

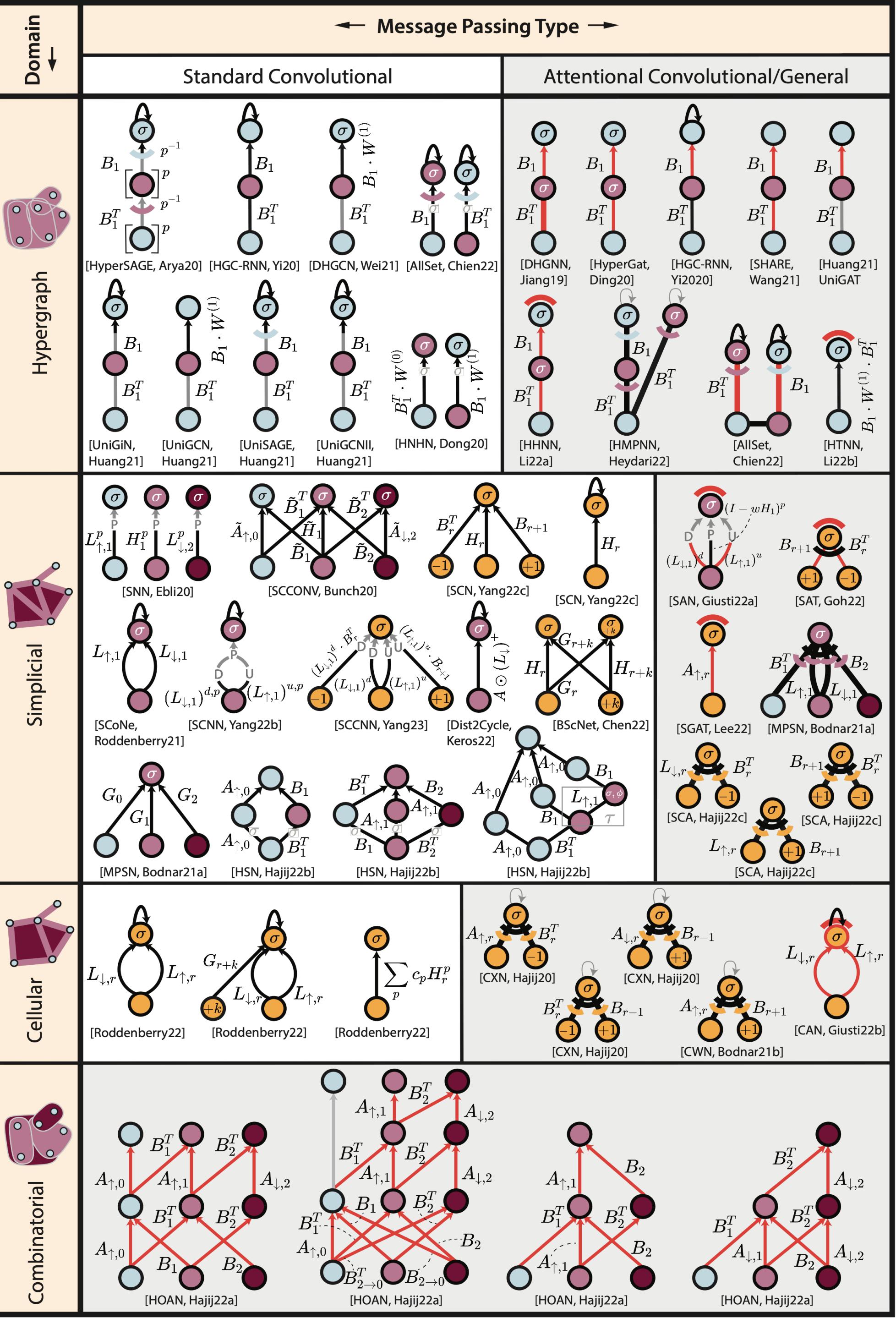
A Survey of Message Passing

Topological Neural Networks

Nina Miolane, UC Santa Barbara

Joint work with Mathilde Papillon, Sophia Sanborn & Mustafa Hajij

CoSyNe 2025 @ It's All Connected!



