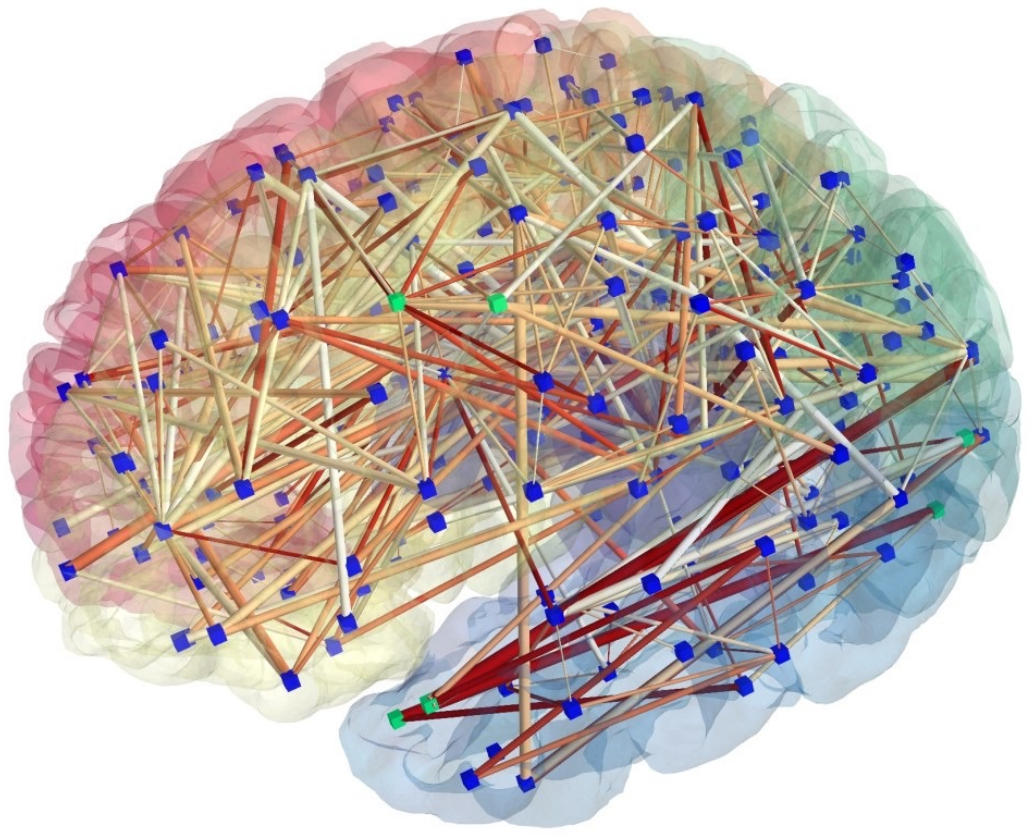
by leveraging non-binary relations
to give "better" answers & answer more questions.



Node-level prediction



Edge-level prediction



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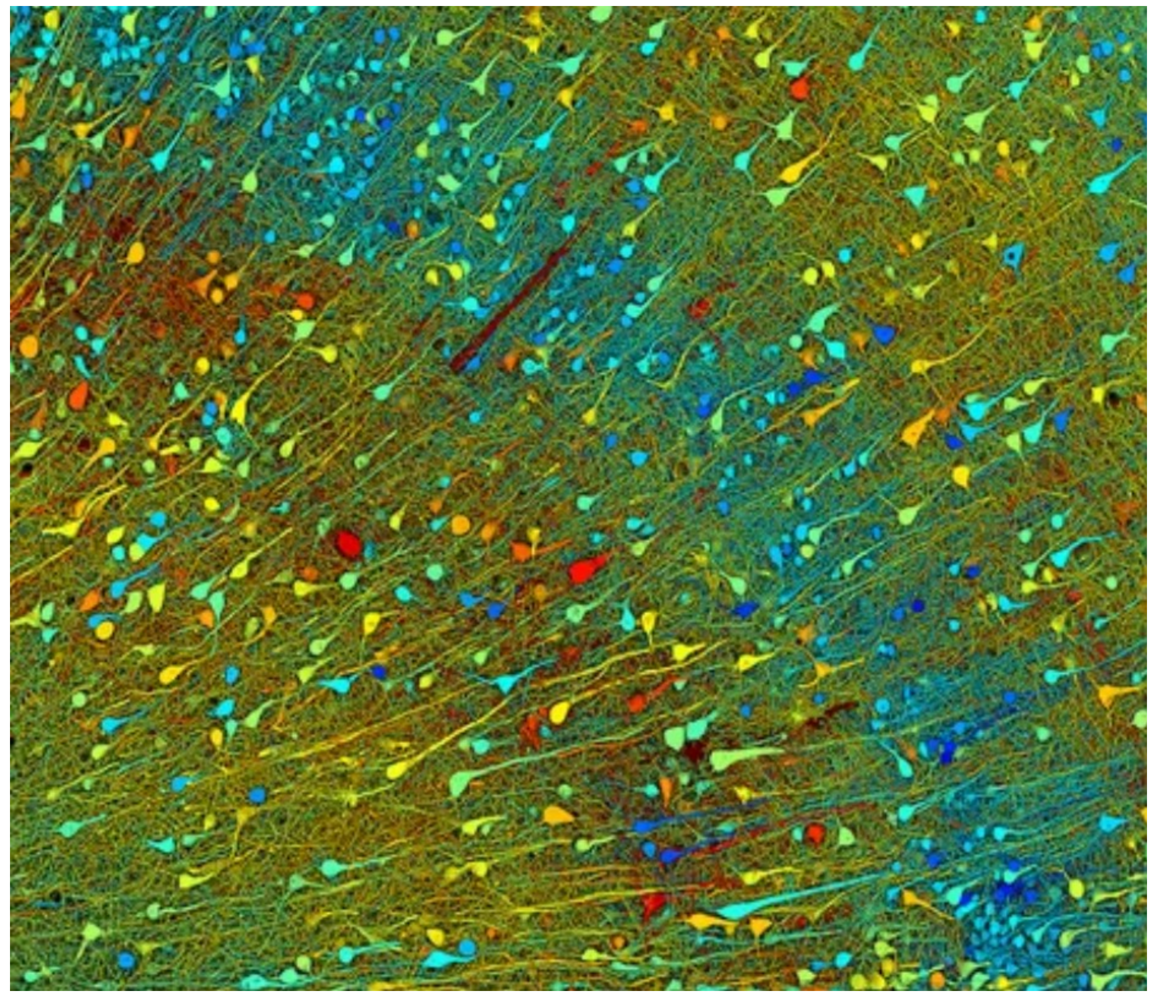
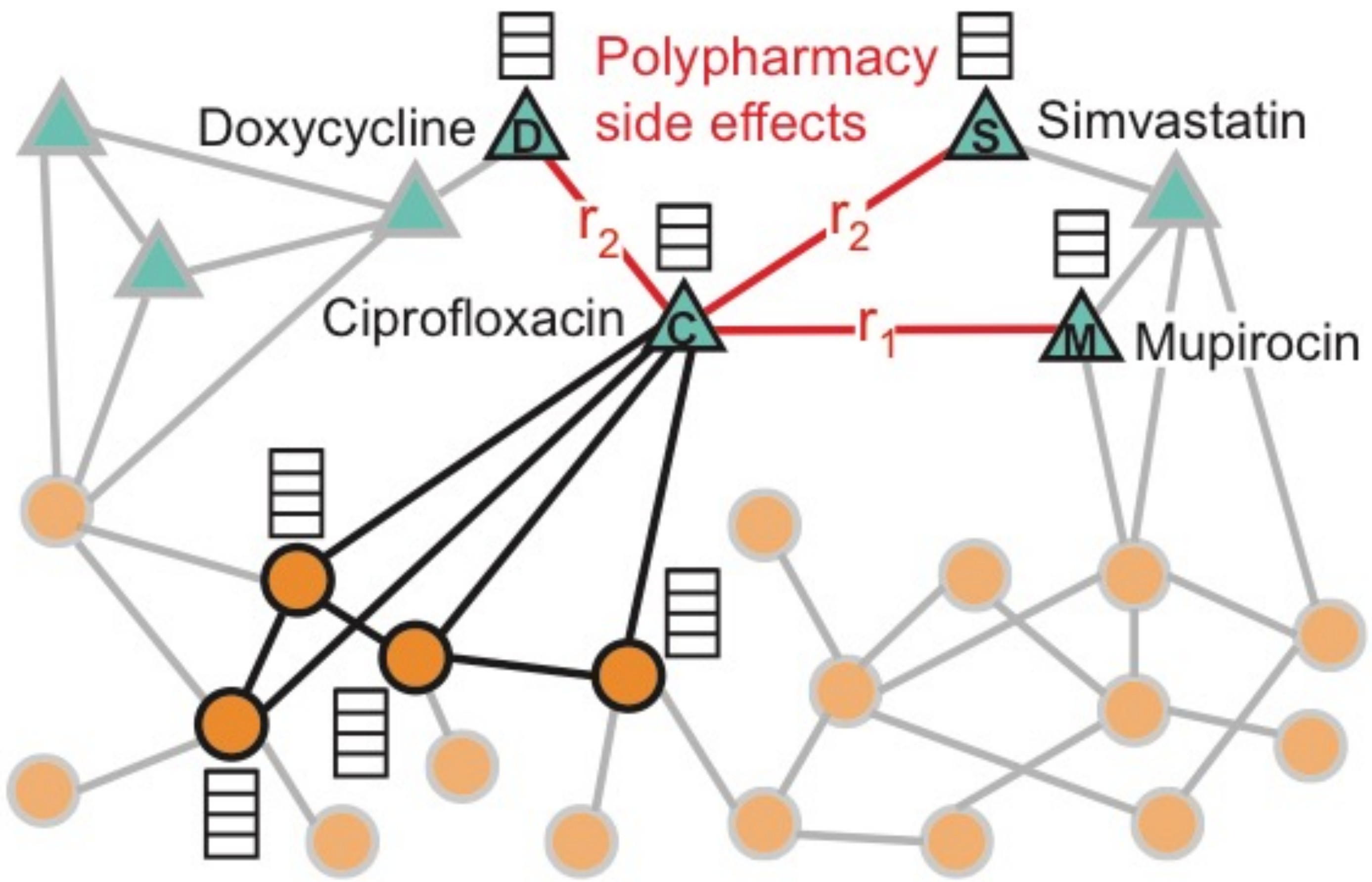
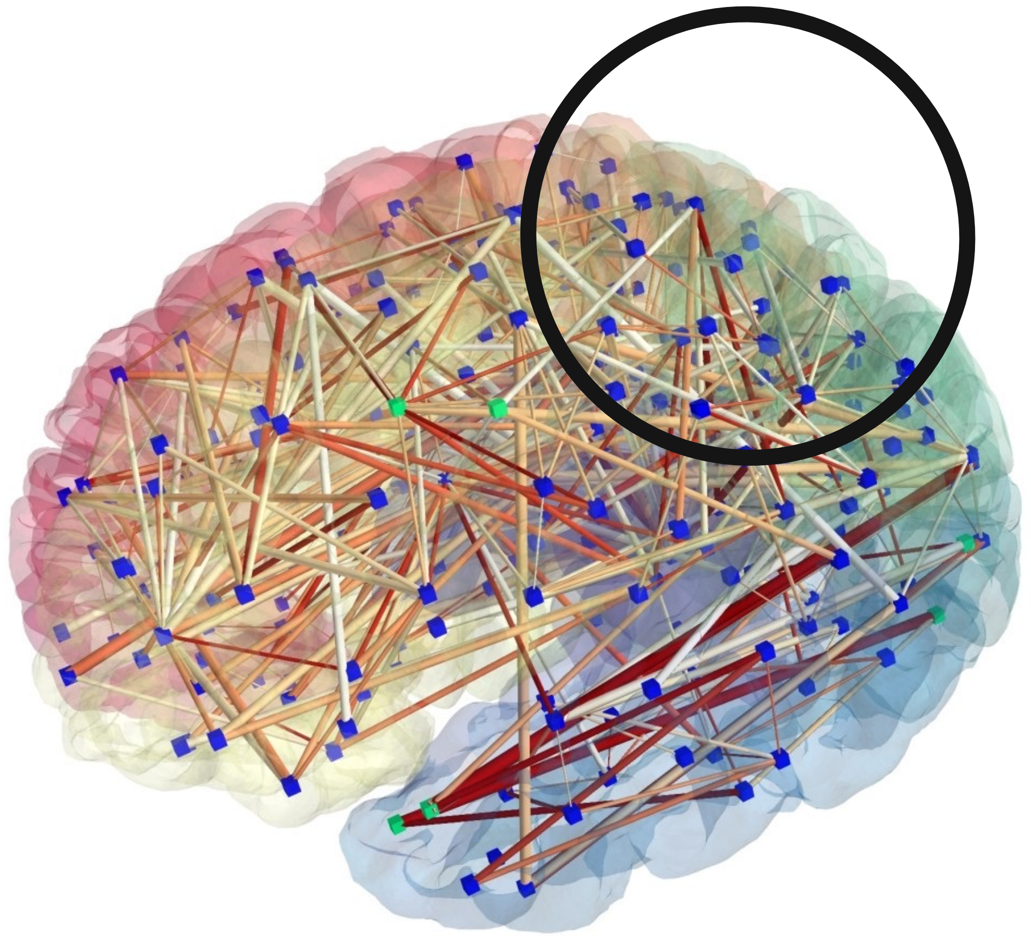


Node-level prediction



Edge-level prediction



System-level prediction

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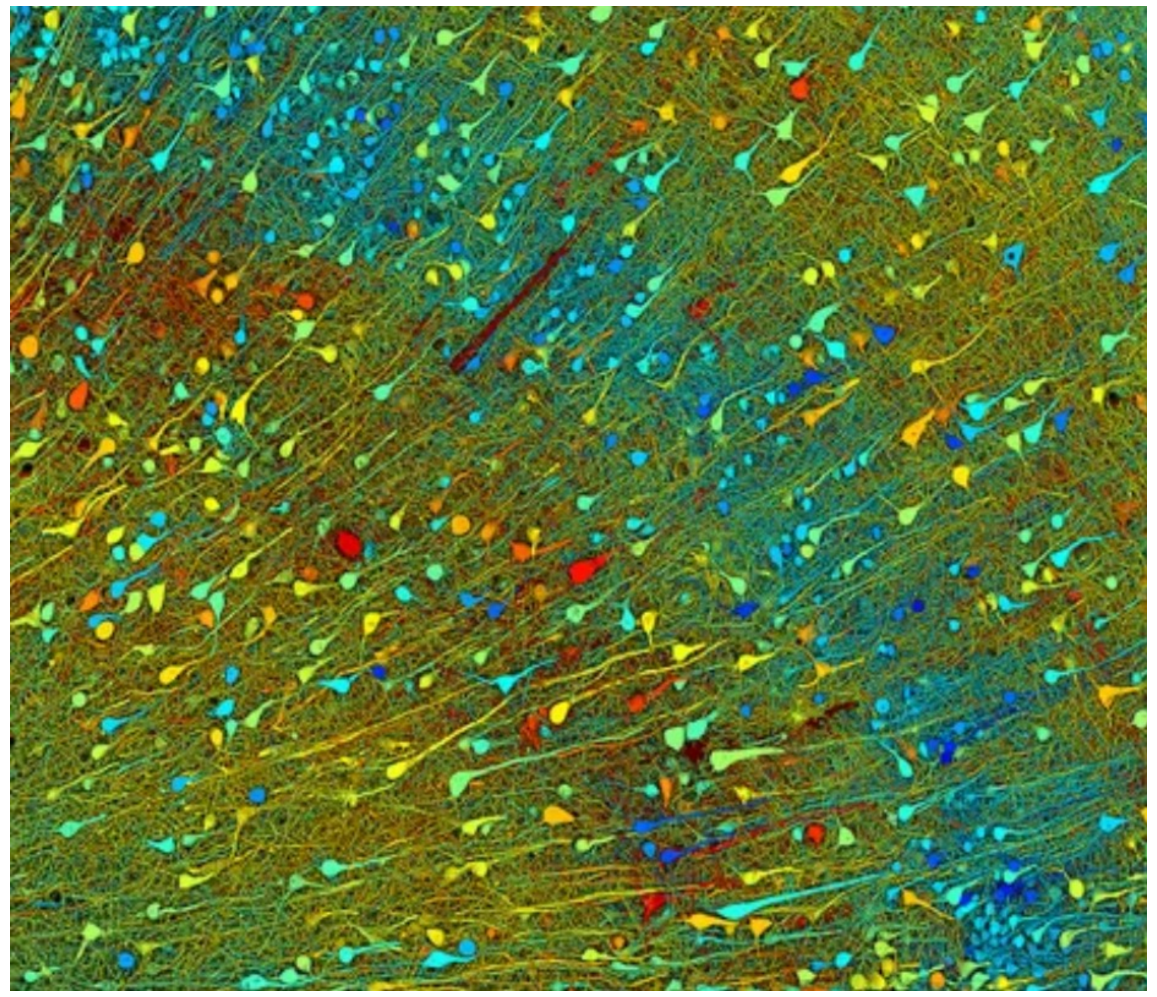

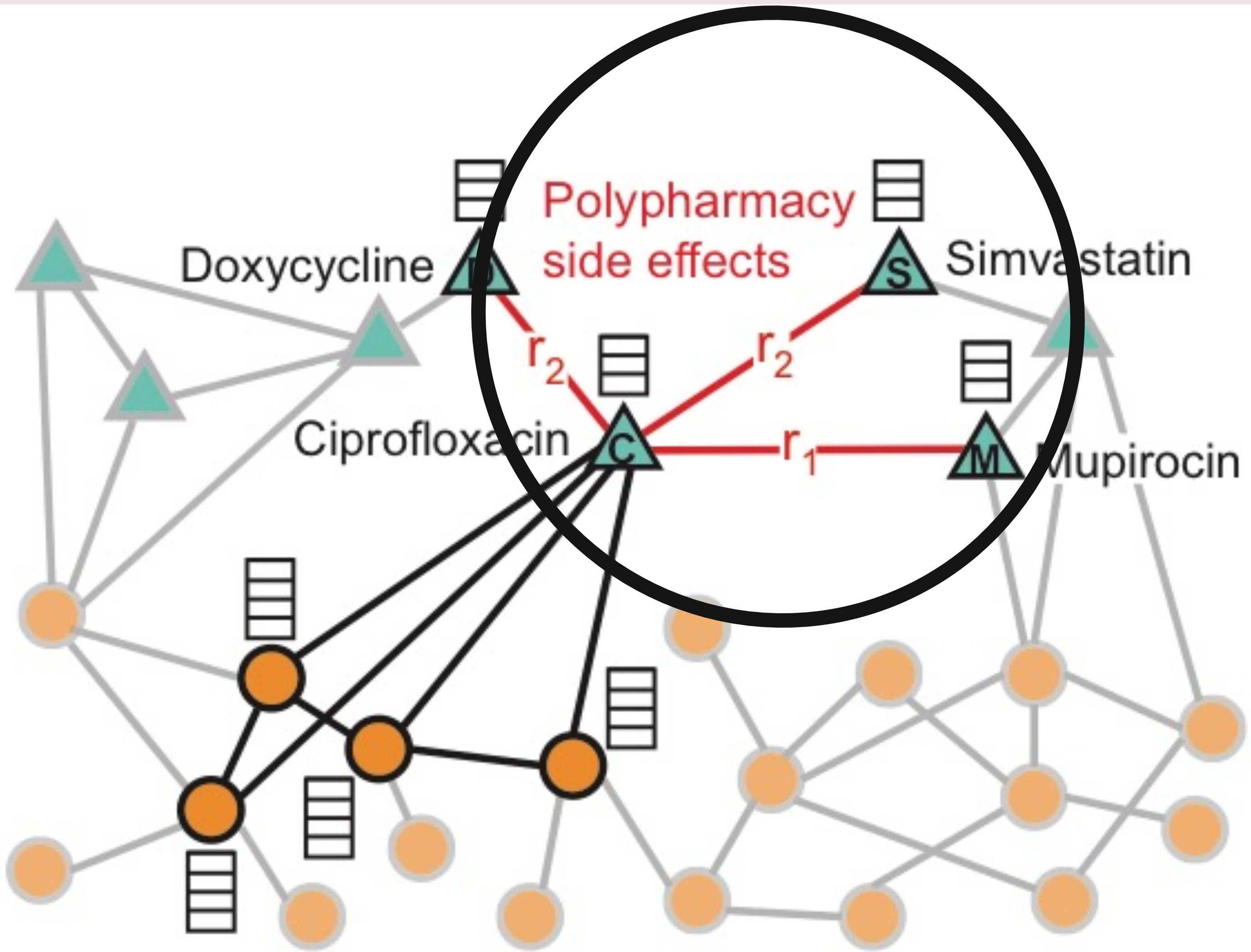

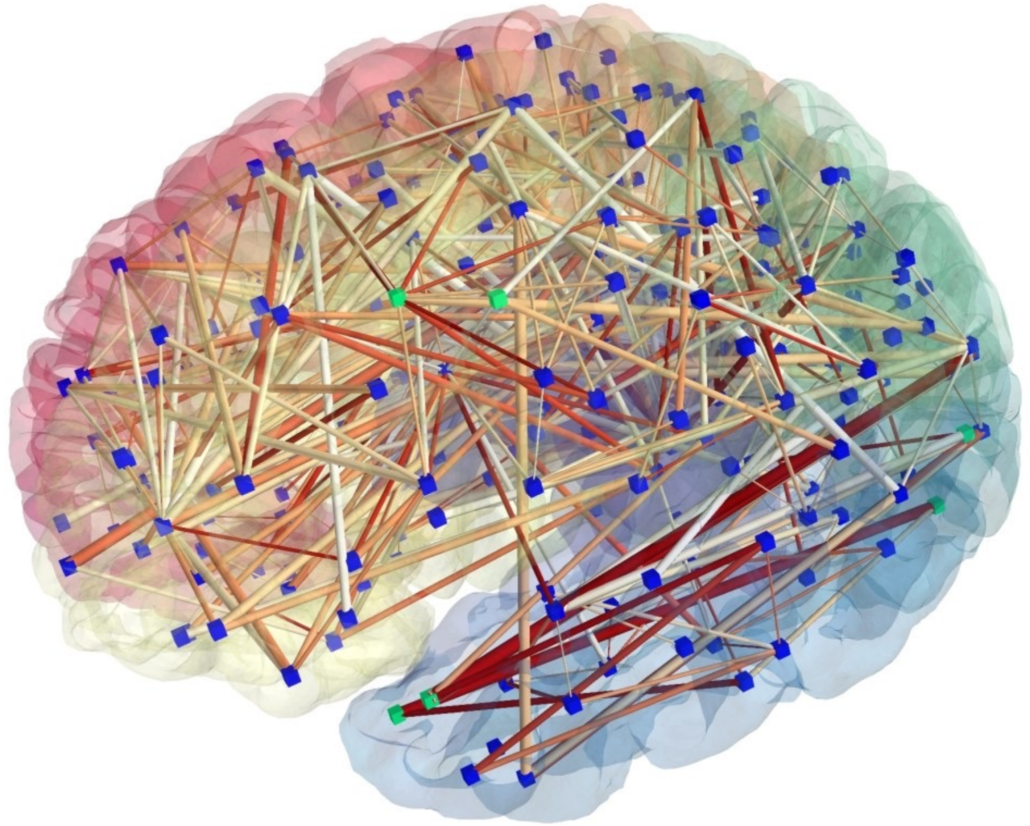

What is the interaction resulting from taking these four drugs?

Topological Neural Networks extend <u>Graph Neural Networks</u>

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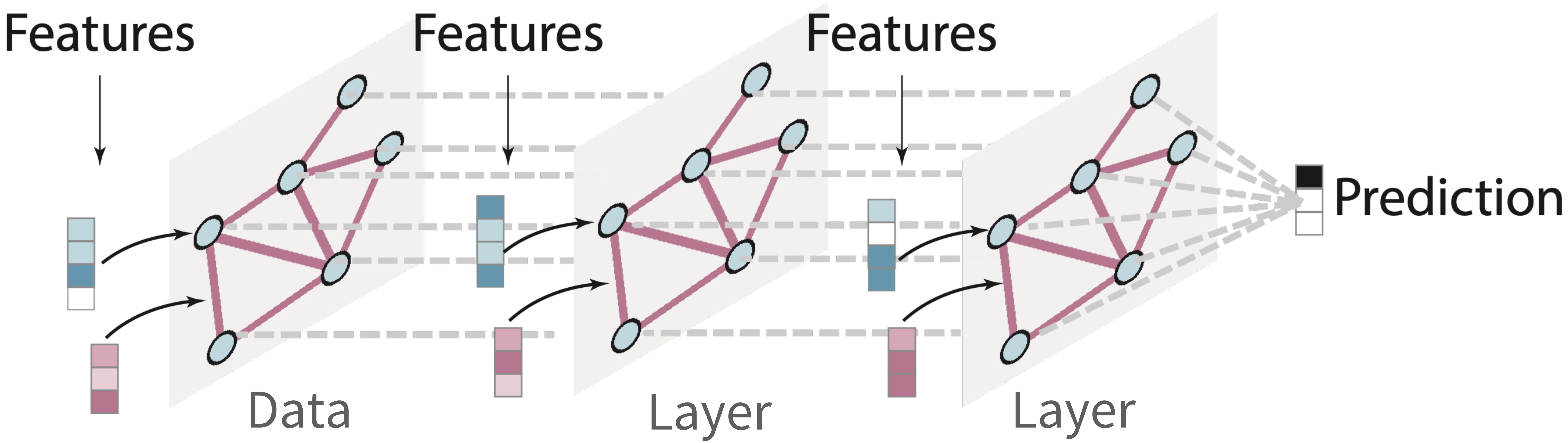
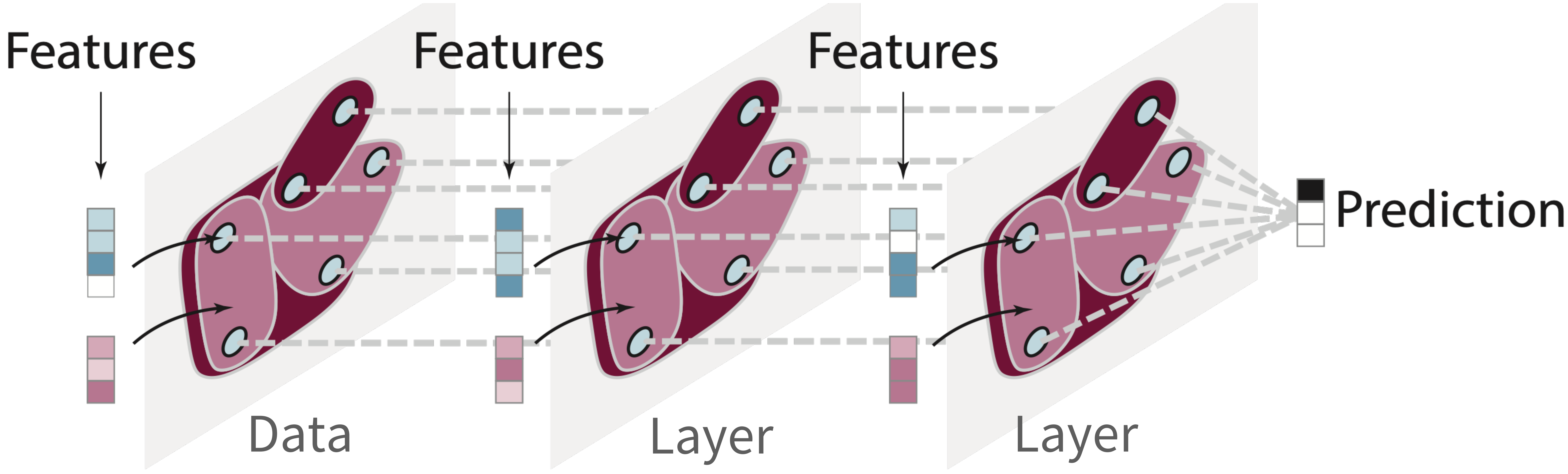


Topological Neural Networks
extend Graph Neural Networks



Why do we need a literature review of TNNs?