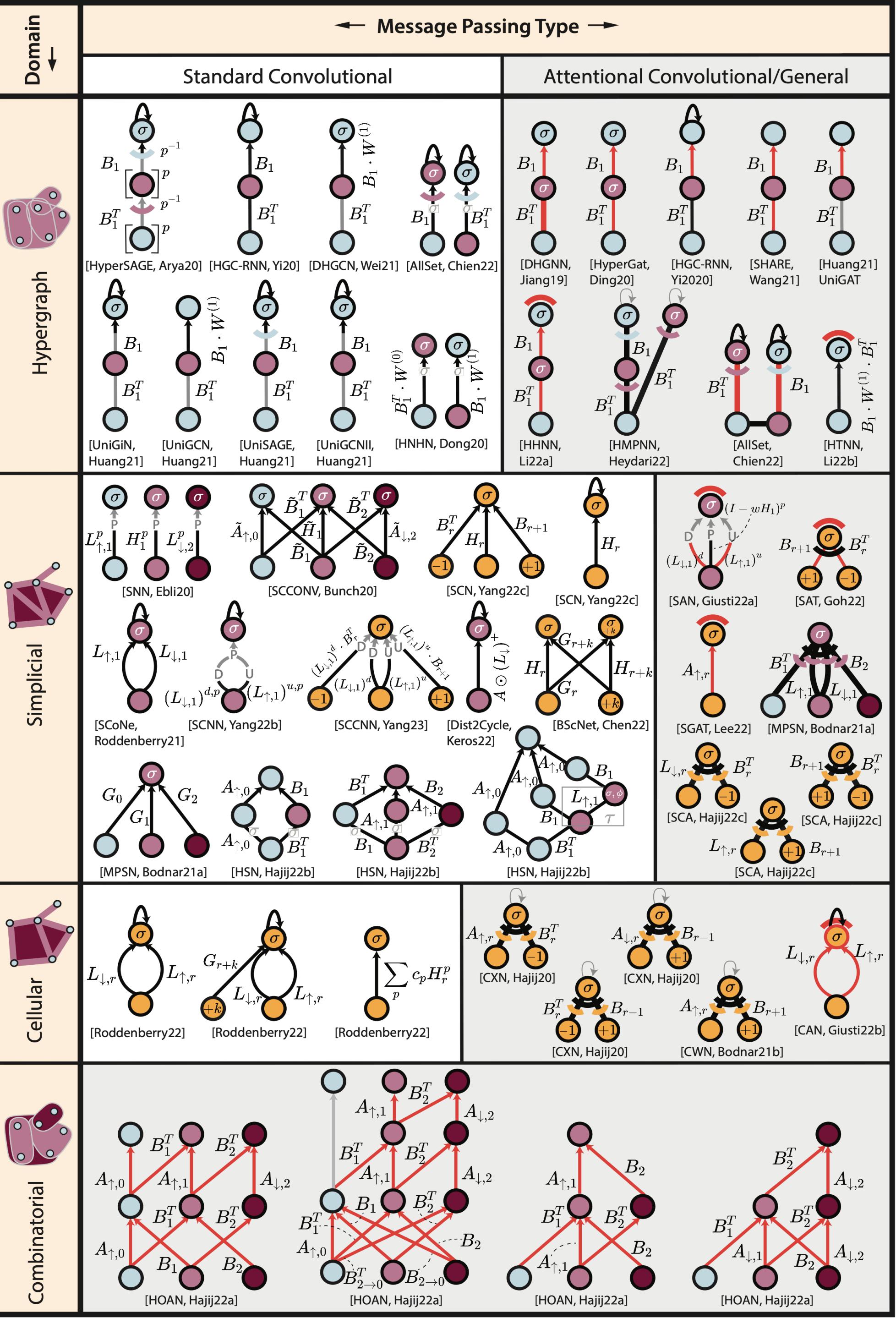
A Survey of Message Passing

Topological Neural Networks

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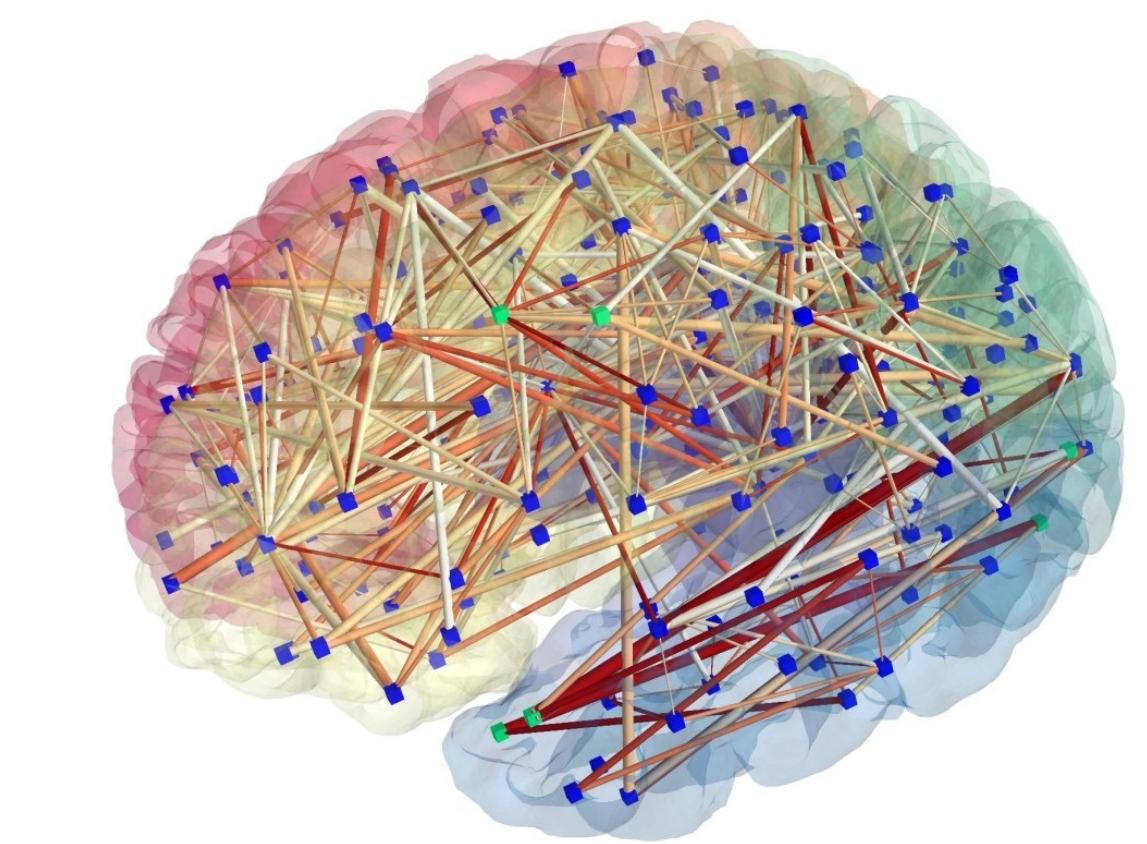
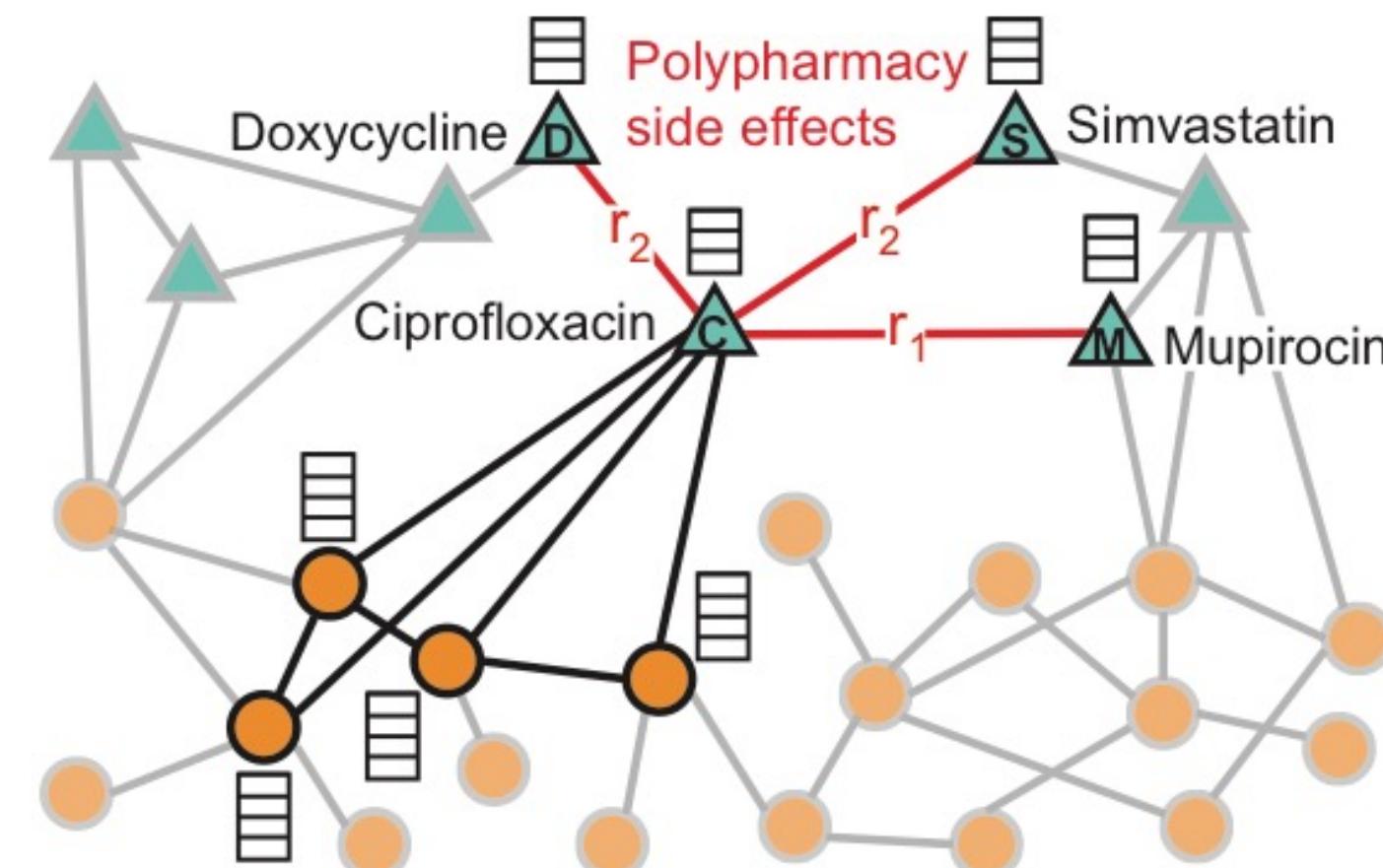
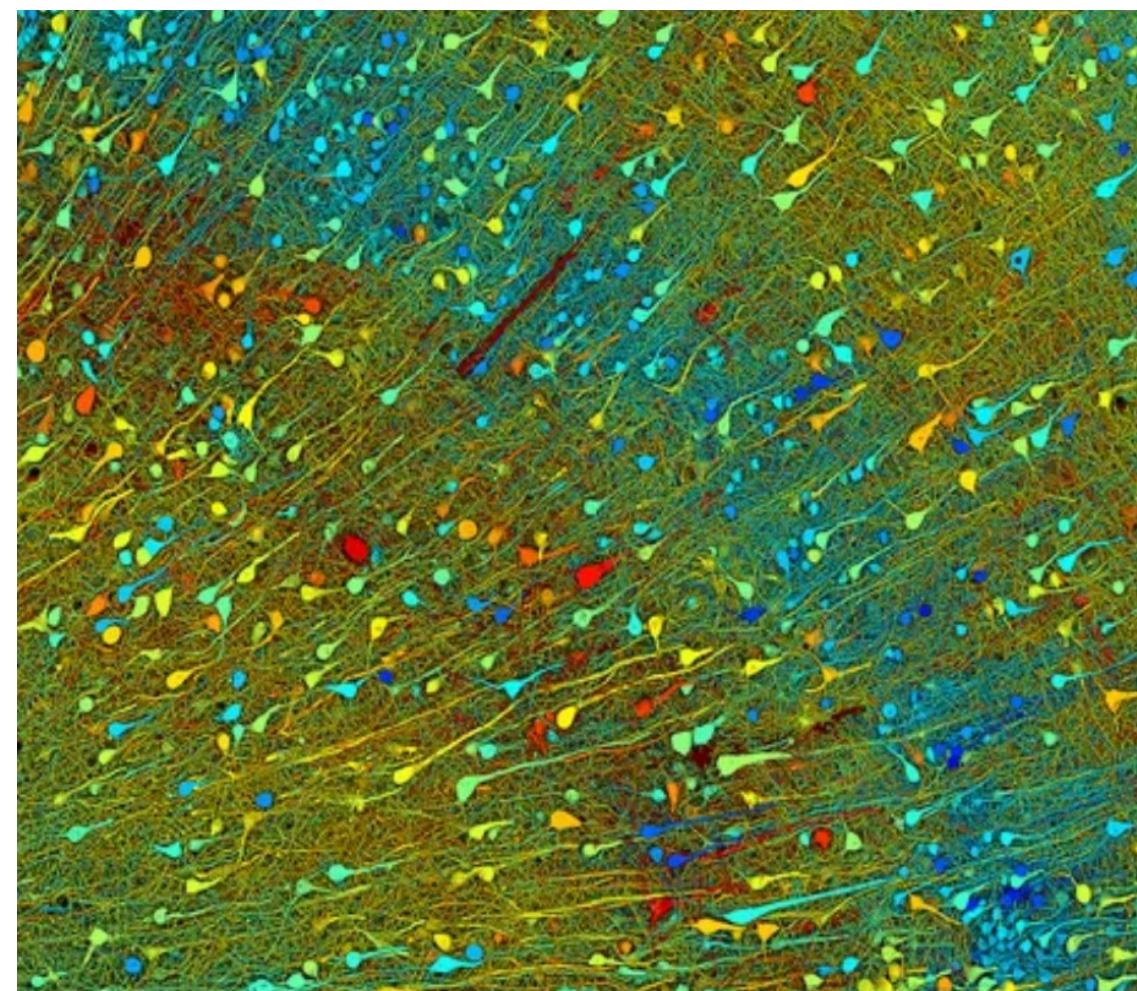
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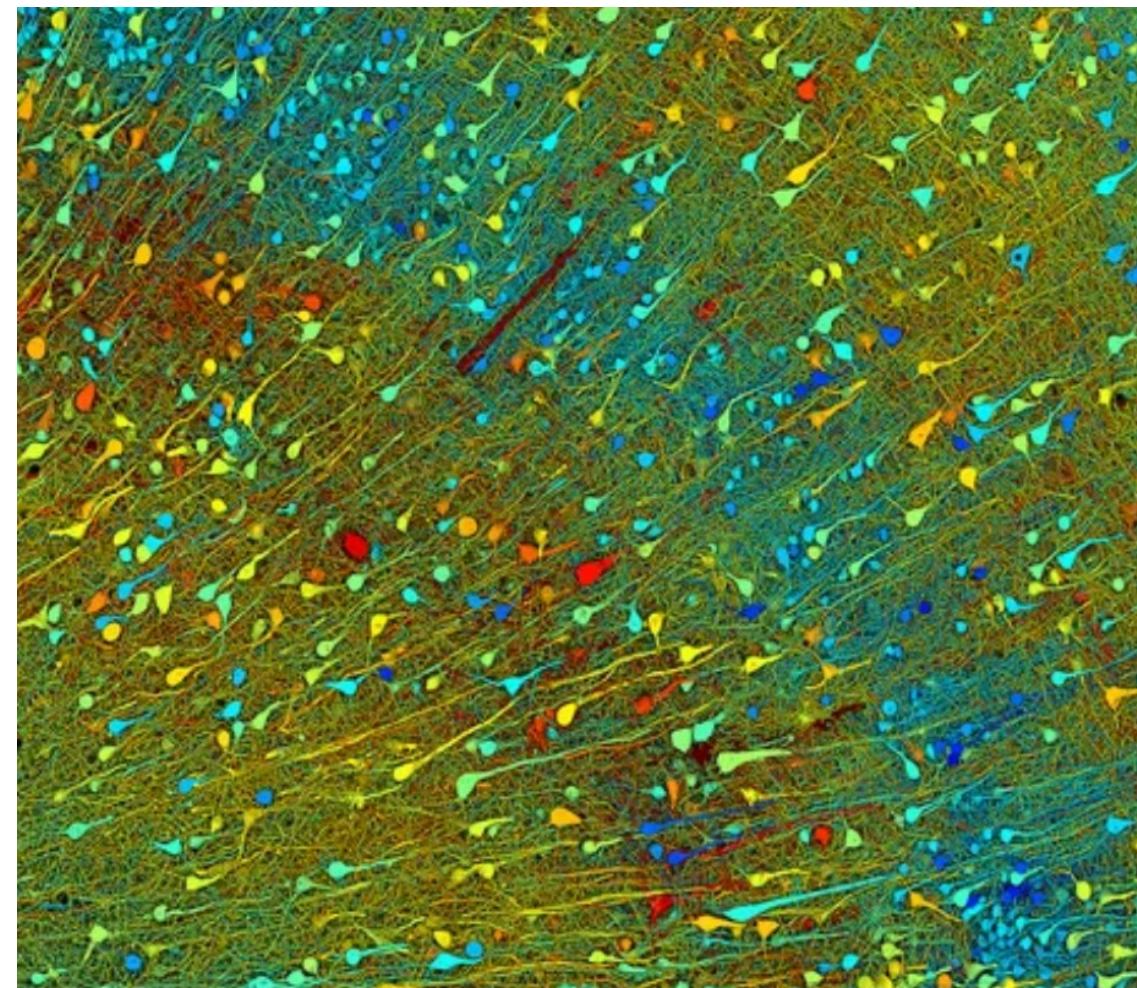
Topological Neural Networks

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



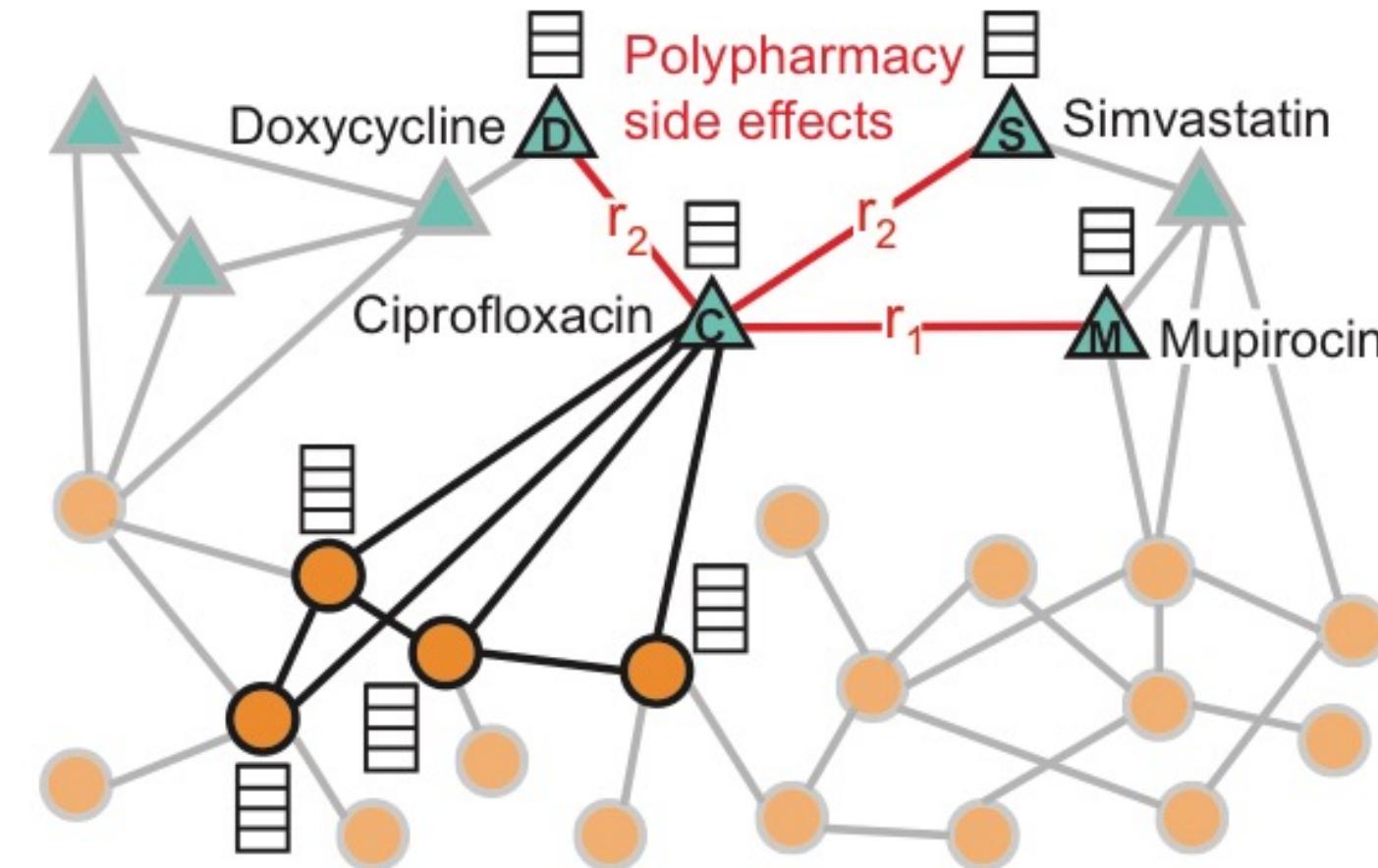
Topological Neural Networks answer questions such as:

Is this neuron
inhibitory or
excitatory?