Mass confusion #1
An important distinction

[1] Hensel, Moor, Rieck. A Survey of Topological Machine Learning Methods. Frontiers in AI (2021).
[2] Horn, de Brouwer, Moor, Moreau, Rieck, Borgwardt. Topological Graph Neural Networks. ICLR (2022).

Mass confusion #2
Notation chaos

$$m_{\mathcal{B}}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{B}(\sigma)}\left(M_{\mathcal{B}}\left(h_\sigma^t, h_\tau^t\right)\right)$$
$$m_{\mathcal{C}}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{C}(\sigma)}\left(M_{\mathcal{C}}\left(h_\sigma^t, h_\tau^t\right)\right)$$
$$m_{\downarrow}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{N}_\downarrow(\sigma)}\left(M_{\downarrow}\left(h_\sigma^t, h_\tau^t, h_{\sigma\cap\tau}^t\right)\right)$$
$$m_{\uparrow}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{N}_\uparrow(\sigma)}\left(M_{\uparrow}\left(h_\sigma^t, h_\tau^t, h_{\sigma\cup\tau}^t\right)\right)$$
$$h_\sigma^{t+1} = U\left(h_\sigma^t, m_{\mathcal{B}}^t(\sigma), m_{\mathcal{C}}^t(\sigma), m_{\downarrow}^{t+1}(\sigma), m_{\uparrow}^{t+1}(\sigma)\right)$$

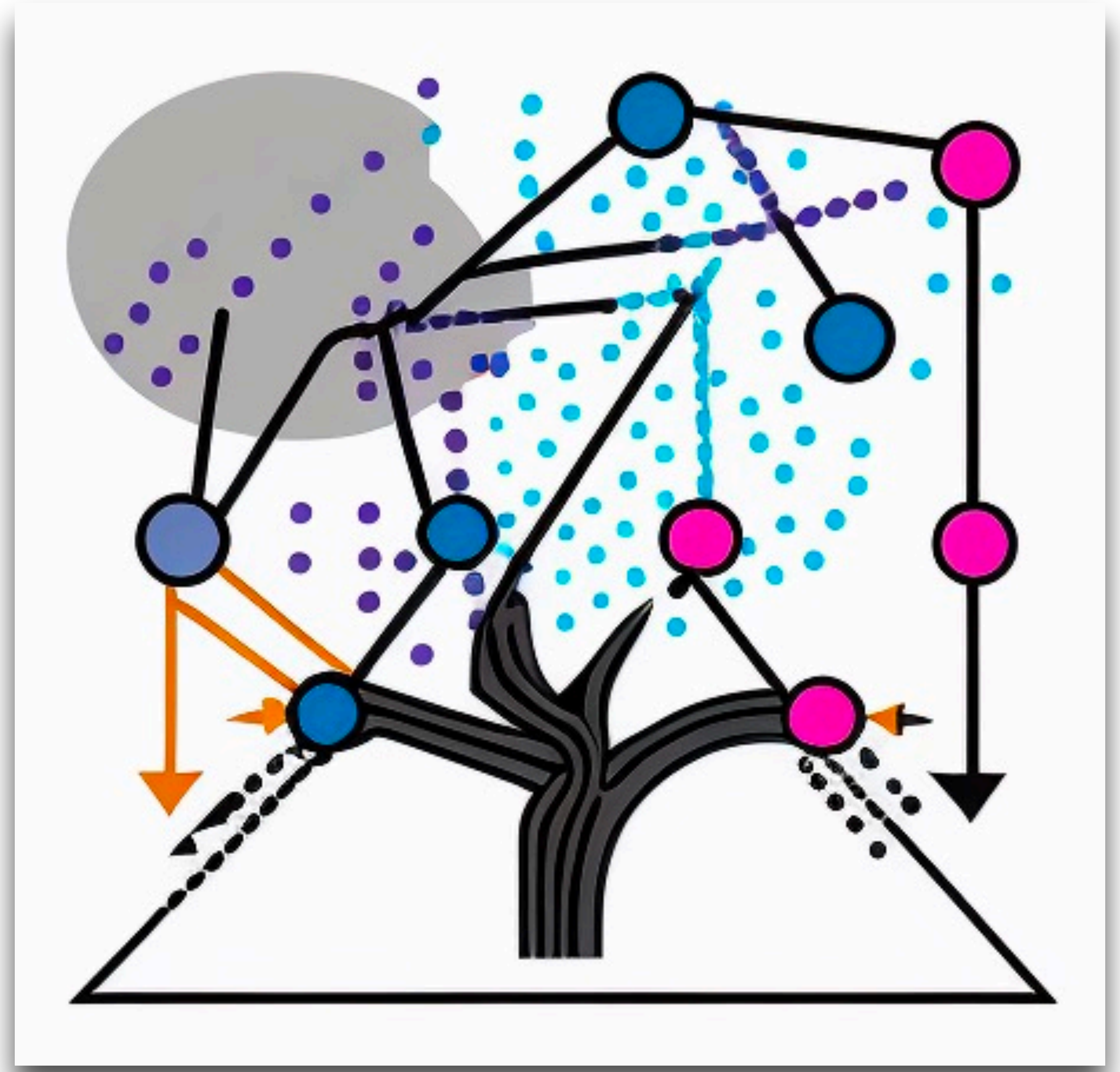
$$\mathcal{F}_p^{-1}\left(\varphi_W\right) *_p c = \textstyle\sum_{i=0}^N W_i U \operatorname{diag}\left(\Lambda^i\right) U^\top c =$$
$$\textstyle\sum_{i=0}^N W_i \left(U \operatorname{diag}(\Lambda) U^\top\right)^i c = \sum_{i=0}^N W_i L_p^i c$$

$$\psi\left(M_n H_n^{\text{in}} W_n + U_n H_{n-1}^{\text{in}} W_{n-1} + O_n H_{n+1}^{\text{in}} W_{n+1}\right)$$

$$X_0^{(h+1)} = \sigma\left(\mathbf{D}_1^{-1}\mathbf{B}_1 X_1^{(h)} W_{0,1}^{(h)} + \widetilde{\mathbf{A}}_0^u X_0^{(h)} W_{0,0}^{(h)}\right)$$
$$X_1^{(h+1)} =$$
$$\sigma\left(\mathbf{B}_2\mathbf{D}_3 X_2^{(h)} W_{1,2}^{(h)} + \left(\widetilde{\mathbf{A}}_1^d + \widetilde{\mathbf{A}}_1^u\right) X_1^{(h)} W_{1,1}^{(h)} + \mathbf{D}_2\mathbf{B}_1^*\mathbf{D}_1^{-1} X_0^{(h)} W_{1,0}^{(h)}\right)$$
$$X_2^{(h+1)} = \sigma\left(\widetilde{\mathbf{A}}_2^d X_2^{(h)} W_{2,2}^{(h)} + \mathbf{D}_4\mathbf{B}_2^*\mathbf{D}_5^{-1} X_1^{(h)} W_{2,1}^{(h)}\right)$$

$$\boldsymbol{x}^1 = \left(\textstyle\sum_{k=1}^{K_l} a_k^I (\mathbf{L}_1^l)^k + \sum_{k=1}^{K_u} a_k^s (\mathbf{L}_1^u)^k\right)\boldsymbol{s}^1$$

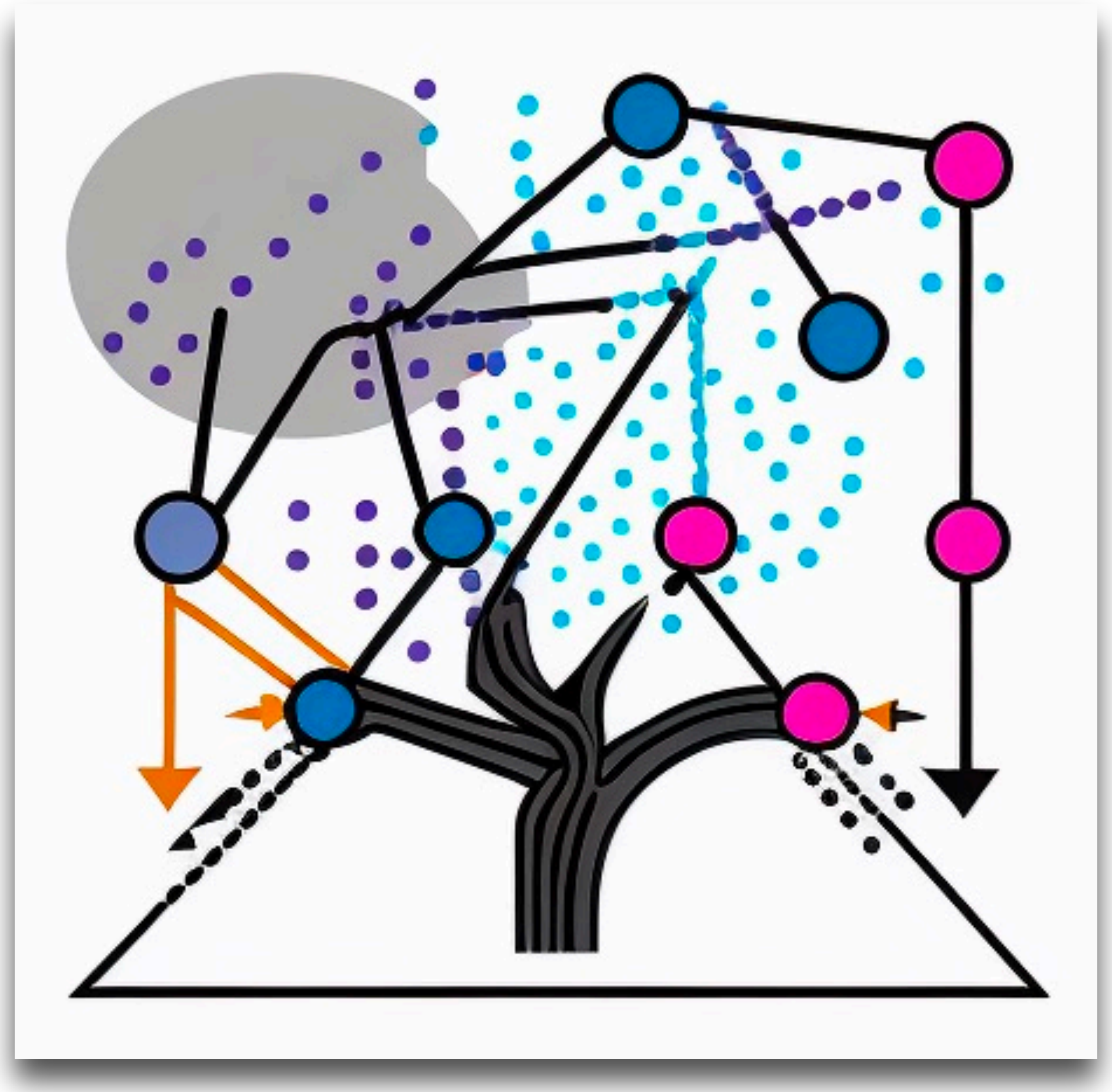
Outline



Graphical Framework

Survey of the literature

Outline



Graphical Framework

1. Topological domain
2. Message passing mechanism

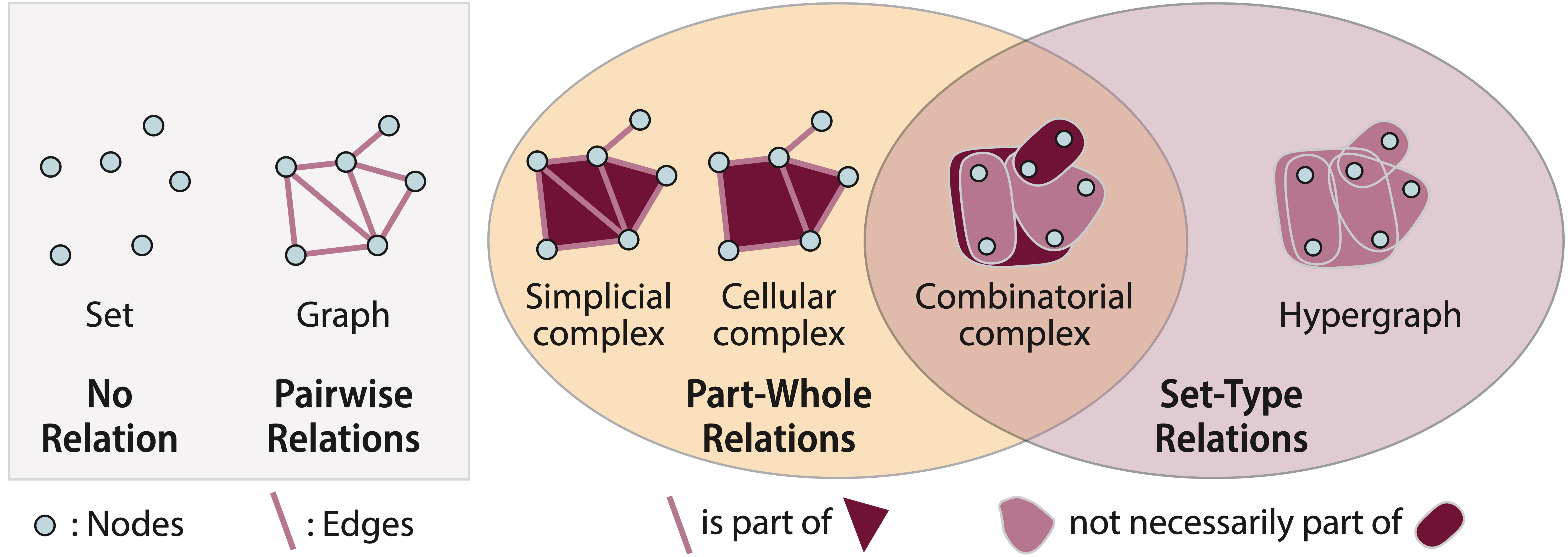
Survey of the literature

1. Topological Domain

The Framework

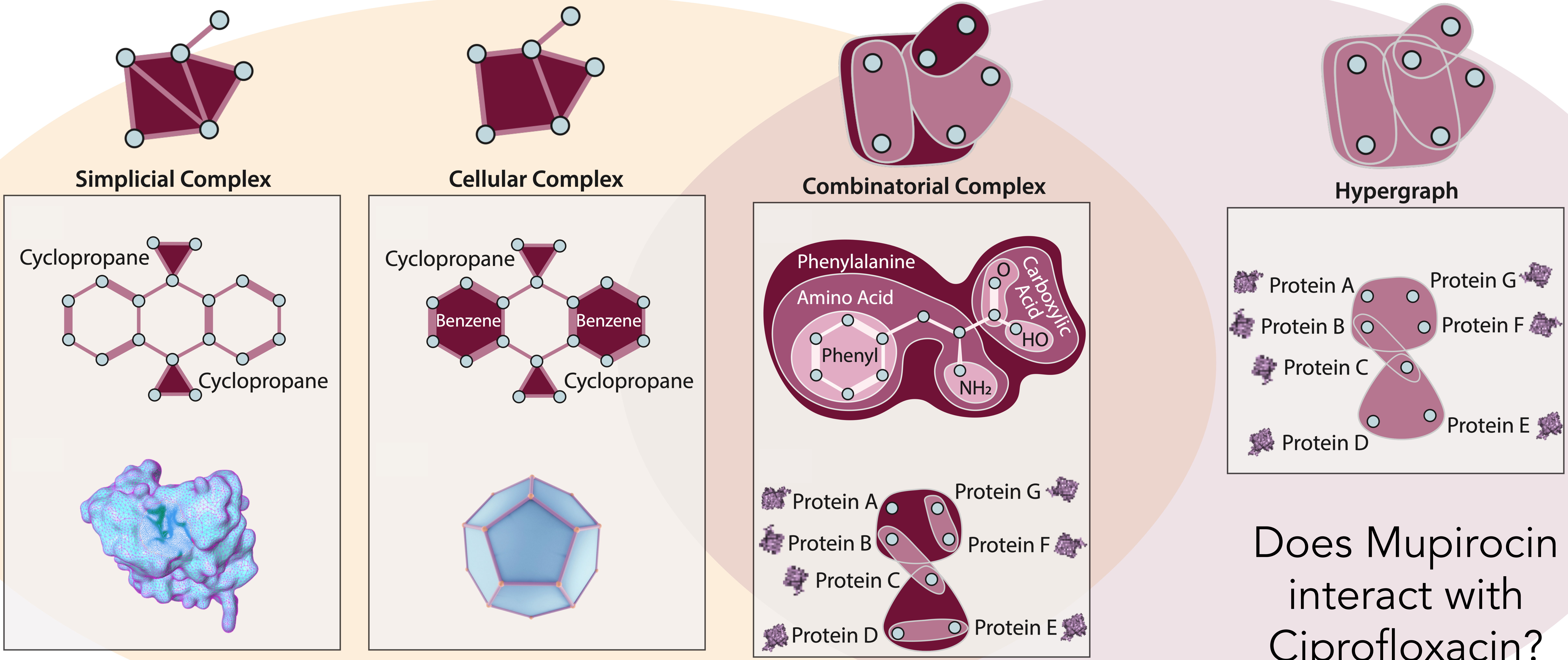
Traditional Discrete Domains

Domains of Topological Deep Learning



How to Choose?

1. Topological Domain



Does Mupirocin interact with Ciprofloxacin?

What are the properties of this molecule?

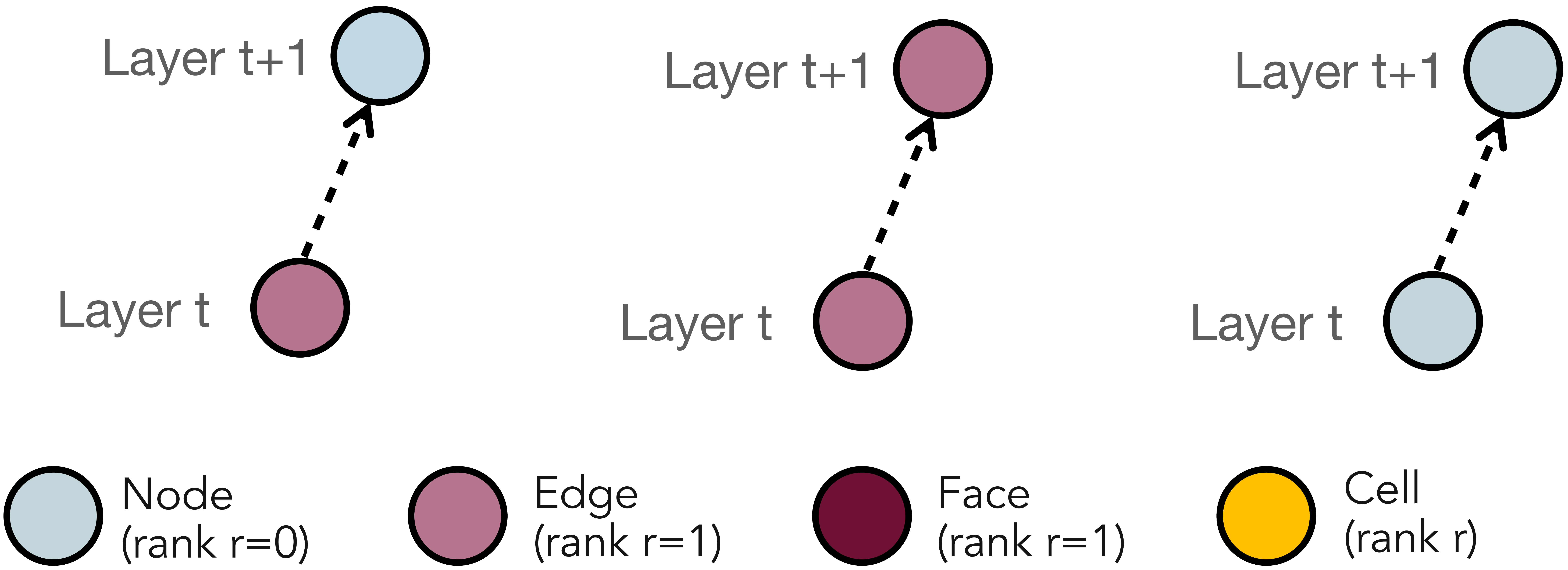
The Framework

2. Mechanism: Message passing

The Framework

2. Mechanism: Message passing

Which "cells" send messages to which "cells":