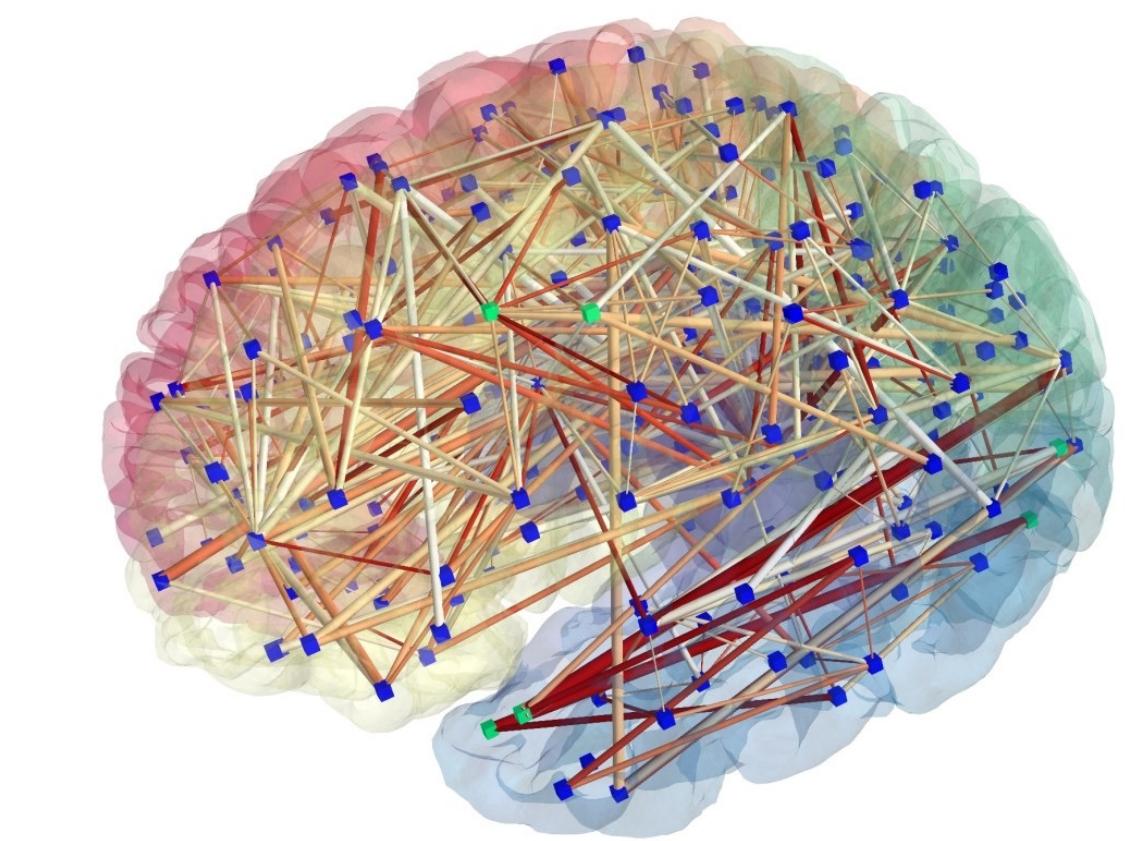
Node-level prediction

Does Fluoxetine
interact with
Venlafaxine?



Edge-level prediction

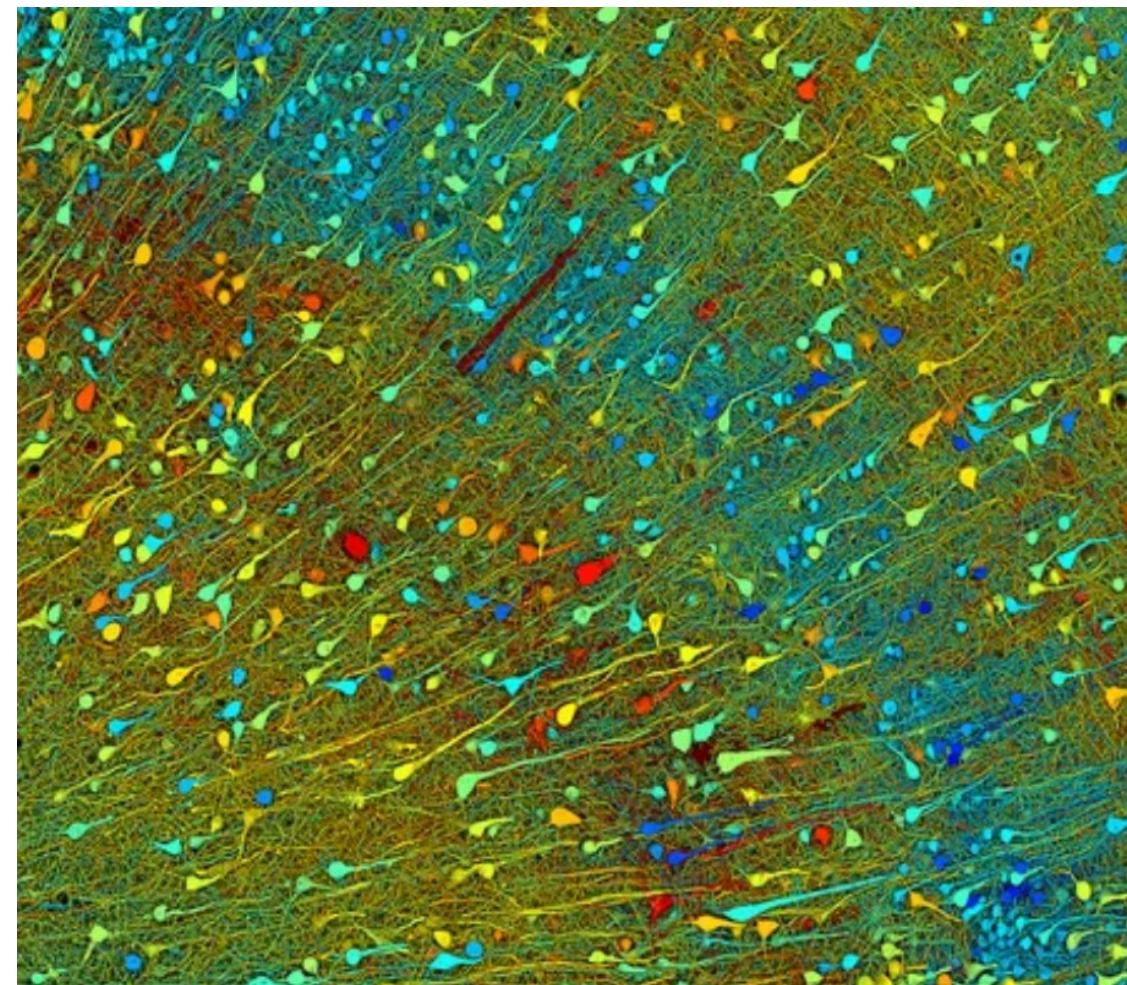
What is the brain
state associated with
this connectome?



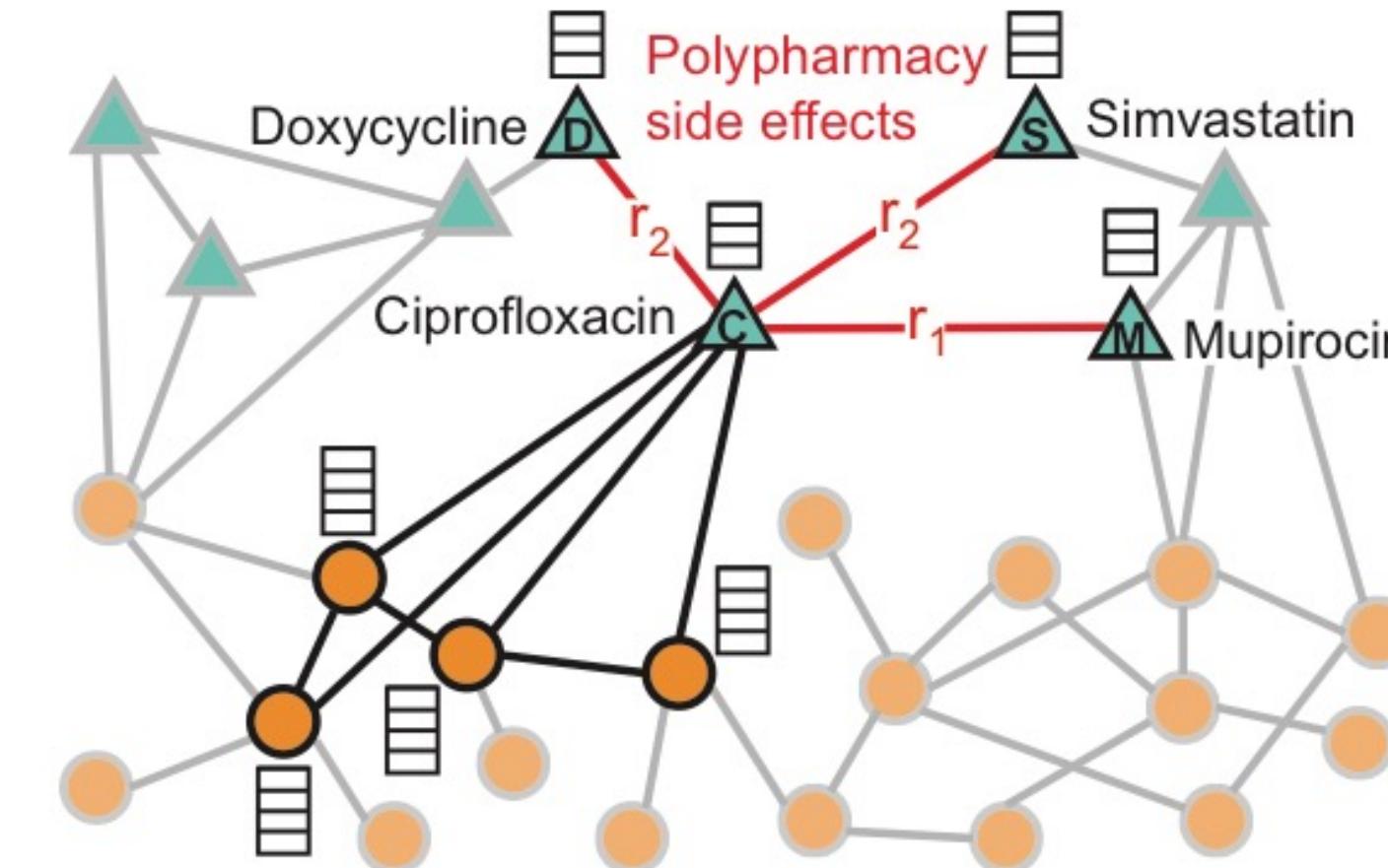
System-level prediction

Topological Neural Networks extend Graph Neural Networks

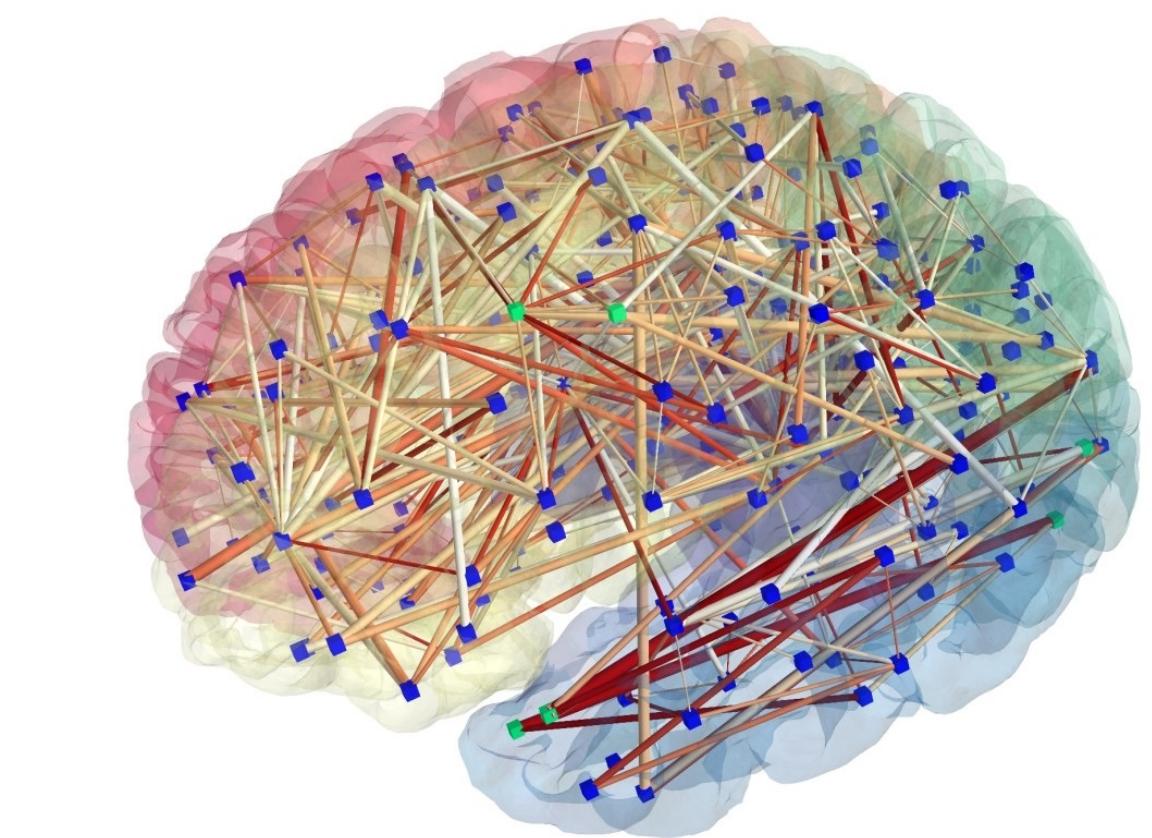
by leveraging non-binary relations
to give “better” answers & answer more questions.



Node-level prediction



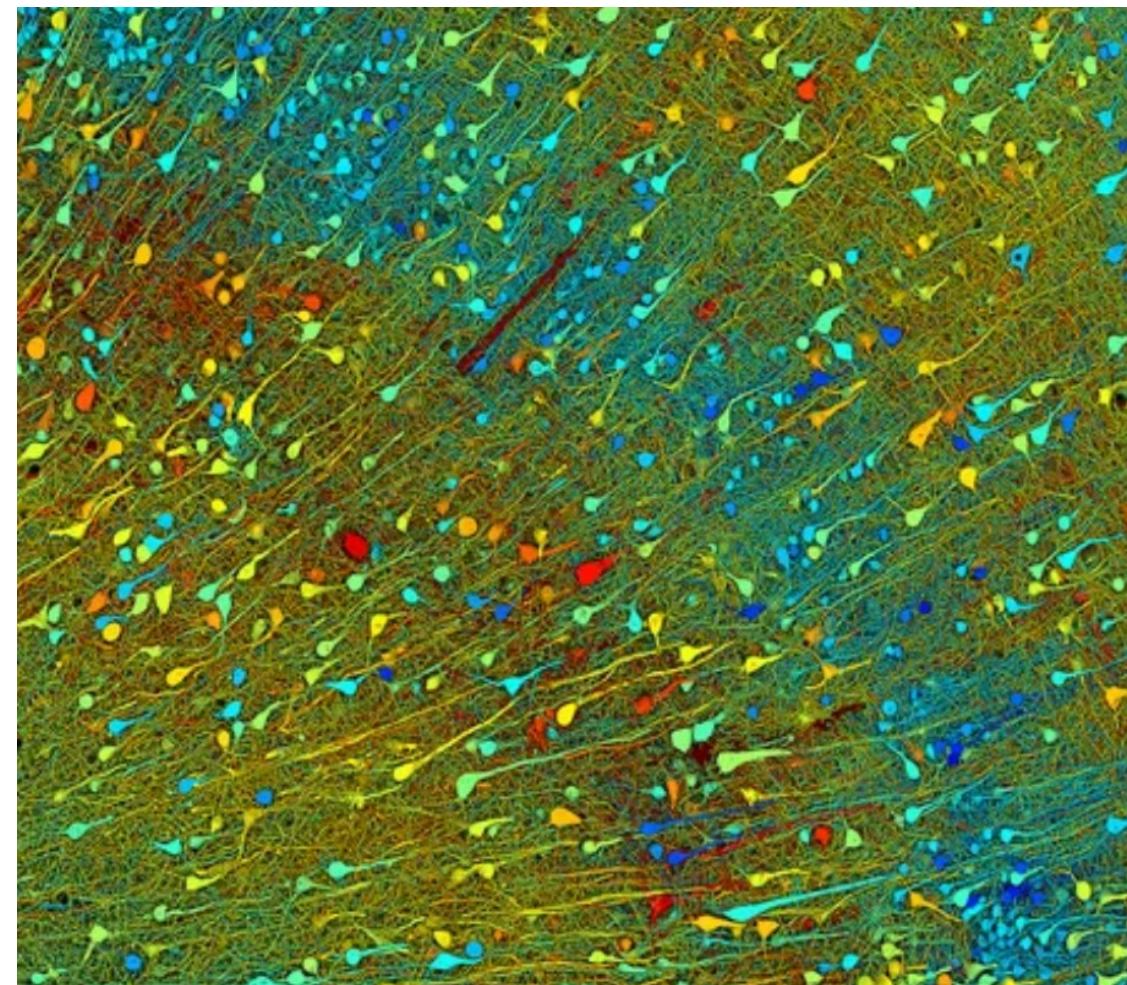
Edge-level prediction



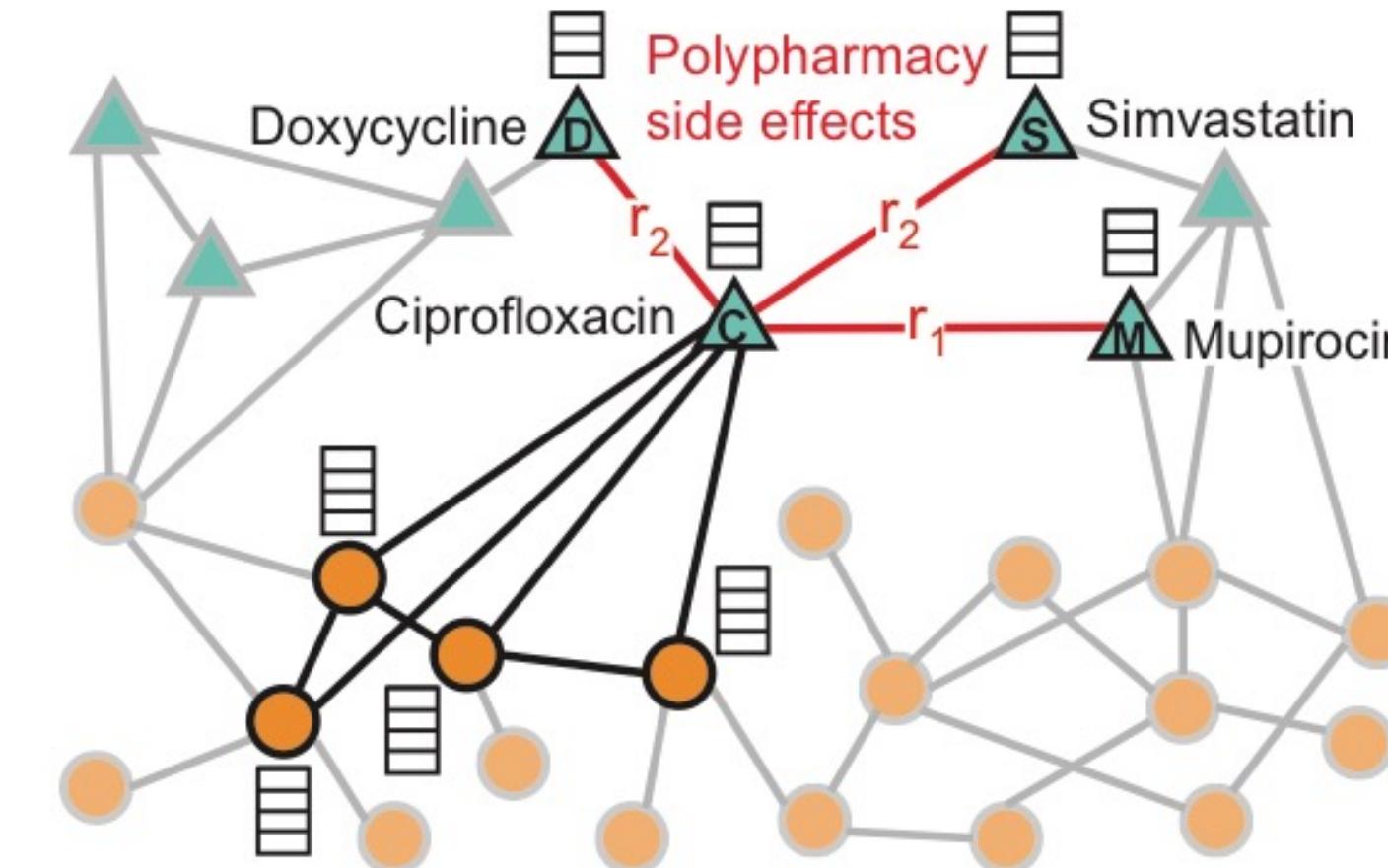
System-level prediction

Topological Neural Networks extend Graph Neural Networks

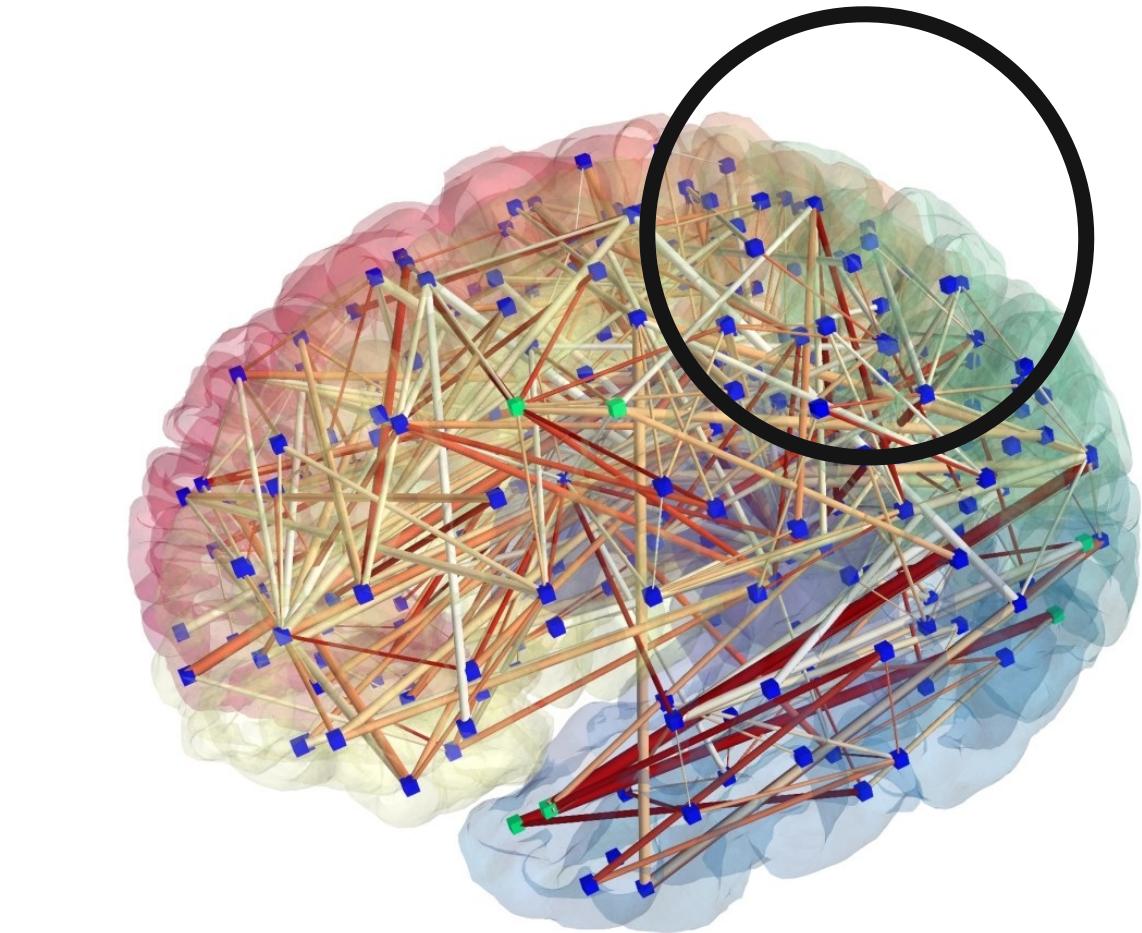
by leveraging non-binary relations
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Node-level prediction