The Framework

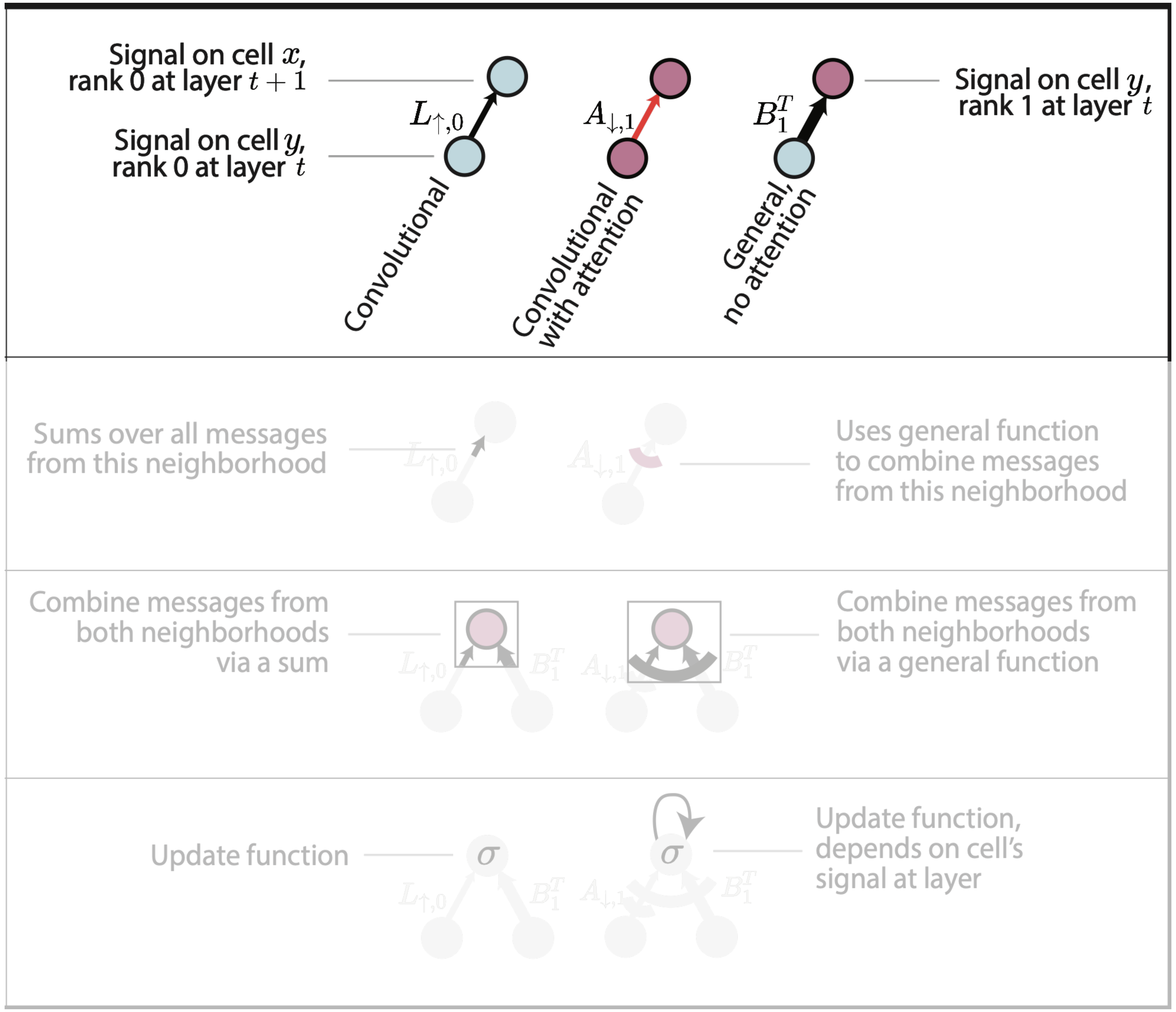
2. Mechanism: Message passing

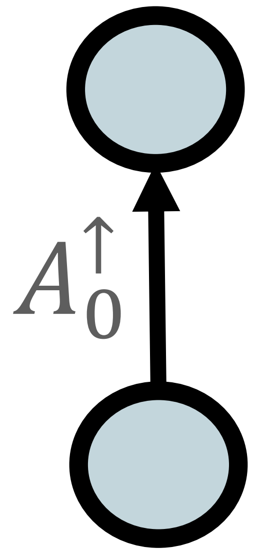
1. Define message

2. Aggregate intra-neighborhood

3. Aggregate inter-neighborhood

4. Update





Graph Convolutional Network

The Framework

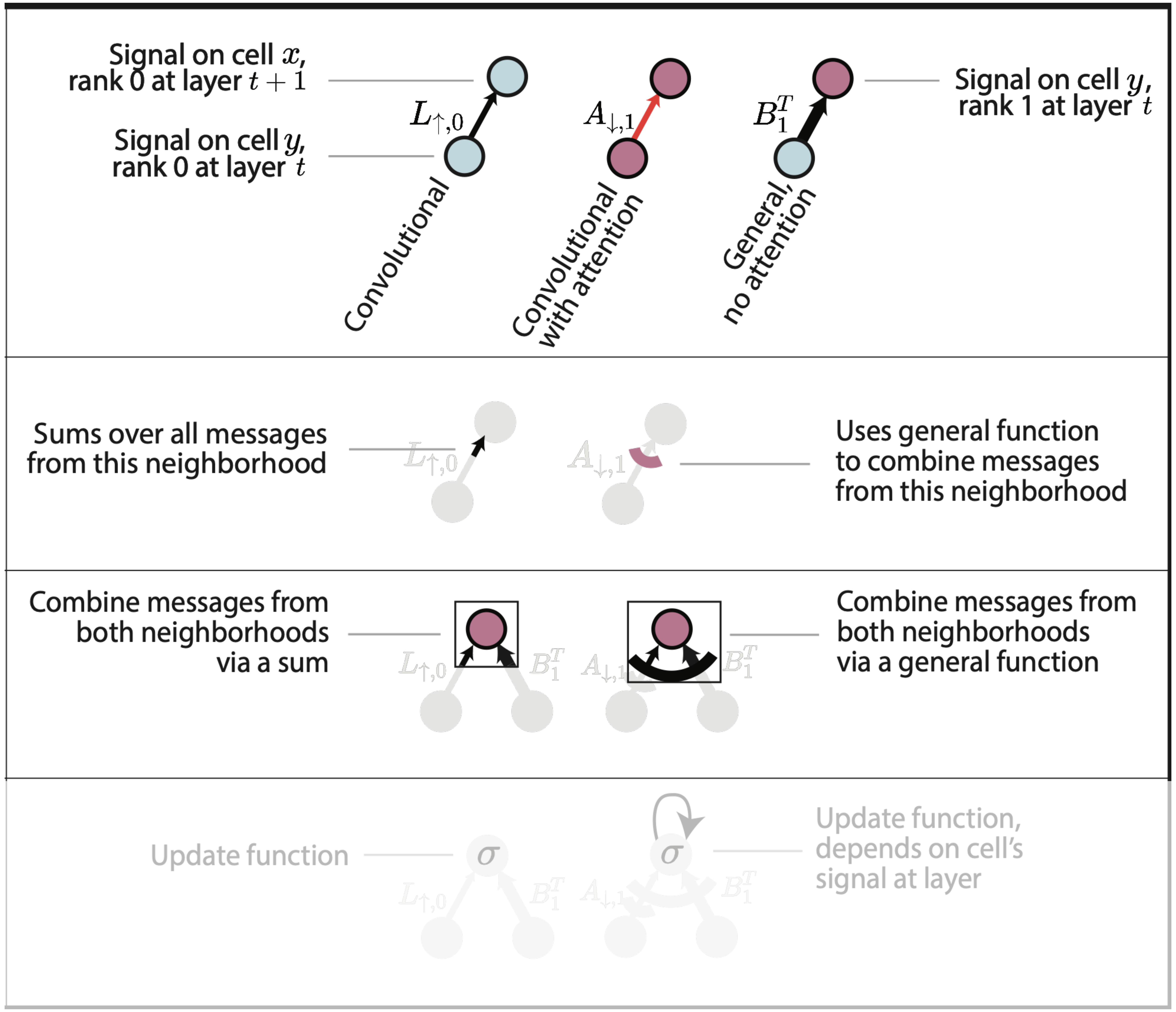
2. Mechanism: Message passing

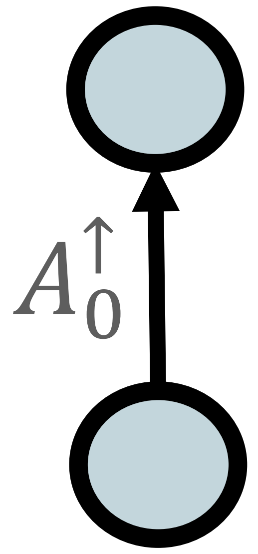
1. Define message

2. Aggregate intra-neighborhood

3. Aggregate inter-neighborhood

4. Update





Graph Convolutional Network

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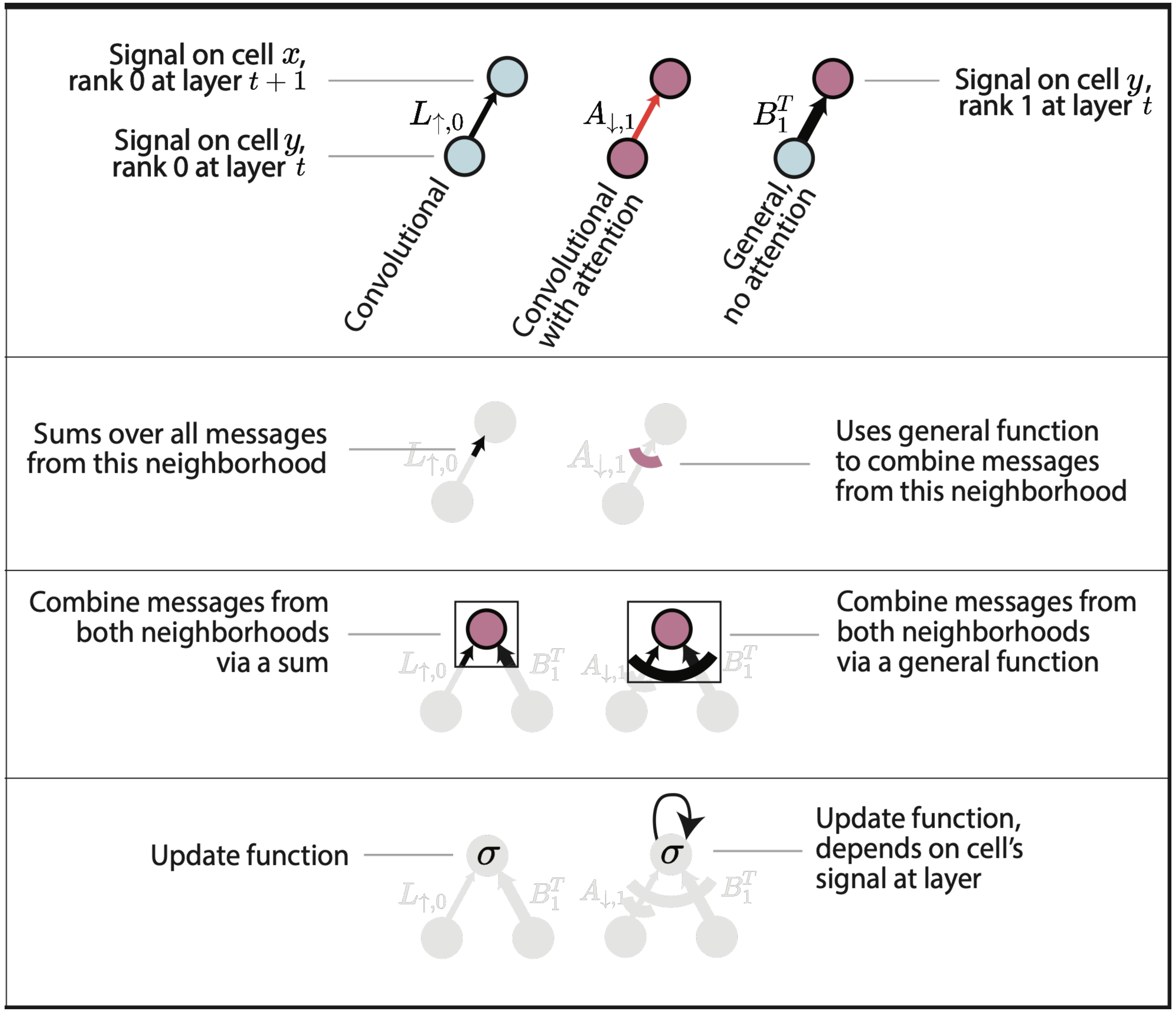

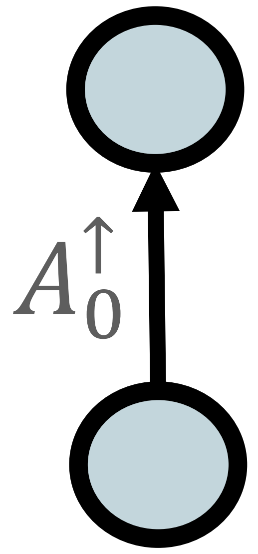

Graph Convolutional Network

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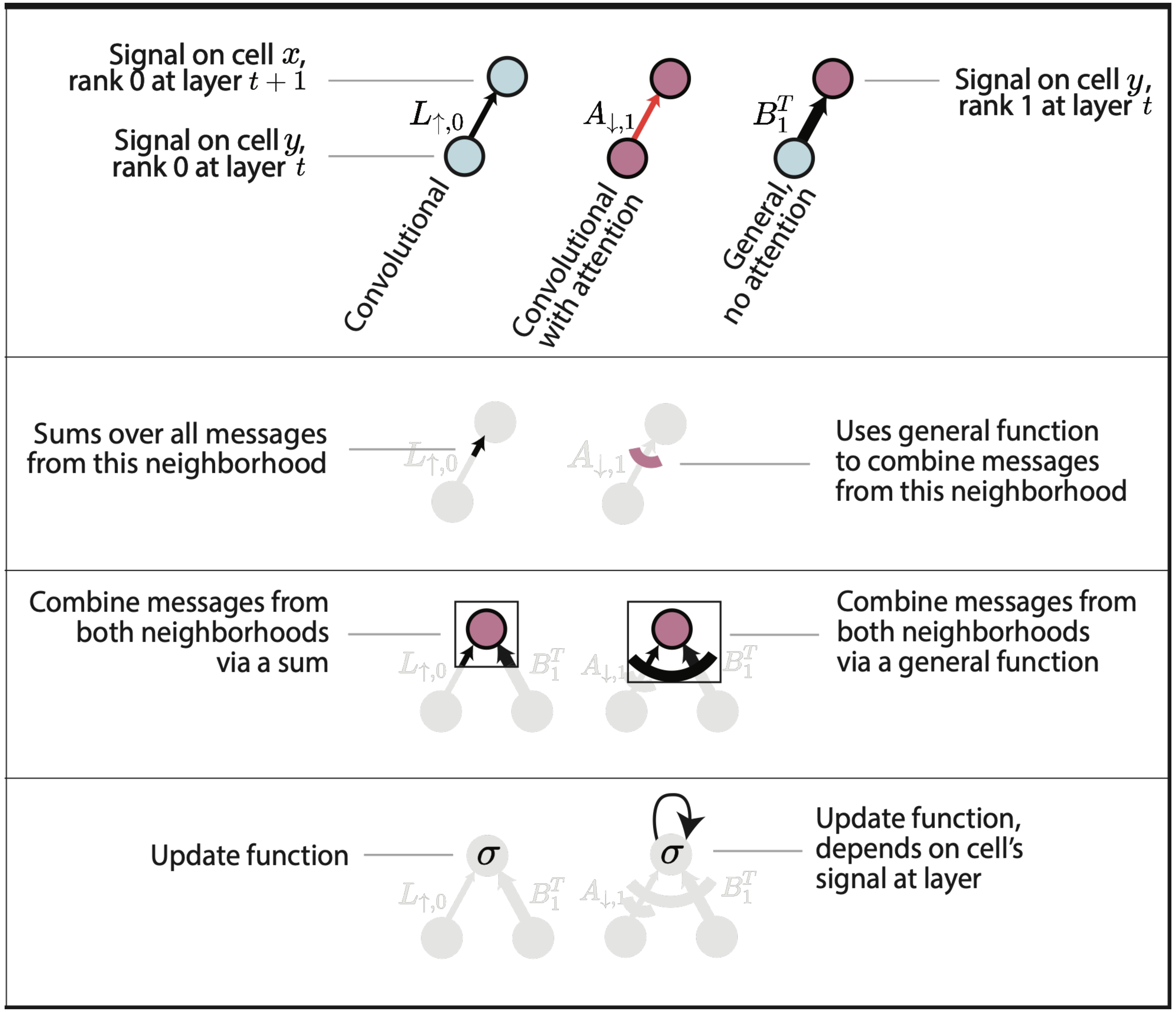
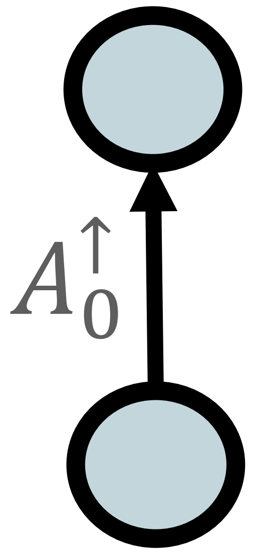
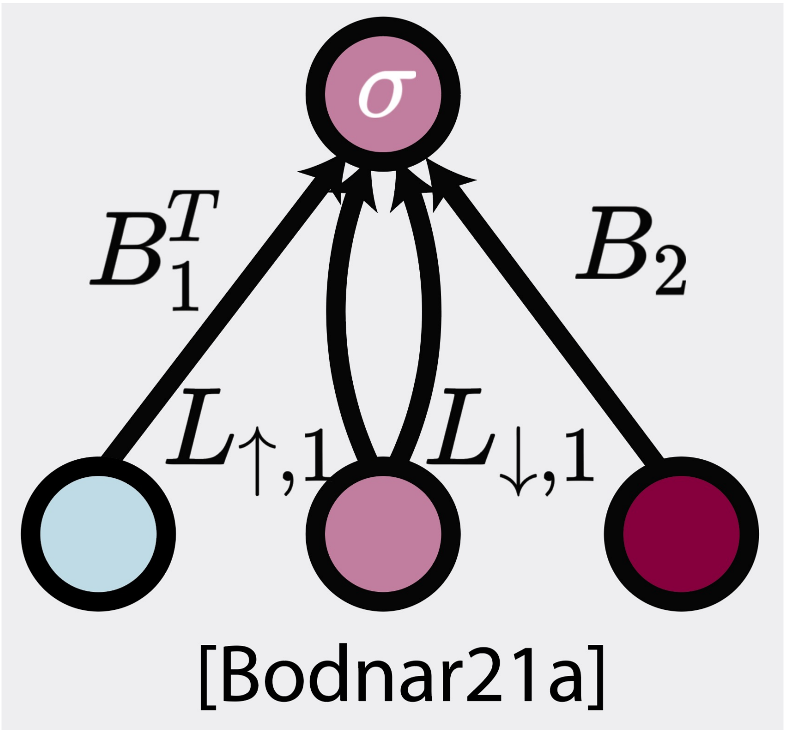