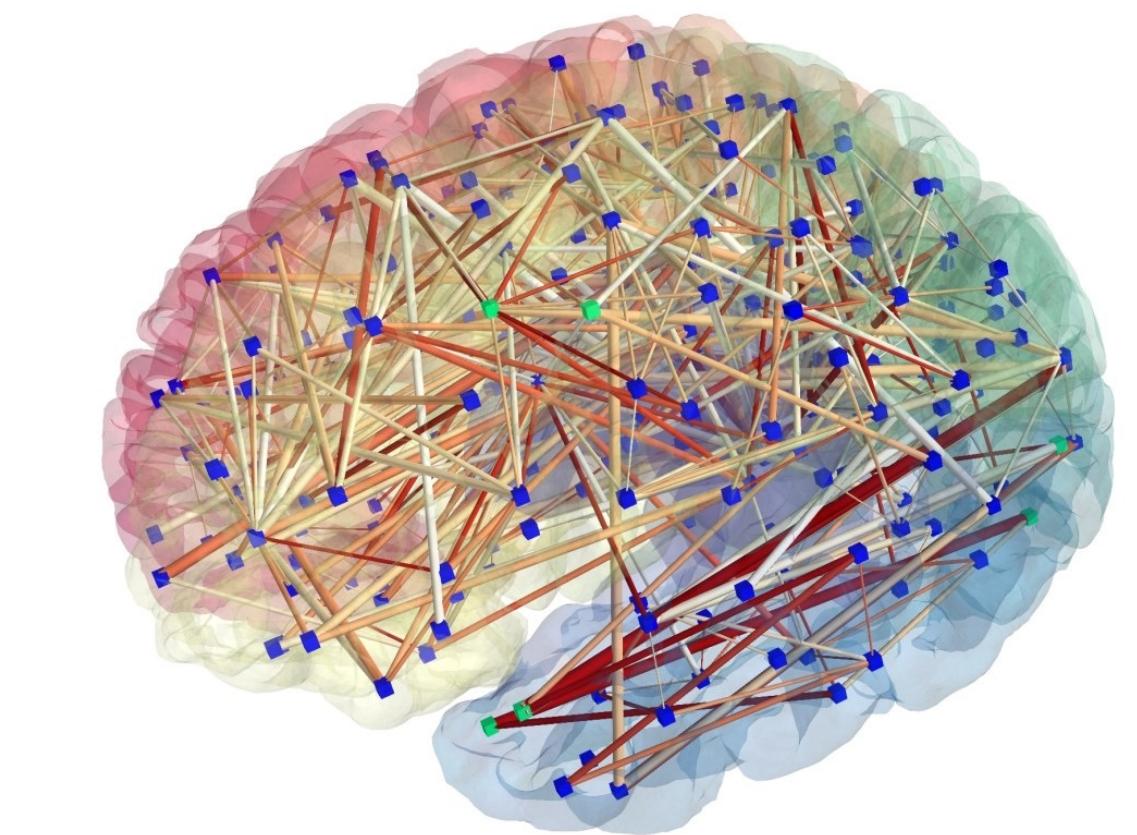
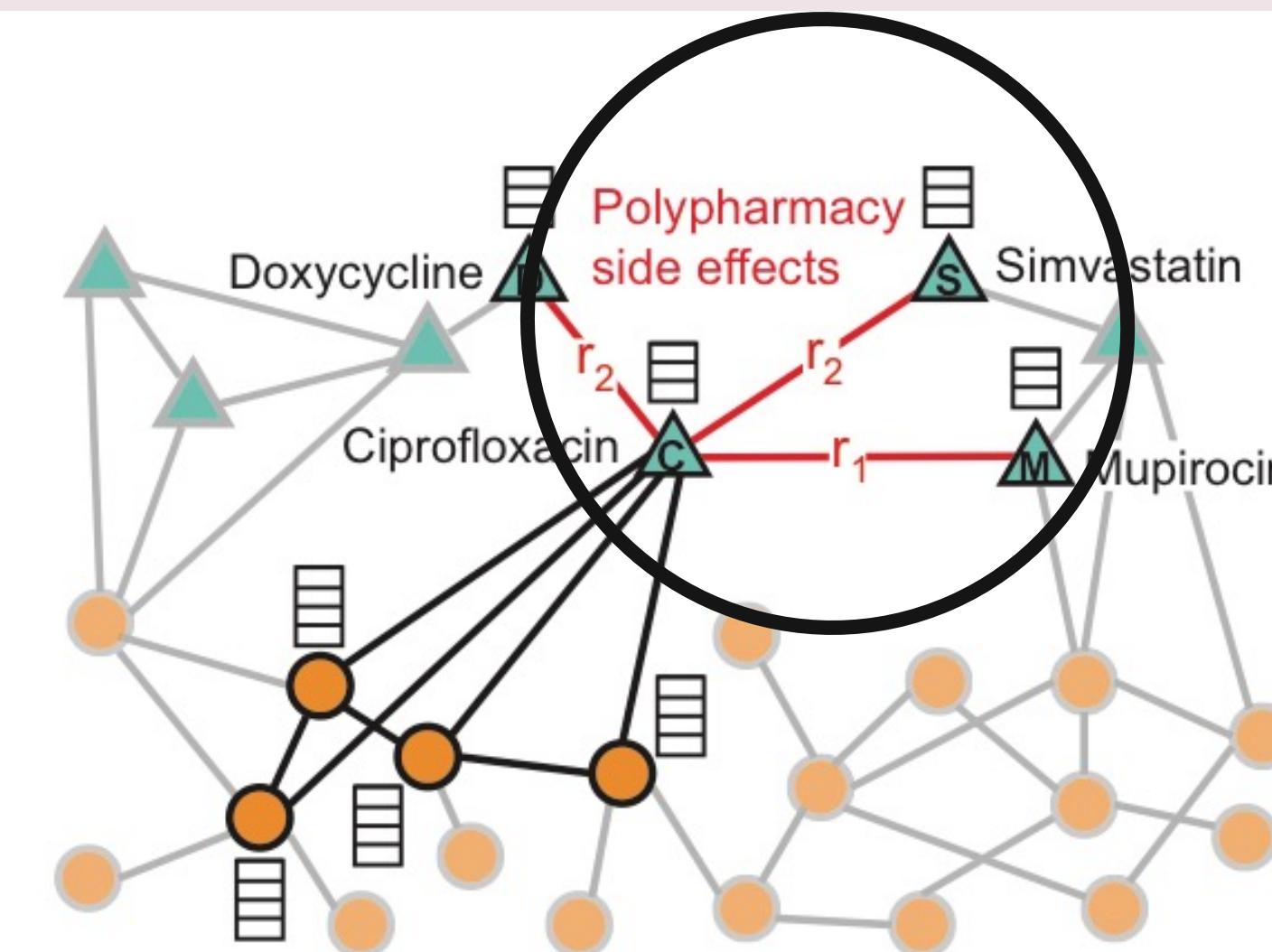
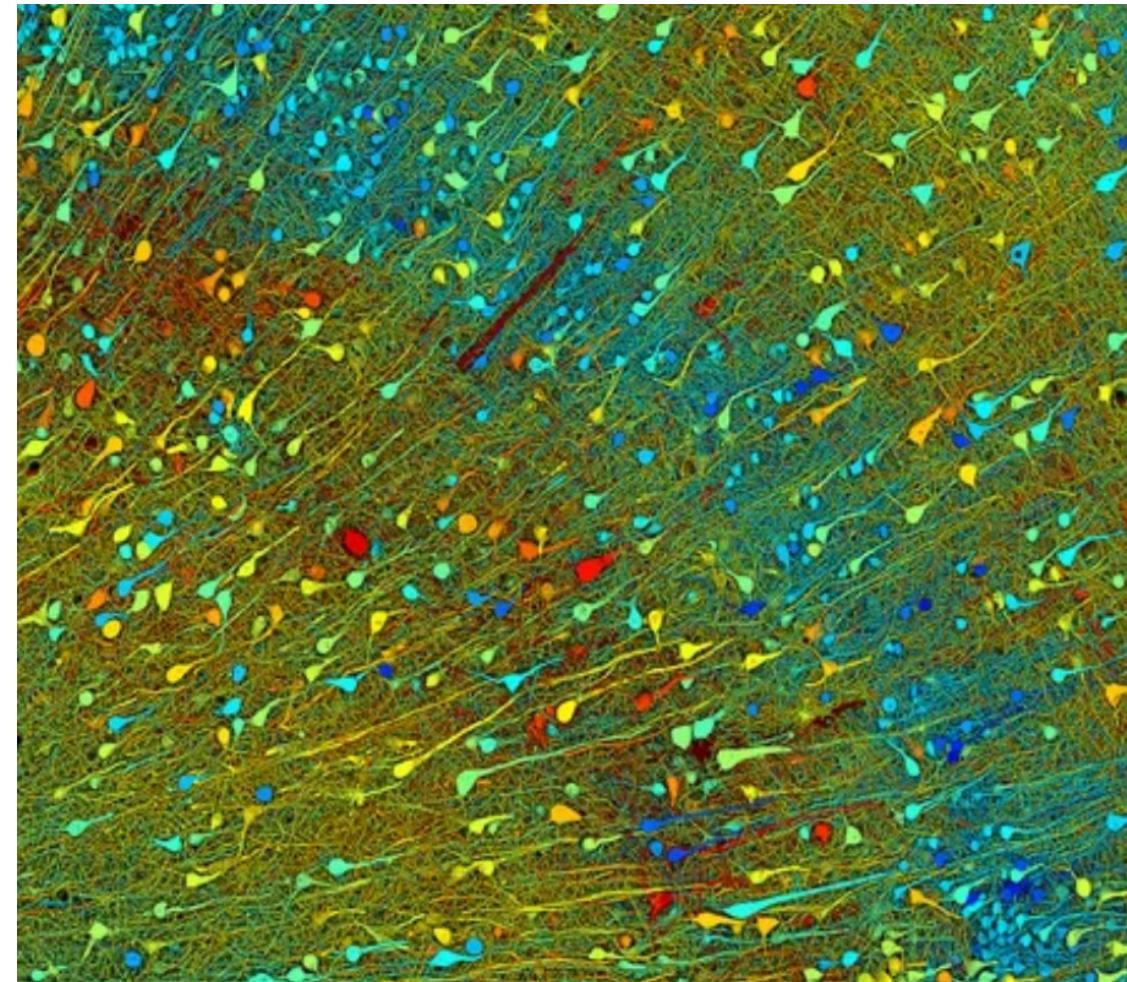
Edge-level prediction



System-level prediction

Topological Neural Networks extend Graph Neural Networks

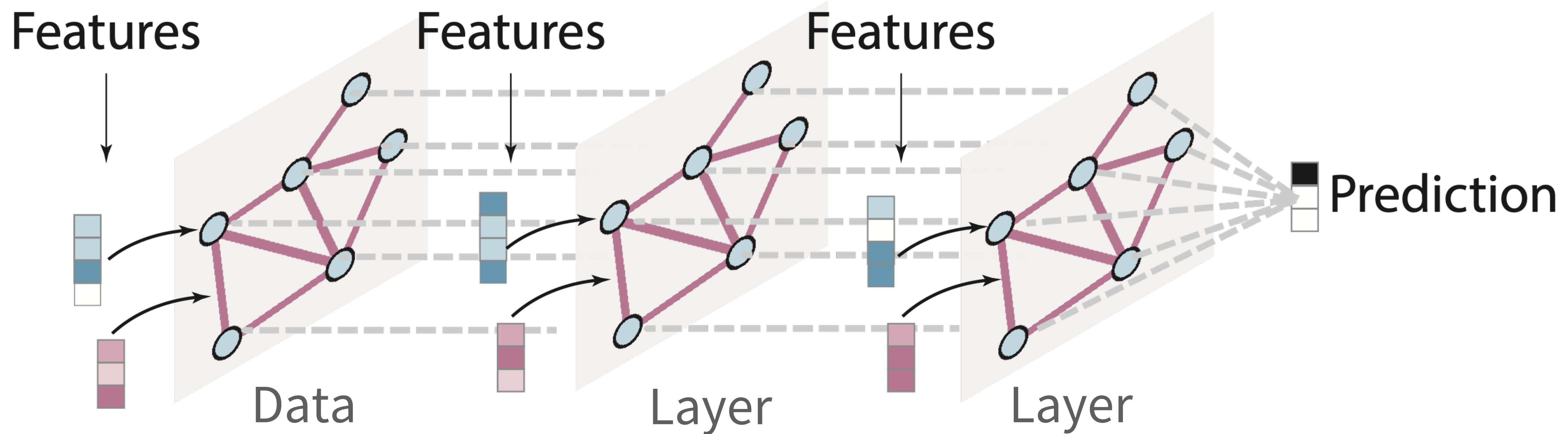
by leveraging non-binary relations
to give “better” answers & answer more questions.



What is the interaction resulting from taking these four drugs?

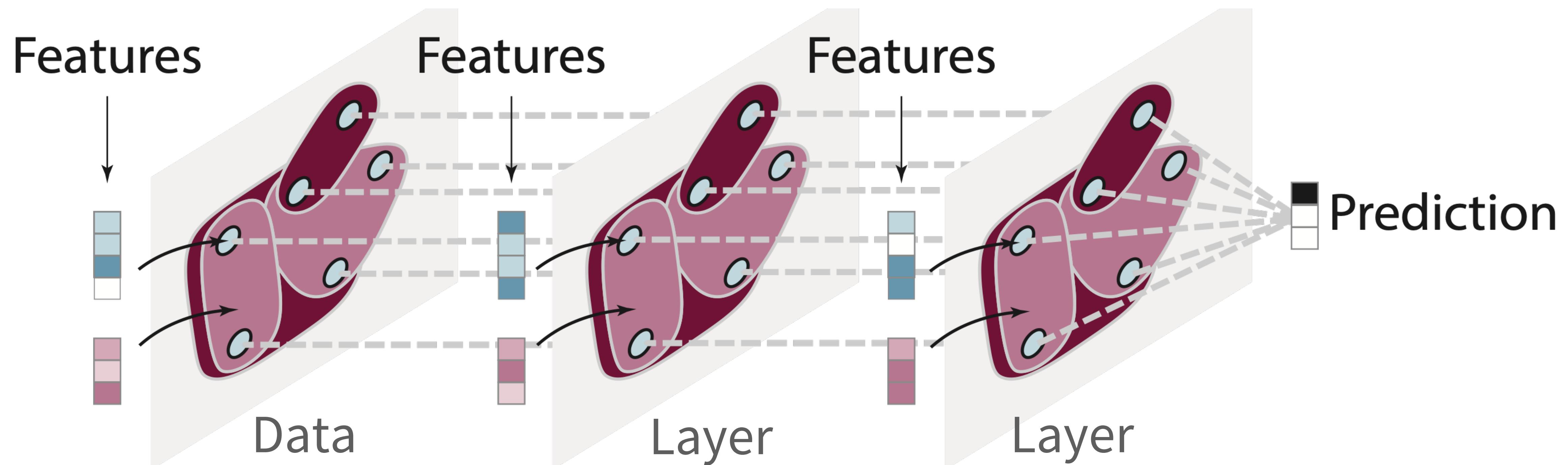
Topological Neural Networks
extend Graph Neural Networks

Topological Neural Networks extend Graph Neural Networks



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

$$m_{\mathcal{B}}^{t+1}(\sigma) = \text{AGG}_{\tau \in \mathcal{B}(\sigma)} \left(M_{\mathcal{B}} \left(h_{\sigma}^t, h_{\tau}^t \right) \right)$$

$$m_{\mathcal{C}}^{t+1}(\sigma) = \text{AGG}_{\tau \in \mathcal{C}(\sigma)} \left(M_{\mathcal{C}} \left(h_{\sigma}^t, h_{\tau}^t \right) \right)$$

$$m_{\downarrow}^{t+1}(\sigma) = \text{AGG}_{\tau \in \mathcal{N}_{\downarrow}(\sigma)} \left(M_{\downarrow} \left(h_{\sigma}^t, h_{\tau}^t, h_{\sigma \cap \tau}^t \right) \right)$$

$$m_{\uparrow}^{t+1}(\sigma) = \text{AGG}_{\tau \in \mathcal{N}_{\uparrow}(\sigma)} \left(M_{\uparrow} \left(h_{\sigma}^t, h_{\tau}^t, h_{\sigma \cup \tau}^t \right) \right)$$

$$h_{\sigma}^{t+1} = U \left(h_{\sigma}^t, m_{\mathcal{B}}^t(\sigma), m_{\mathcal{C}}^t(\sigma), m_{\downarrow}^{t+1}(\sigma), m_{\uparrow}^{t+1}(\sigma) \right)$$

$$\begin{aligned}\mathcal{F}_p^{-1}\left(\varphi_W\right)*_p c &= \sum\nolimits_{i=0}^N W_i U \operatorname{diag}\left(\Lambda^i\right) U^\top c = \\ \sum\nolimits_{i=0}^N W_i \left(U \operatorname{diag}(\Lambda) U^\top\right)^i c &= \sum\nolimits_{i=0}^N W_i L_p^i c\end{aligned}$$

$$\psi\left(M_nH_n^{\mathrm{in}}W_n+U_nH_{n-1}^{\mathrm{in}}W_{n-1}+O_nH_{n+1}^{\mathrm{in}}W_{n+1}\right)$$

$$X_0^{(h+1)}=\sigma\left(\mathbf{D}_1^{-1}\mathbf{B}_1X_1^{(h)}W_{0,1}^{(h)}+\widetilde{\mathbf{A}}_0^uX_0^{(h)}W_{0,0}^{(h)}\right)$$