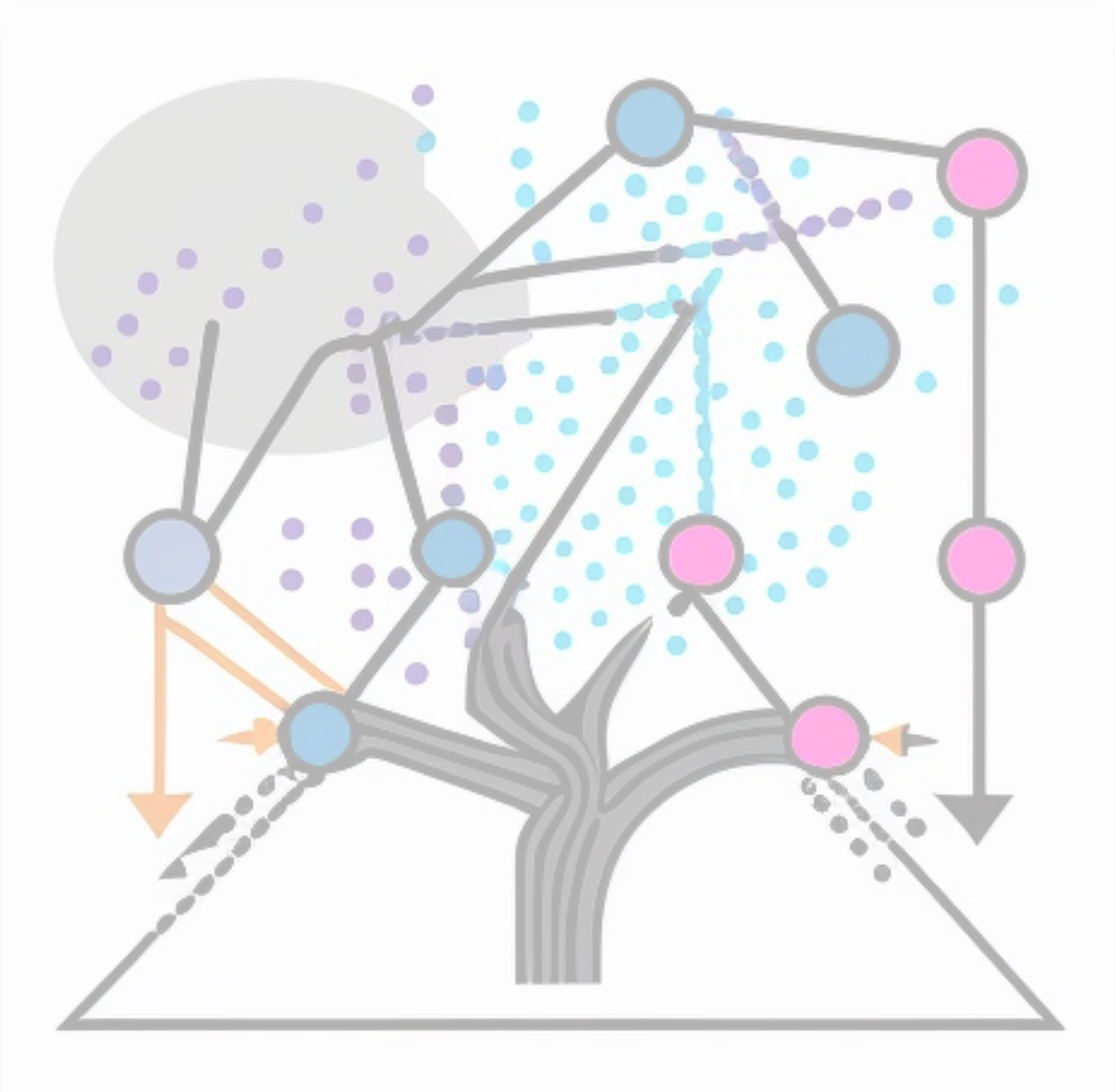


Graph Convolutional Network



Message Passing Simplicial Network

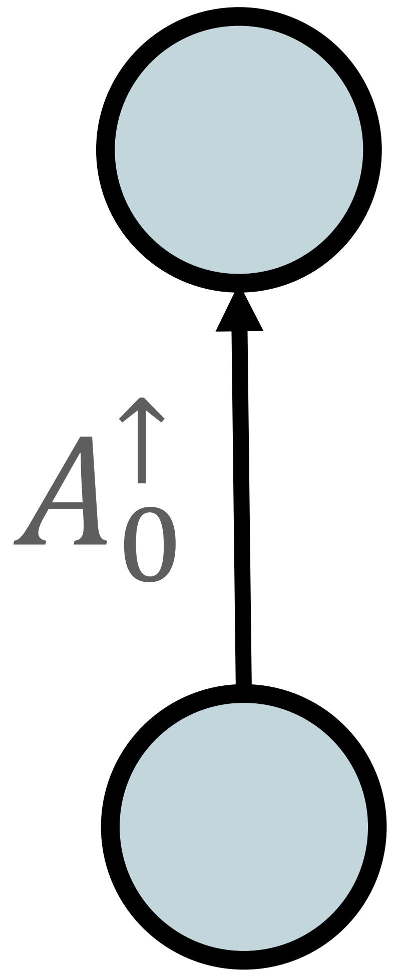
Outline

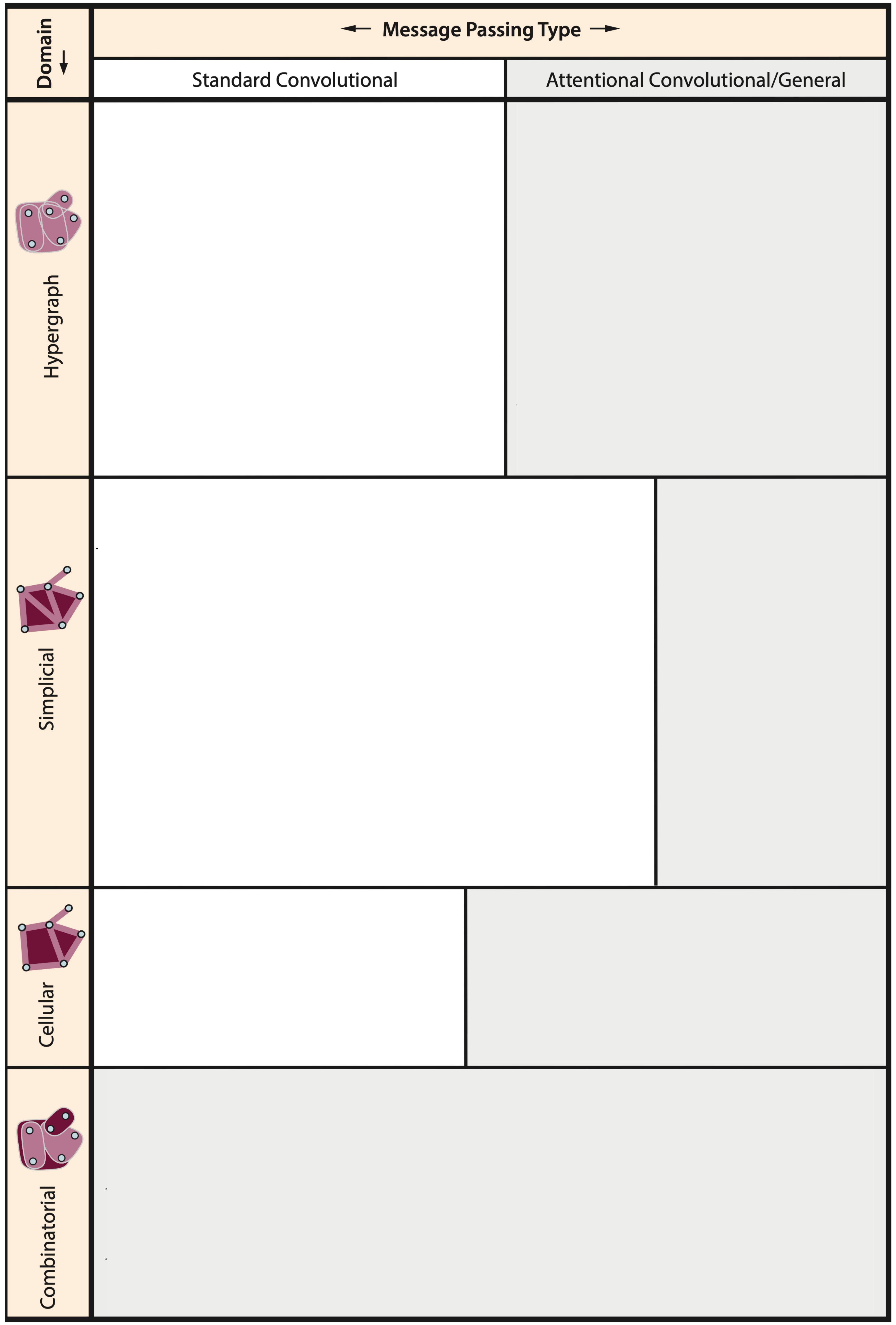


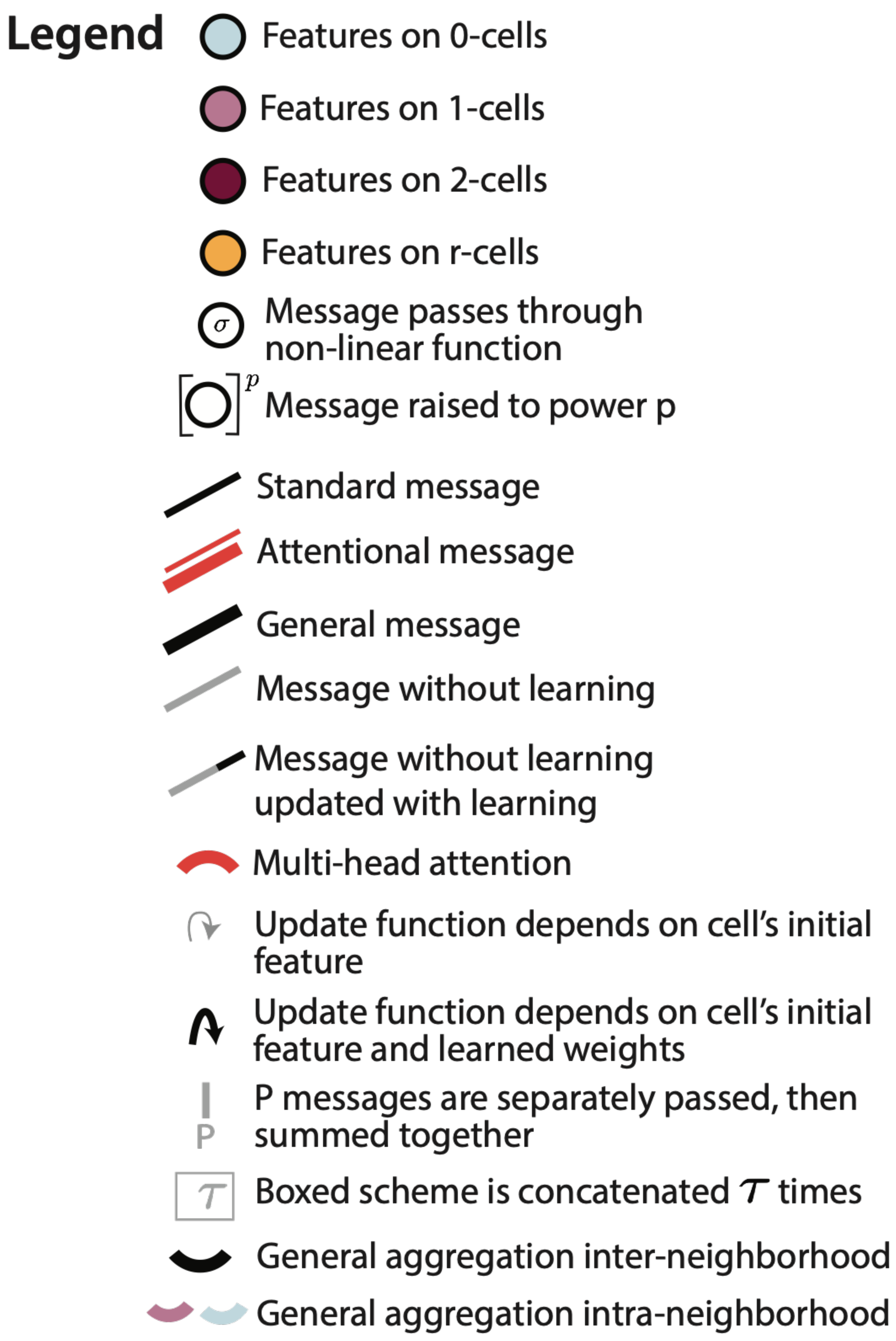
Graphical Framework

Survey of the literature

Beyond Graph Convolutional Network:







Survey of the literature

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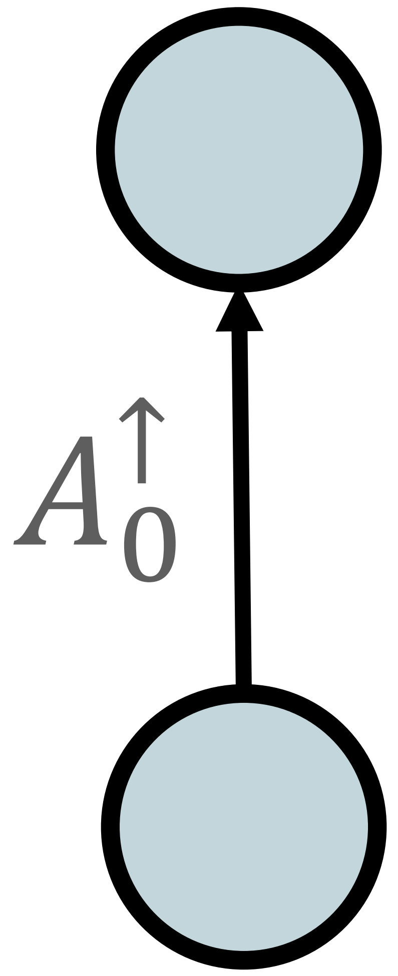
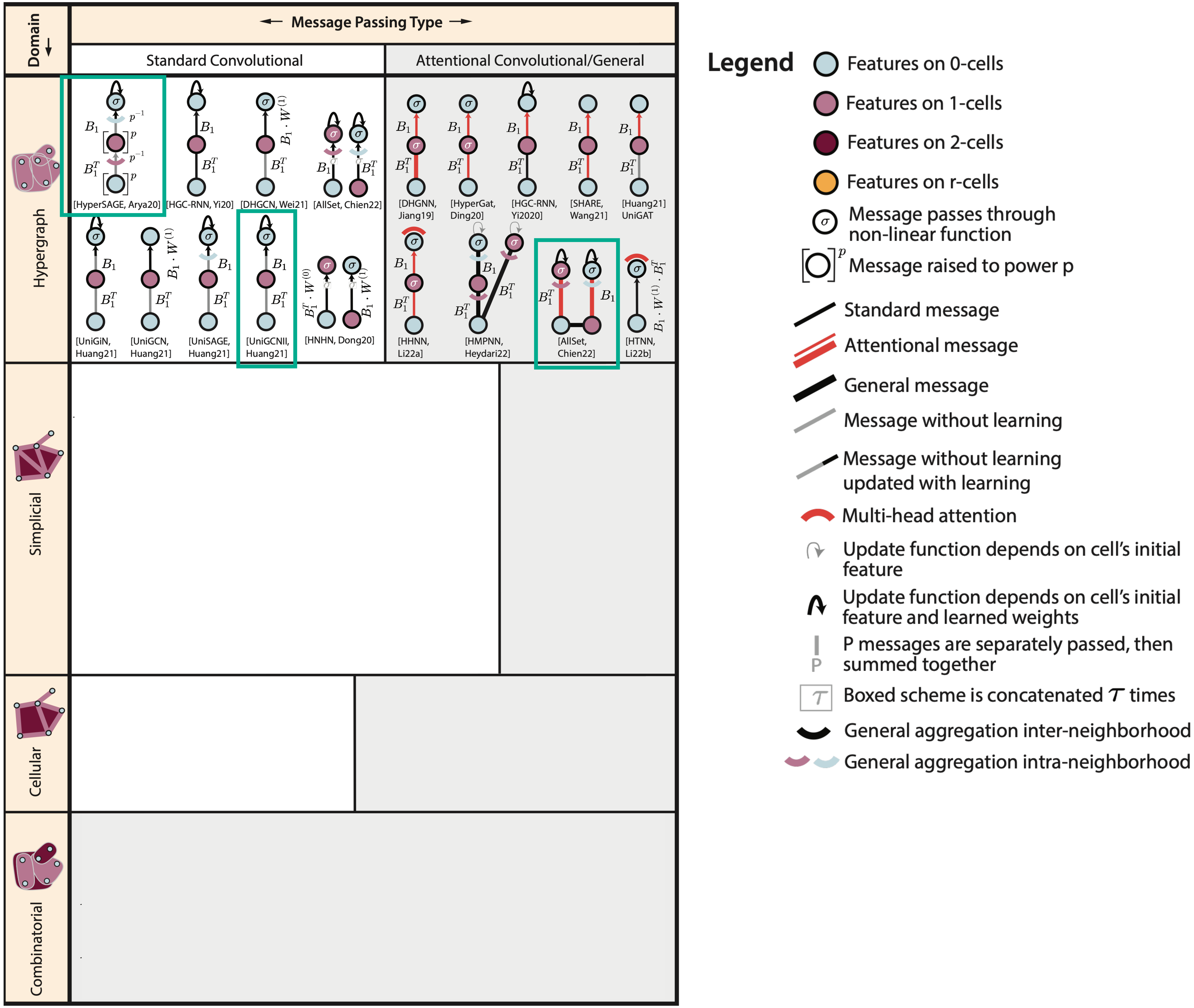
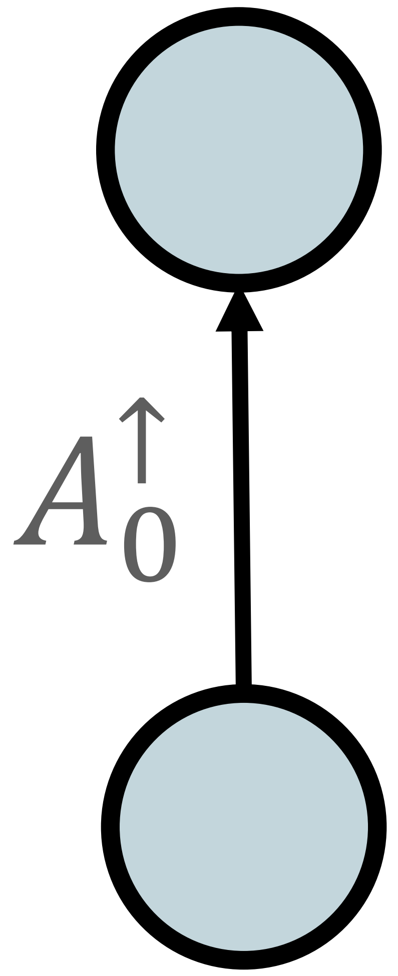
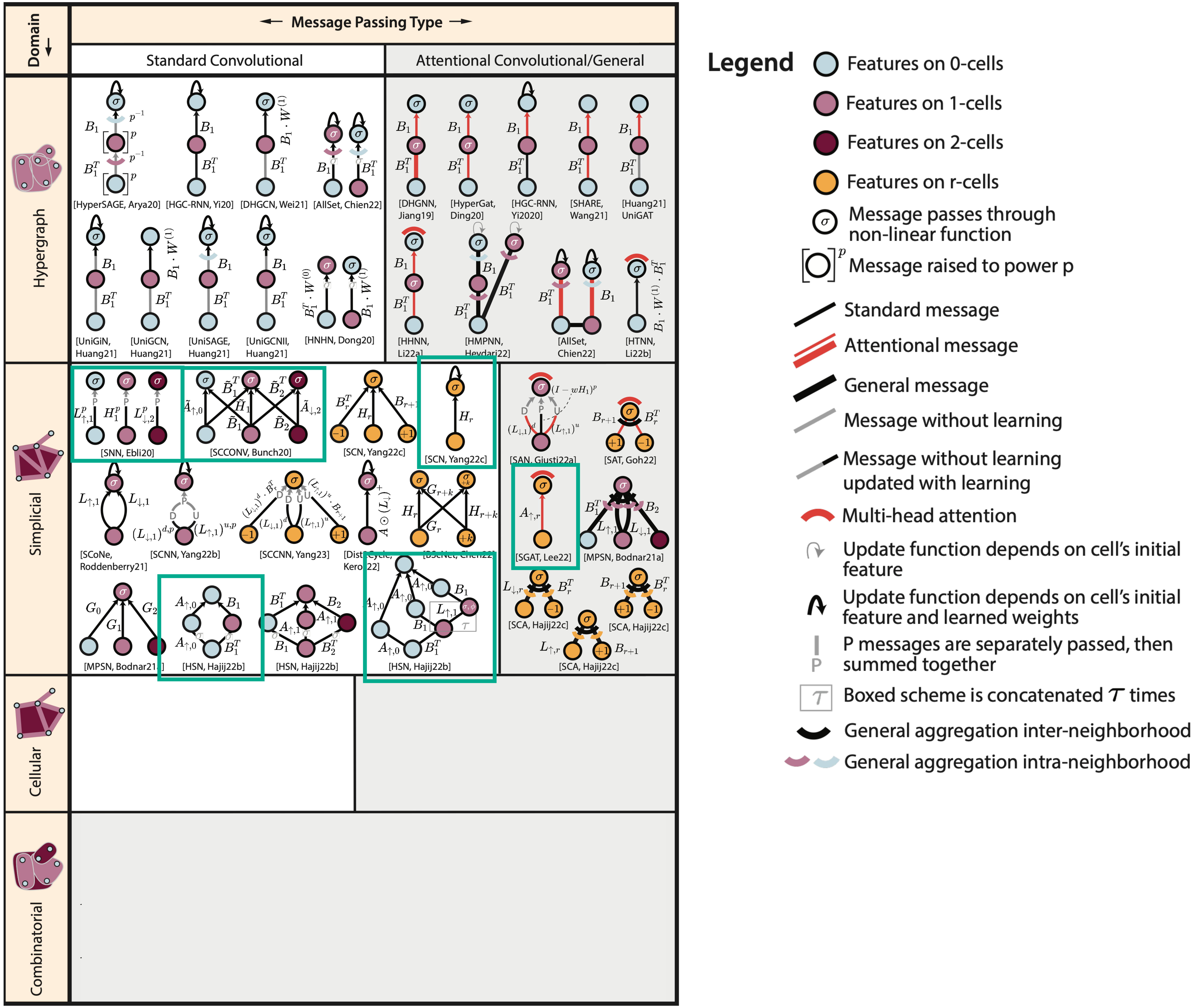




Survey of the literature

Beyond Graph Convolutional Network:





Survey of the literature

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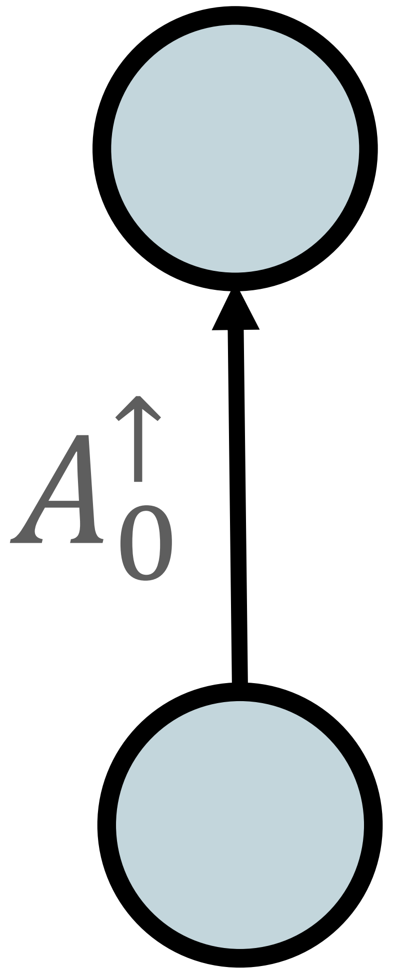
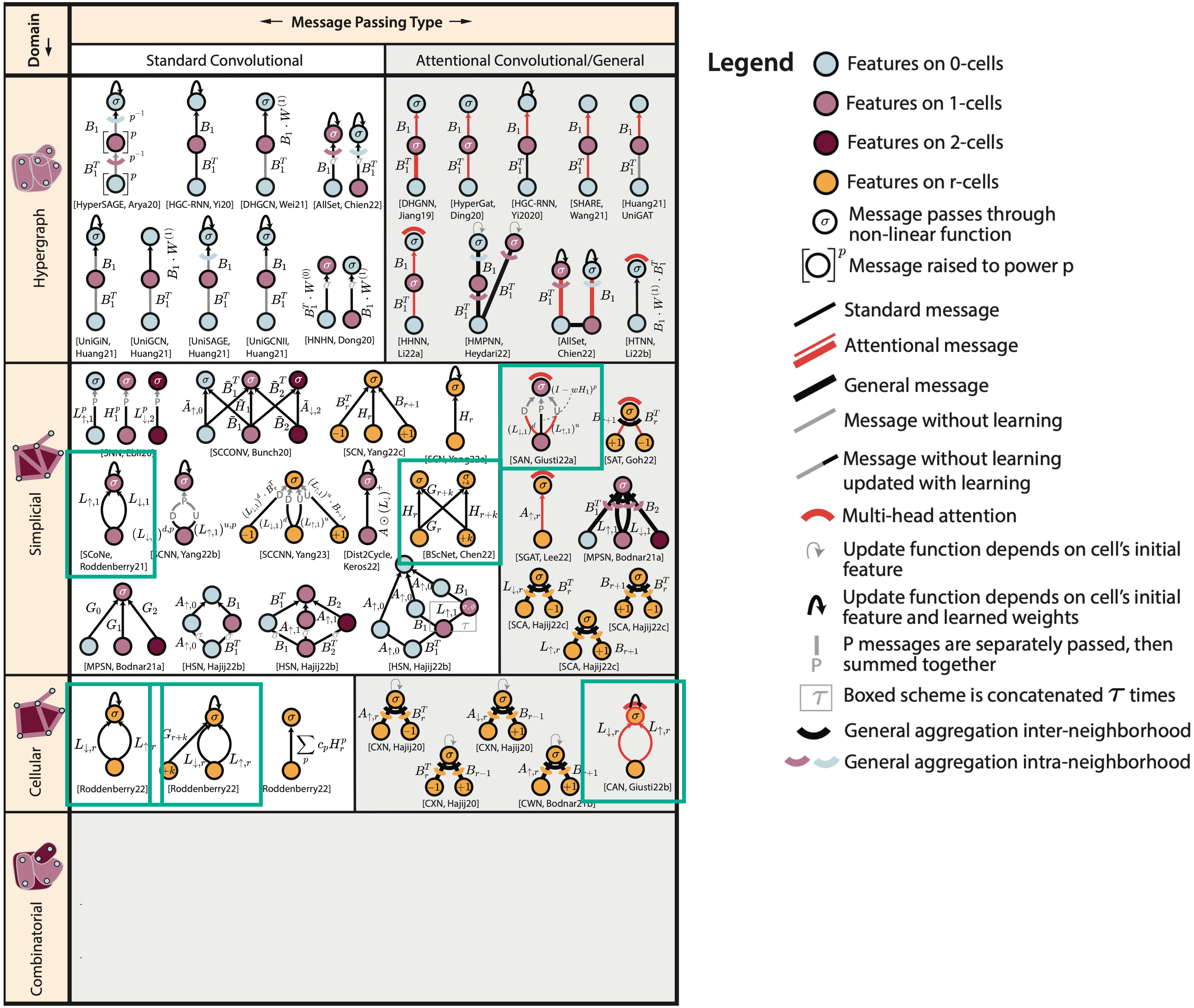
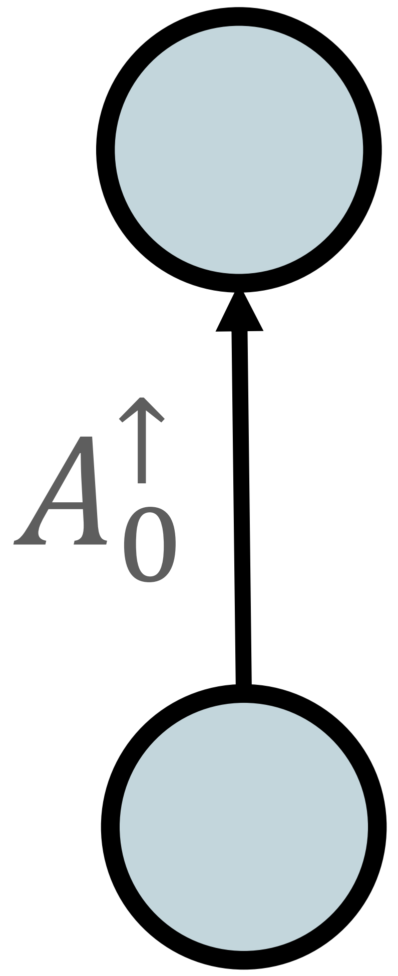
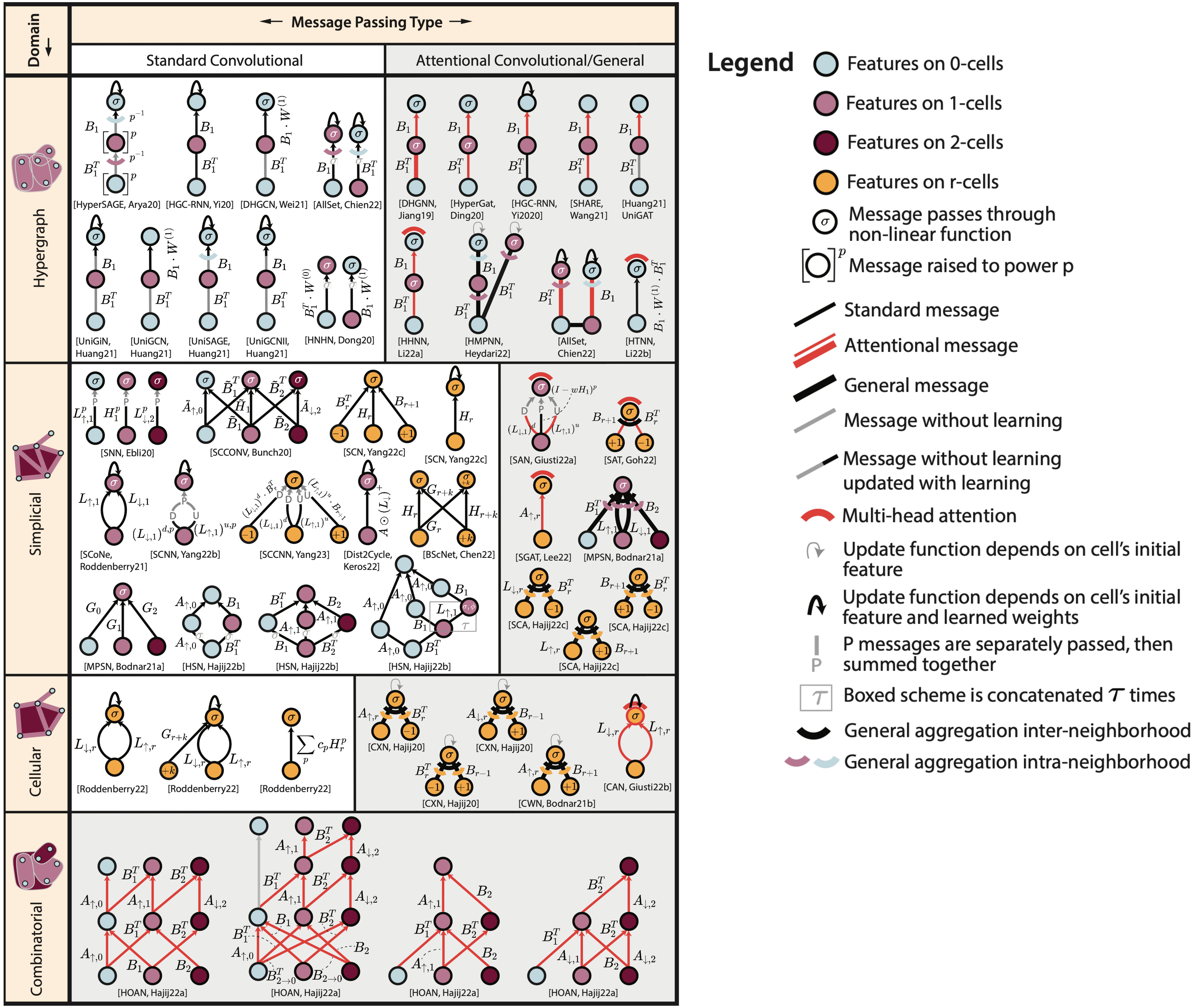