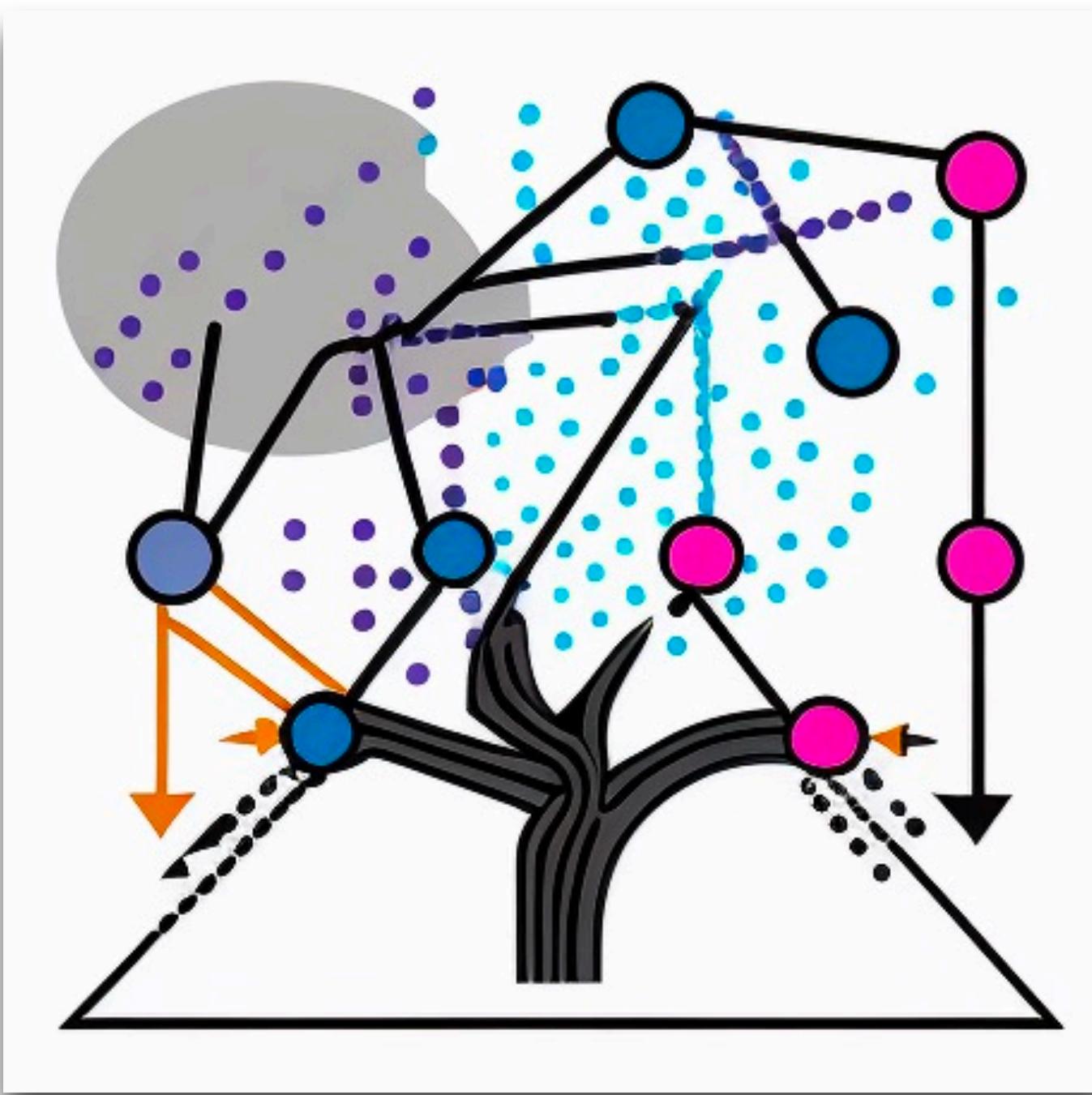
$$X_1^{(h+1)} =$$

$$\sigma\left(\mathbf{B}_2\mathbf{D}_3X_2^{(h)}W_{1,2}^{(h)}+\left(\widetilde{\mathbf{A}}_1^d+\widetilde{\mathbf{A}}_1^u\right)X_1^{(h)}W_{1,1}^{(h)}+\mathbf{D}_2\mathbf{B}_1^*\mathbf{D}_1^{-1}X_0^{(h)}W_{1,0}^{(h)}\right)$$

$$X_2^{(h+1)}=\sigma\left(\widetilde{\mathbf{A}}_2^dX_2^{(h)}W_{2,2}^{(h)}+\mathbf{D}_4\mathbf{B}_2^*\mathbf{D}_5^{-1}X_1^{(h)}W_{2,1}^{(h)}\right)$$

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

Outline

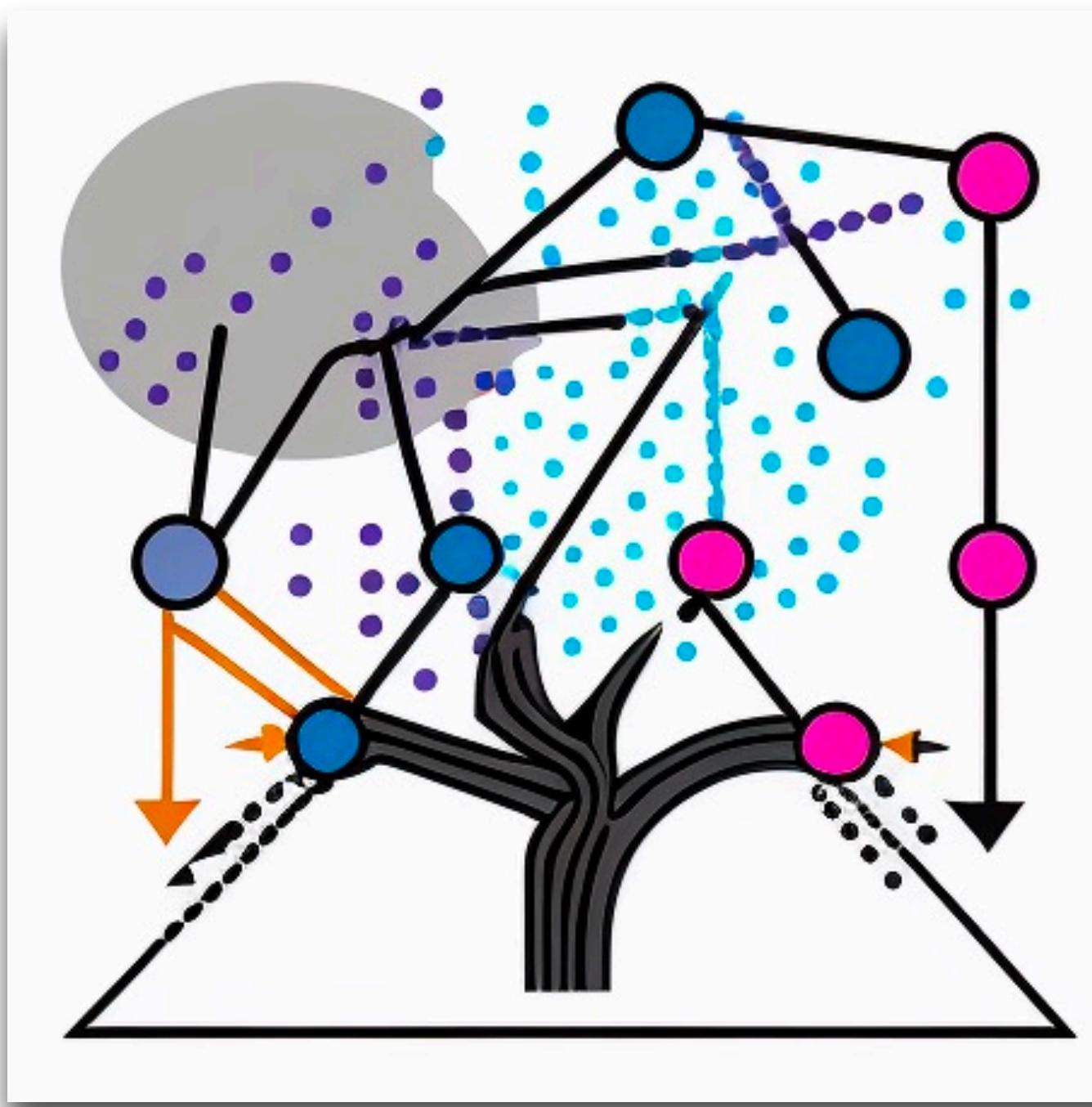


Graphical Framework



Survey of the literature

Outline



Graphical Framework

1. Topological domain
2. Message passing mechanism

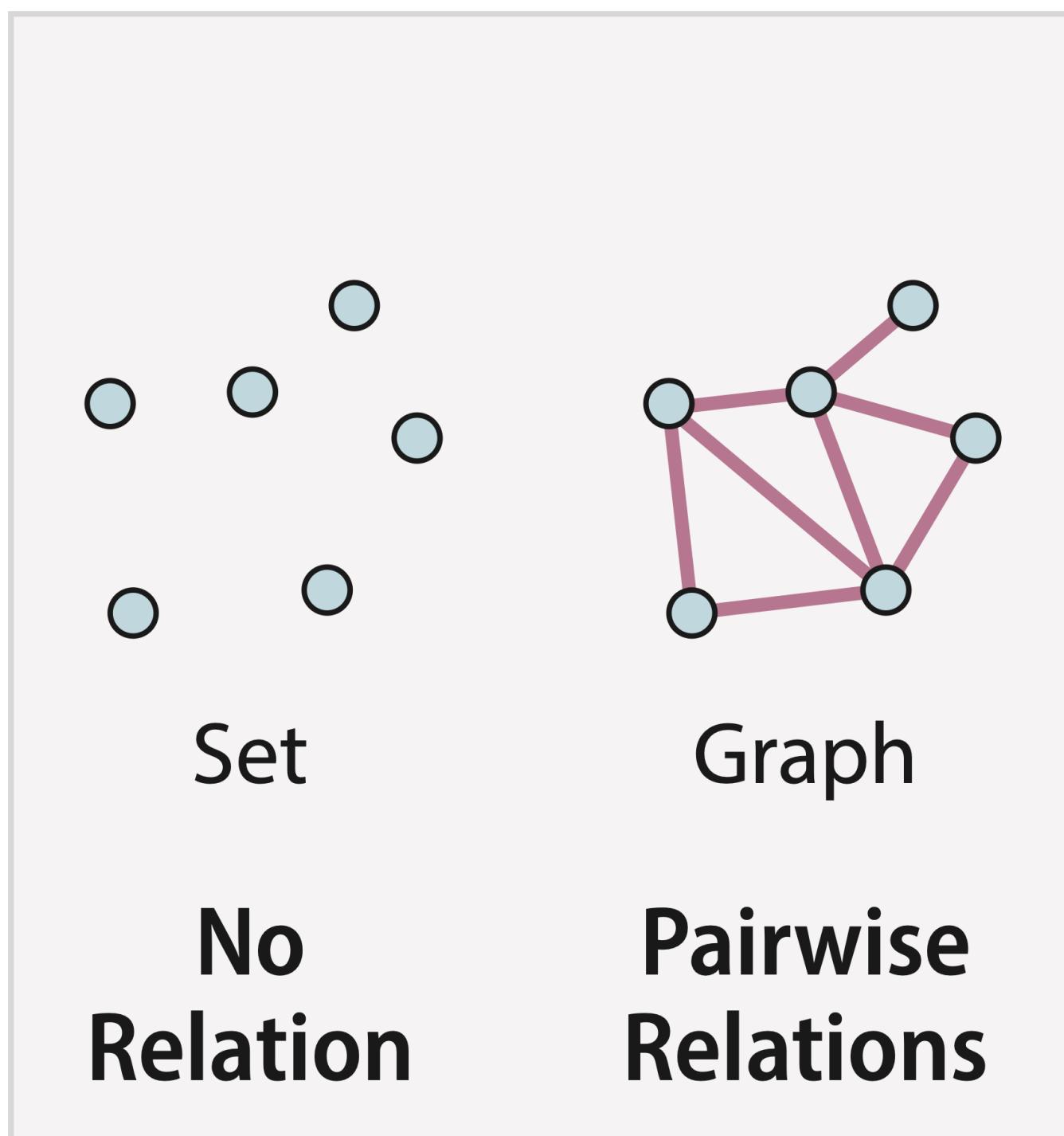


Survey of the literature

1. Topological Domain

The Framework

Traditional Discrete Domains



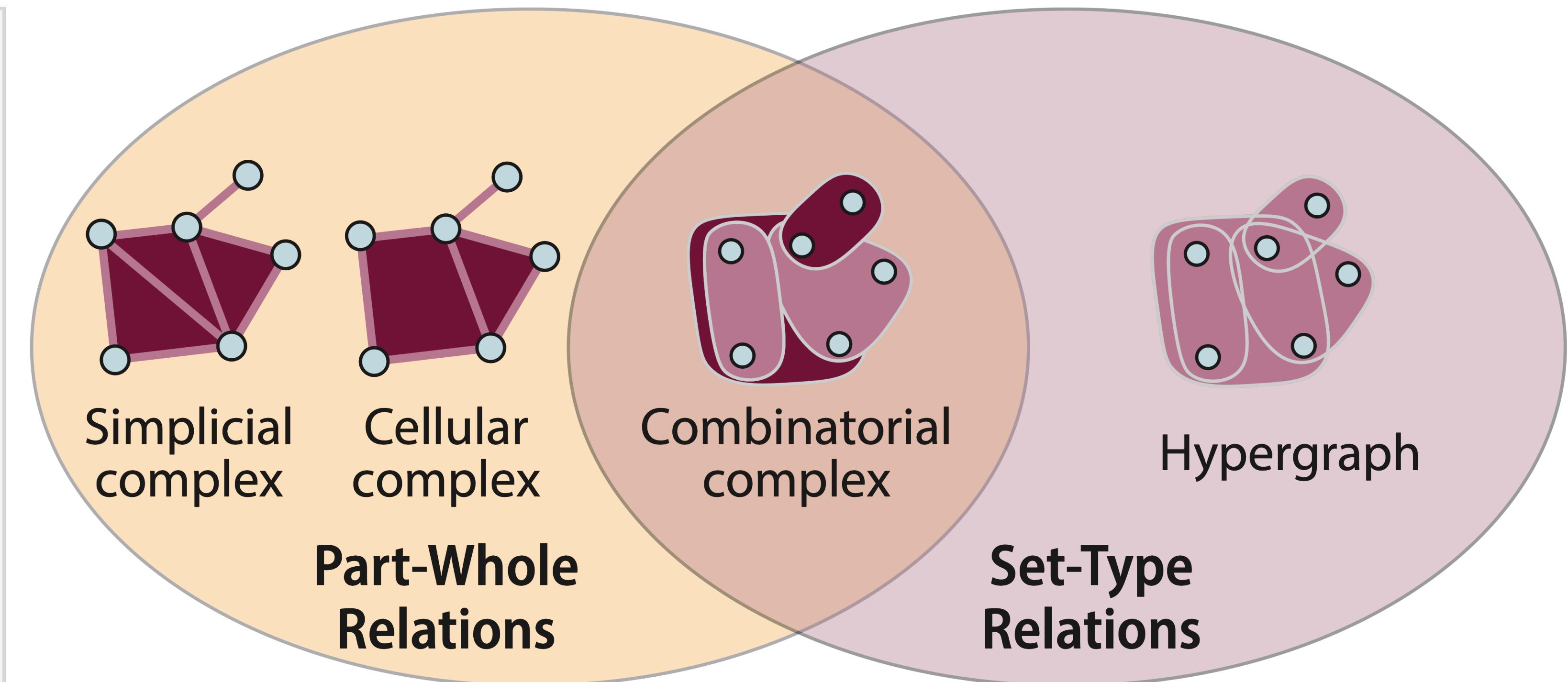
○ : Nodes

— : Edges

is part of

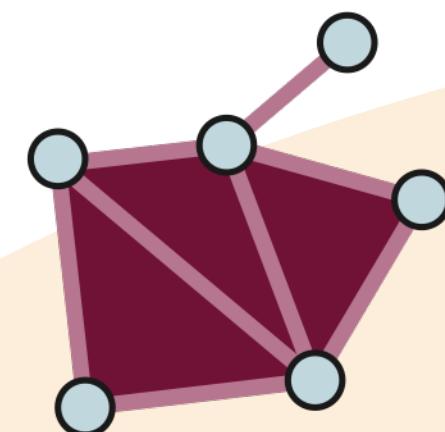
not necessarily part of

Domains of Topological Deep Learning

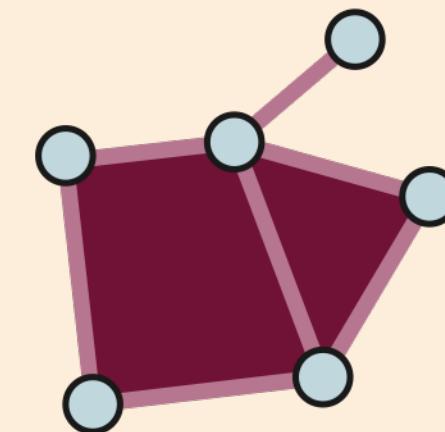


How to Choose?

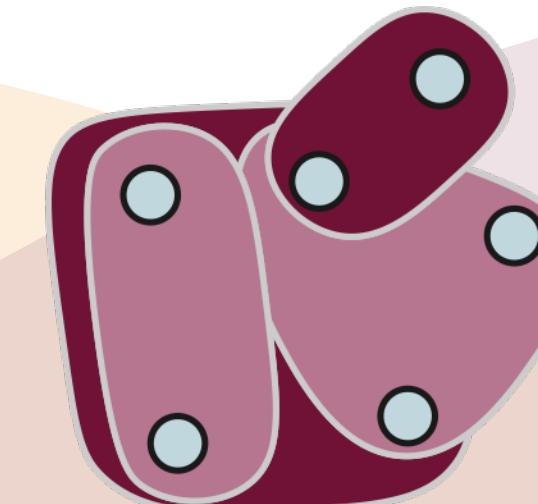
1. Topological Domain



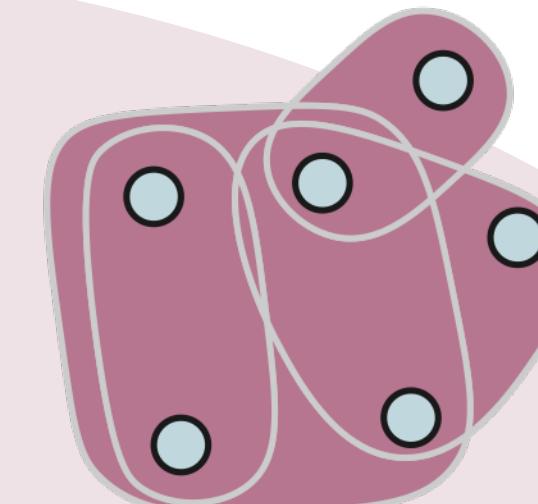
Simplicial Complex



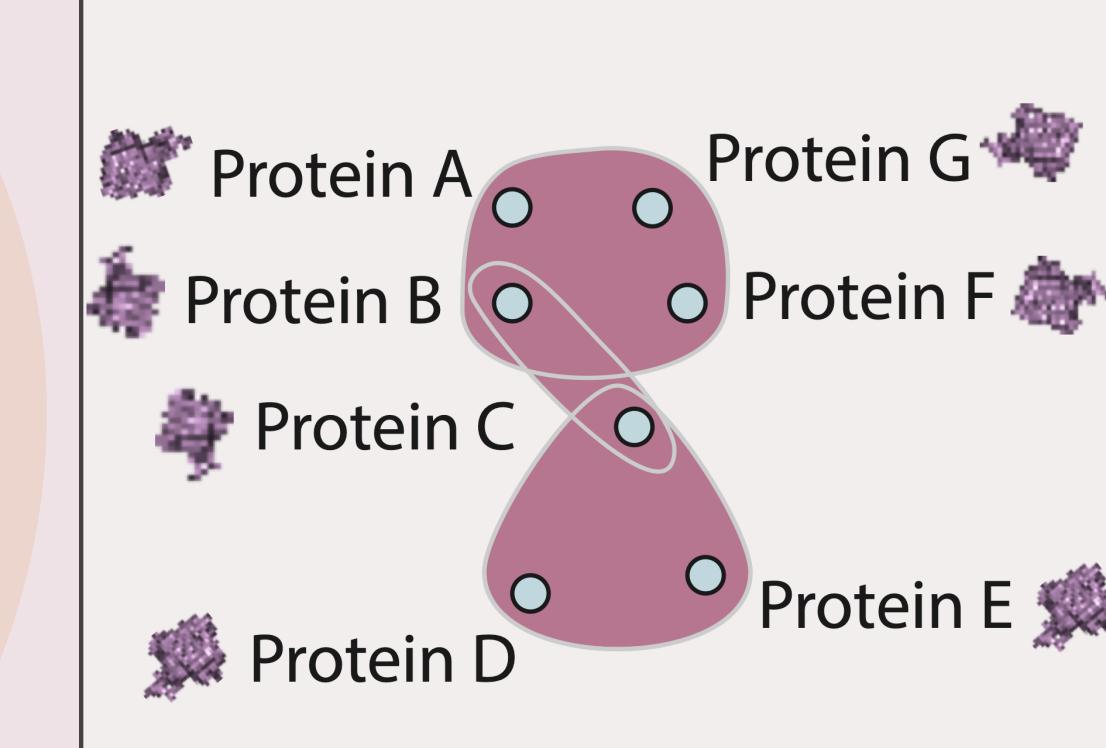
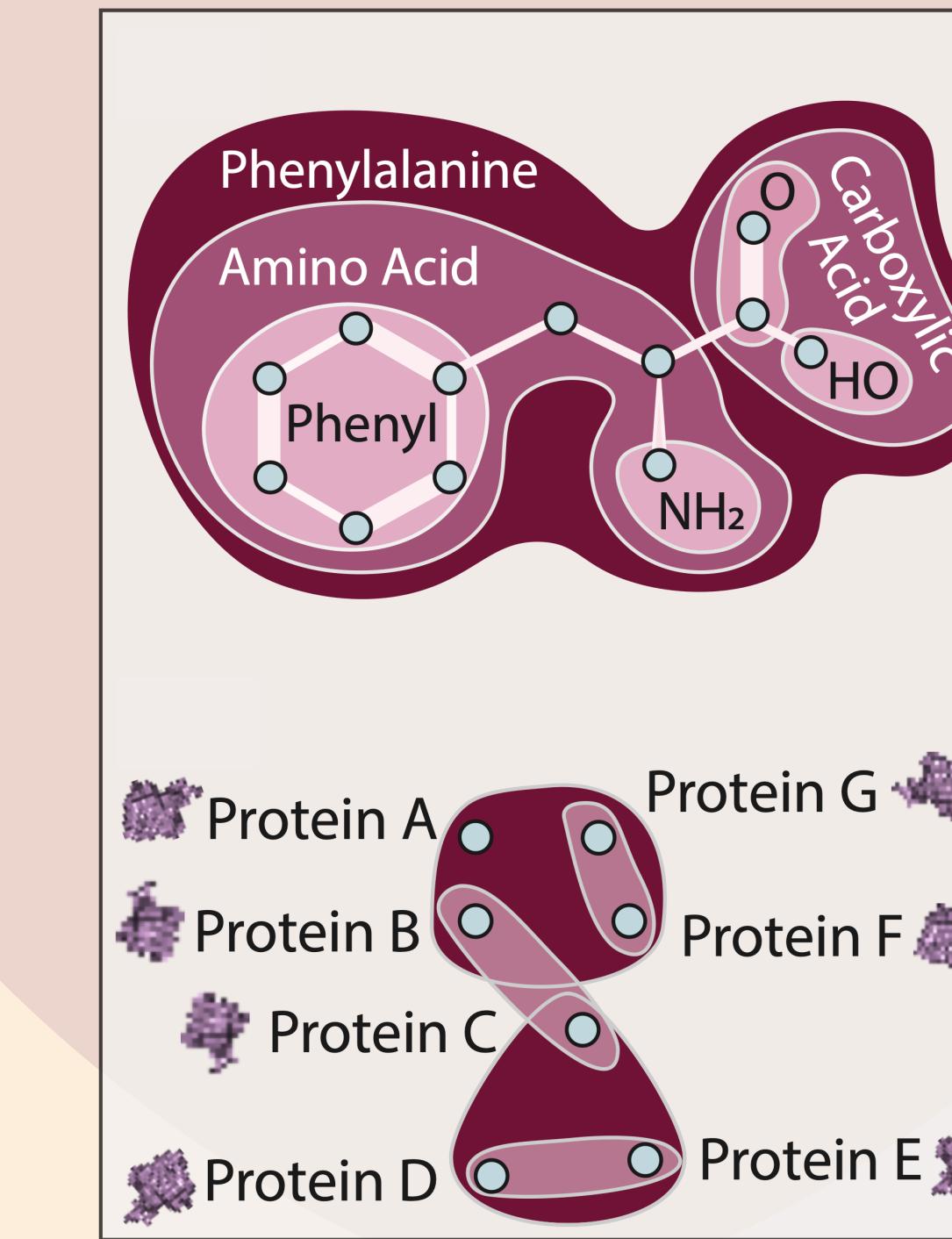
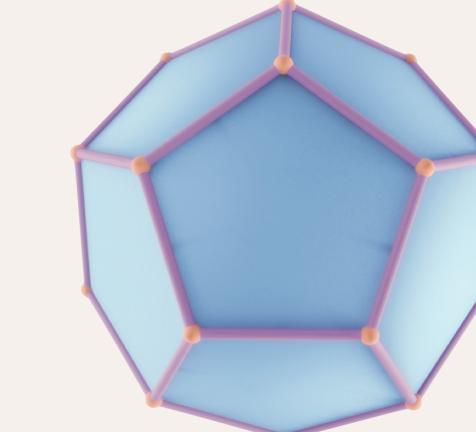
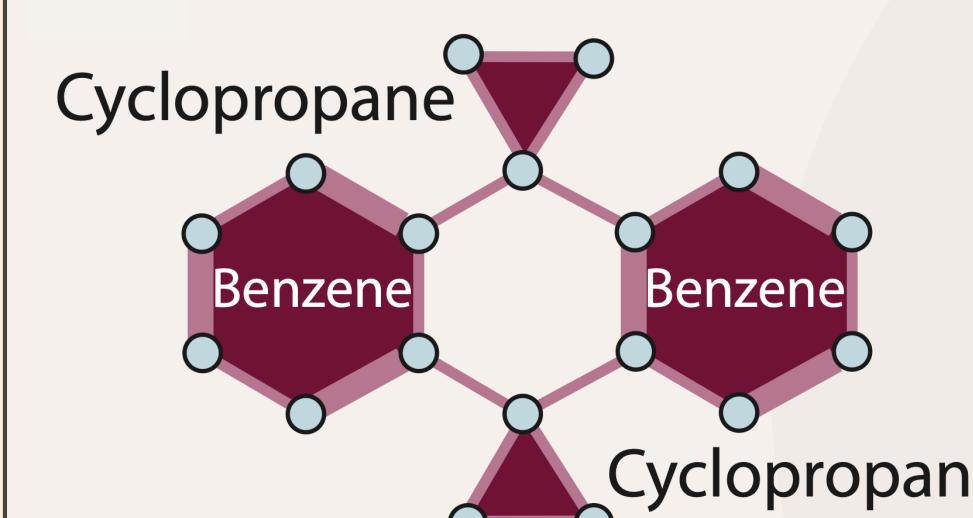
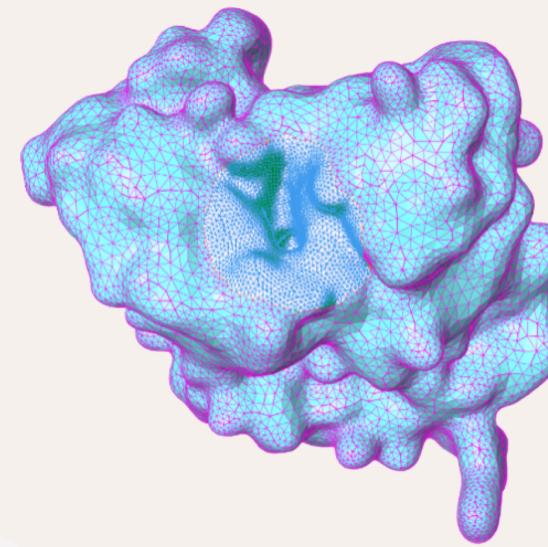
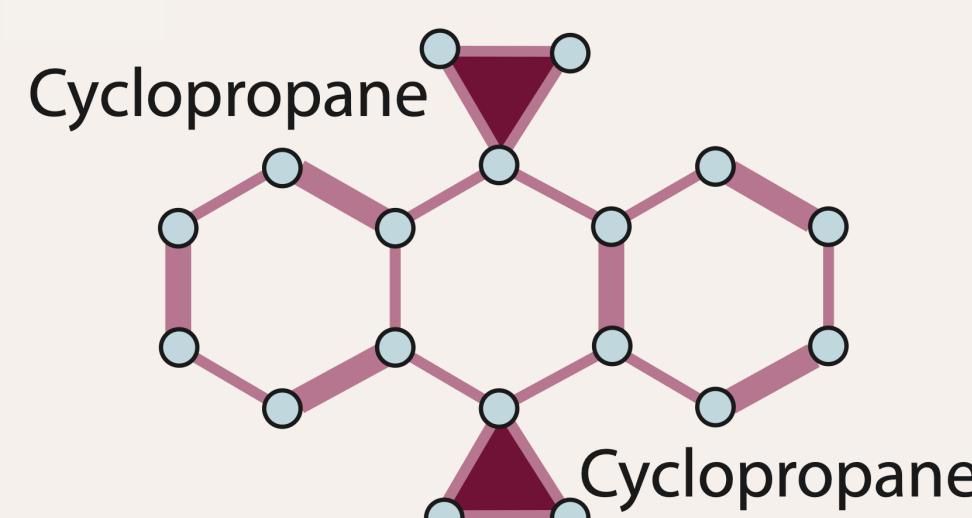
Cellular Complex