Survey of the literature

Beyond Graph Convolutional Network:

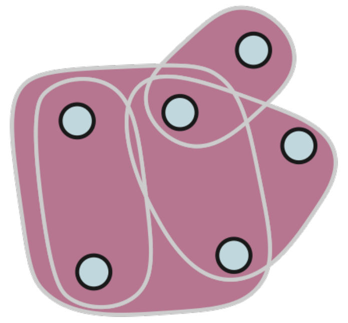


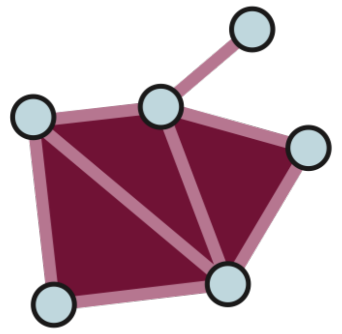


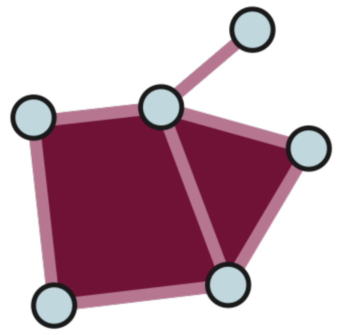
Survey of the literature

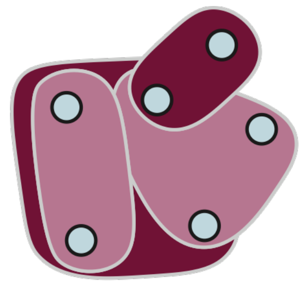
How Do These Models Compare?

Domain	Model	Task Level			Task Purpose	Comparisons
	AllSet Chien et al. (2022)	✓			Classification	TNN SOTA
	HyperGat Ding et al. (2020)	✓			Classification	GNN SOTA
	HNHN Dong et al. (2020)	✓	✓		Classification, Dimensionality Reduction	GNN SOTA
	HMPNN* Heydari and Livi (2022)	✓			Classification	TNN SOTA
	UniGNN Huang and Yang (2021)	✓			Classification (Inductive + Transductive)	TNN SOTA
	DHGNN Jiang et al. (2019)	✓			Classification (Multimodal)	GNN SOTA
	EHNN Kim et al. (2022)	✓			Classification, Keypoint Matching	TNN SOTA
	HHNN Li et al. (2022a)	✓			Link prediction	TNN SOTA
	HTNN Li et al. (2022b)	✓			Classification	TNN SOTA
	SHARE* Wang et al. (2021a)	✓			Prediction	GNN SOTA
	DHGCN* Wei et al. (2021)			✓	Classification	GNN SOTA
	HGC-RNN* (Yi and Park, 2020)	✓			Prediction	GNN SOTA
SC	MPSN Bodnar et al. (2021a)		✓	✓	Classification, Trajectory Classification	GNN SOTA
	SCCONV Bunch et al. (2020)			✓	Classification	Graph
	BScNet Chen et al. (2022)		✓		Link prediction	GNN SOTA
	SNN Ebli et al. (2020)		✓		Imputation	None
	SAN Giusti et al. (2022a)		✓		Classification, Trajectory Classification	TNN SOTA
	SAT Goh et al. (2022)		✓	✓	Classification, Trajectory Classification	TNN SOTA
	HSN* Hajij et al. (2022b)	✓	✓	✓	Classification, Link prediction, Vector embedding	Graph
	SCA* Hajij et al. (2022c)			✓	Clustering	Graph
	Dist2Cycle Keros et al. (2022)		✓		Homology Localization	GNN SOTA
	SGAT Lee et al. (2022)	✓			Classification	GNN SOTA
	SCoNe Roddenberry et al. (2021)		✓		Trajectory Classification	TNN SOTA
	SCNN* Yang et al. (2022b)		✓		Imputation	TNN SOTA
	SCCNN Yang and Isufi (2023)		✓		Link prediction, Trajectory Classification	TNN SOTA
	SCN Yang et al. (2022c)		✓		Classification	TNN SOTA
CC	CWN Bodnar et al. (2021b)		✓	✓	Classification, prediction, regression	GNN SOTA
	CAN Giusti et al. (2022b)			✓	Classification	GNN SOTA
CCC	HOAN* Hajij et al. (2022a)		✓	✓	Classification	GNN SOTA









On Performance:

Outperform GNNs

- Hypergraph > graph
- Simplicial > graph
- Cellular > graph
- Cellular > simplicial

Outperform other TNNs

- Compare themselves to same domain models
- Difficult to compare across domains

How Do These Models Compare?

github.com/pyt-team

geometric-intelligence/TopoBench

Hajij, M., Papillon, M., Frantzen, F., ... & Miolane, N. (2024). TopoX: a suite of Python packages for machine learning on topological domains. *Journal of Machine Learning Research*, *25*(374), 1-8

Telyanikov, L., Bernárdez, G., Montagna, C., … & Papamarkou, T. (2024). TopoBench: A Framework for Benchmarking Topological Deep Learning. *arXiv preprint arXiv:2406.06642*

How Can You Build New TNNs?

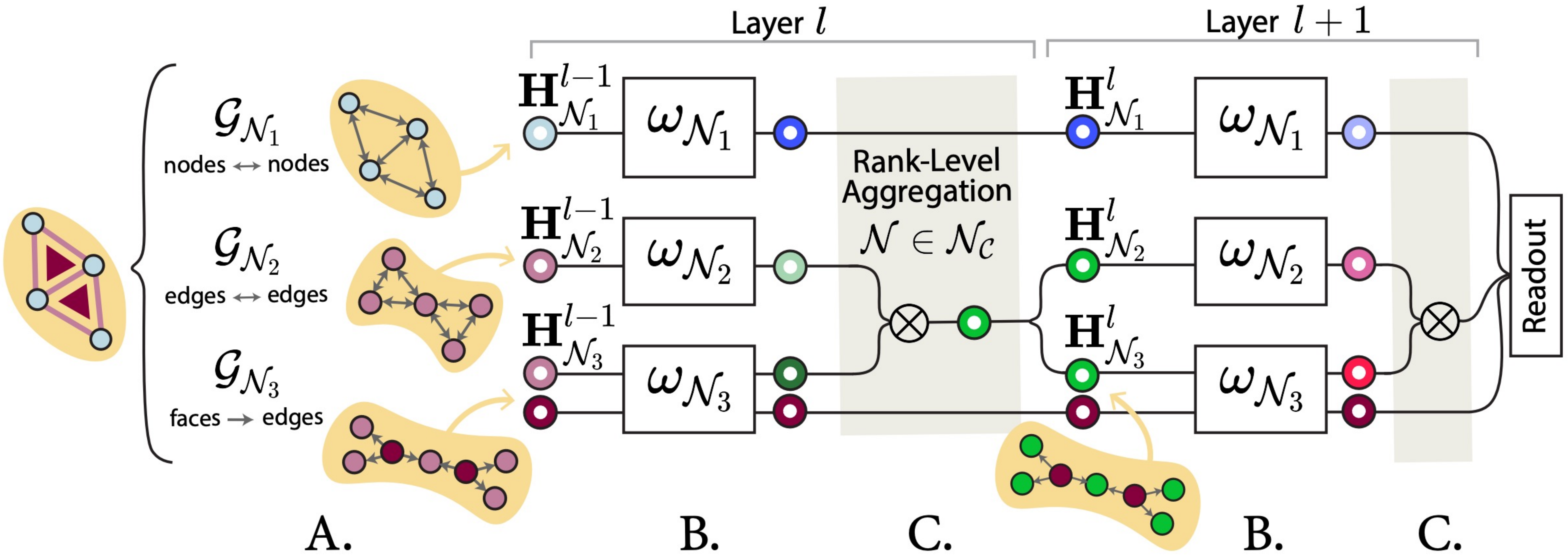


Figure 1. **Generalized Combinatorial Complex Network (GCCN).** The input complex $\mathcal{C}$ has neighborhoods $\mathcal{N}_{\mathcal{C}} = \{\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3\}$. **A.** The complex is expanded into three augmented Hasse graphs $\mathcal{G}_{\mathcal{N}_i}$, $i = \{1, 2, 3\}$, each with features $H_{\mathcal{N}_i}$ represented as a colored disc. **B.** A GCCN layer dedicates one base architecture $\omega_{\mathcal{N}_i}$ (GNN, Transformer, MLP, etc.) to each neighborhood. **C.** The output of all the architectures $\omega_{\mathcal{N}_i}$ is aggregated rank-wise, then updated. In this example, only the complex's edge features (originally pink) are aggregated across multiple neighborhoods ($\mathcal{N}_2$ and $\mathcal{N}_3$).

Papillon, M., Bernárdez, G., Battiloro, C., & Miolane, N. (2024).
TopoTune: A Framework for Generalized Combinatorial Complex Neural Networks. *arXiv preprint arXiv:2410.06530*

Thank you!

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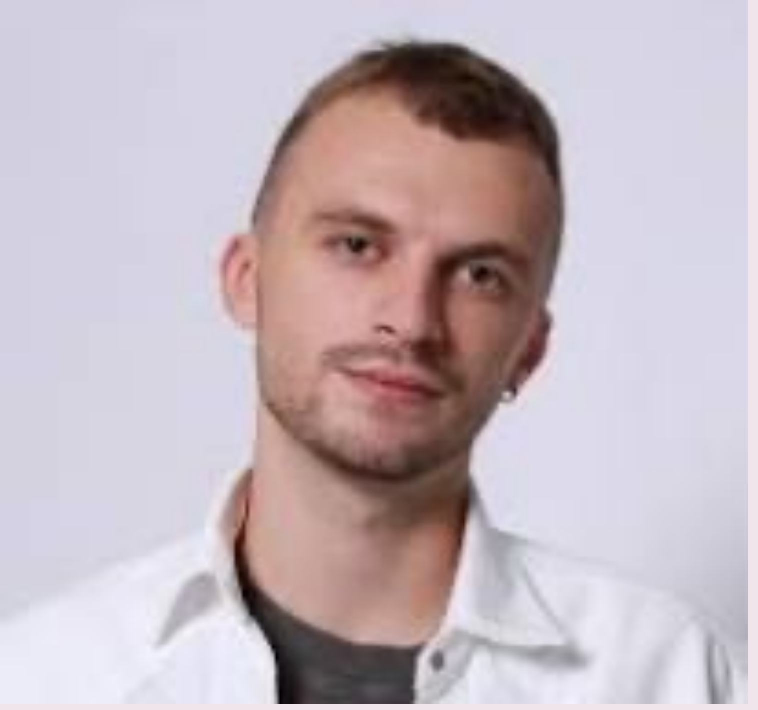

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Telyanikov, Bernárdez et al. (2025). TopoBench: A Framework for Benchmarking Topological Deep Learning.

github.com/awesome-tnns/awesome-tnns
github.com/pyt-team
github.com/geometric-intelligence/TopoBench

NSF SCALE MoDL
Grant 2134241