Combinatorial Complex



Hypergraph



Does Mupirocin
interact with
Ciprofloxacin?

What are the properties of this molecule?

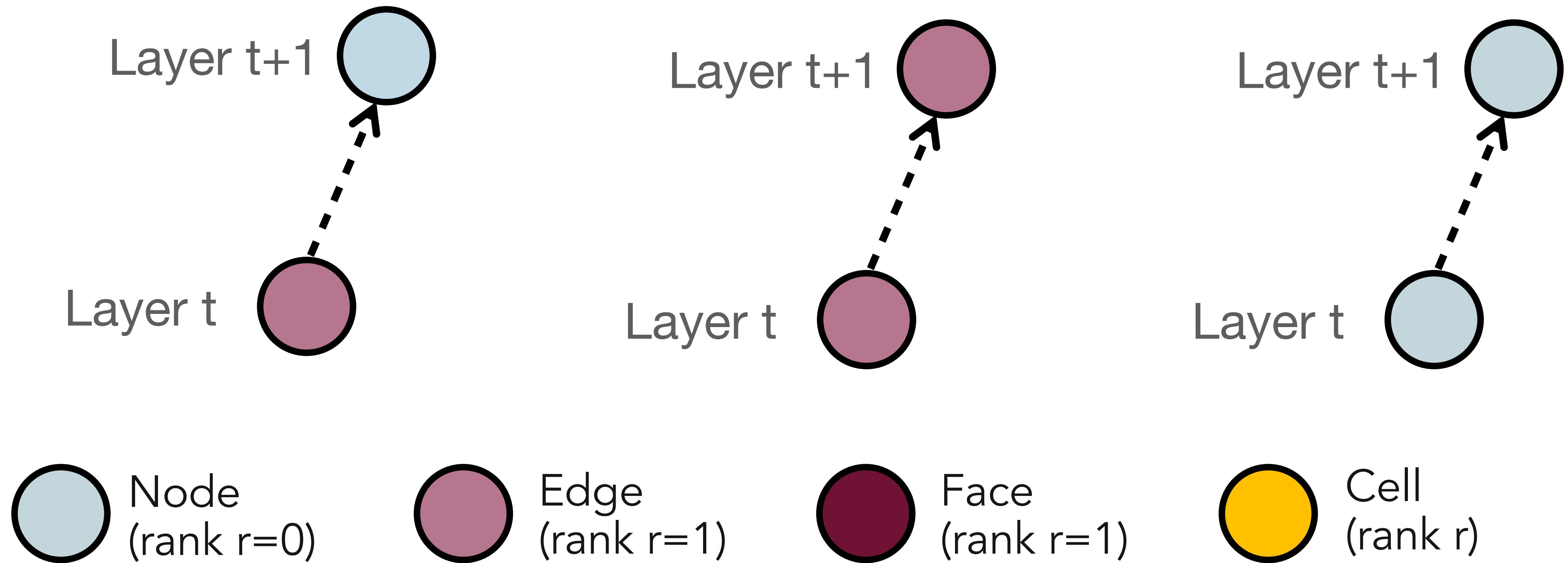
The Framework

2. Mechanism: Message passing

The Framework

2. Mechanism: Message passing

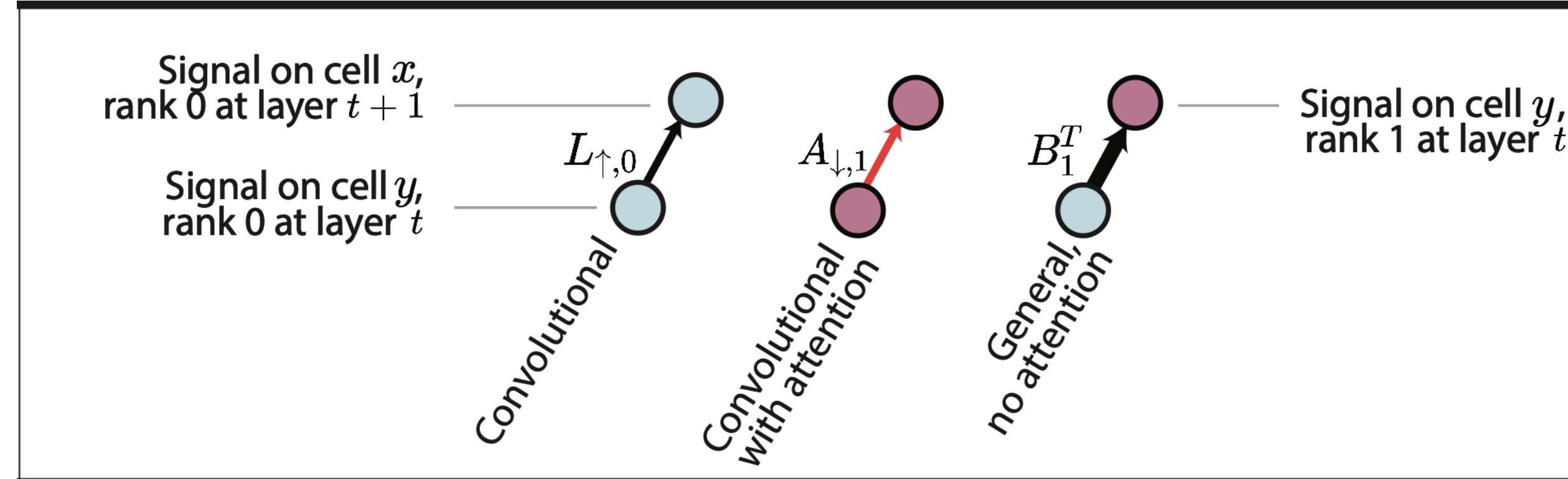
Which “cells” send messages to which “cells”:



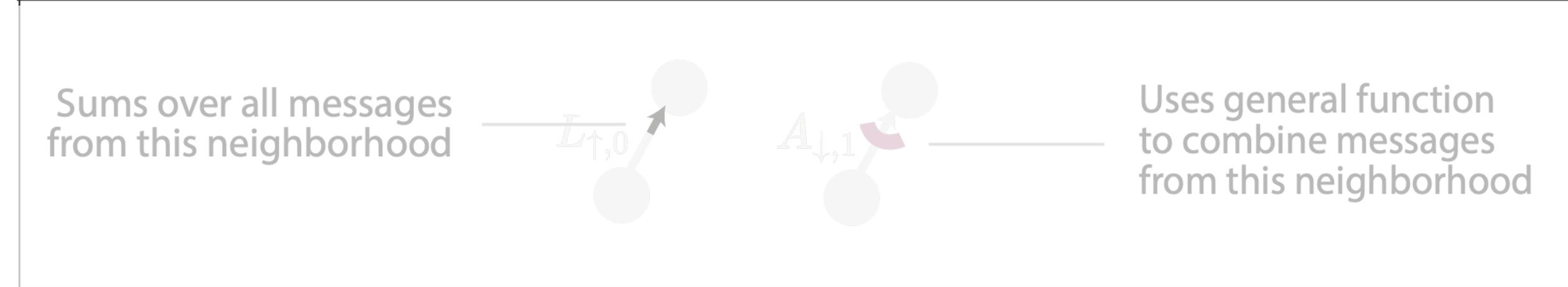
The Framework

2. Mechanism: Message passing

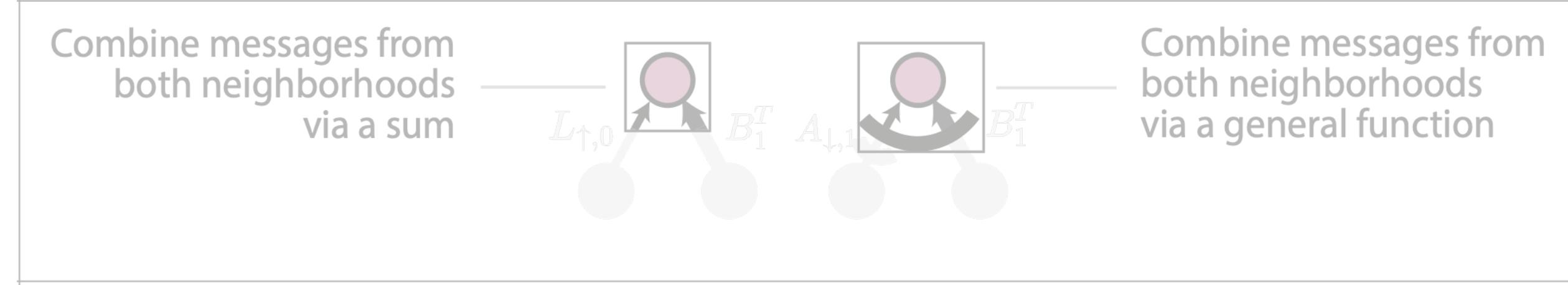
1. Define message



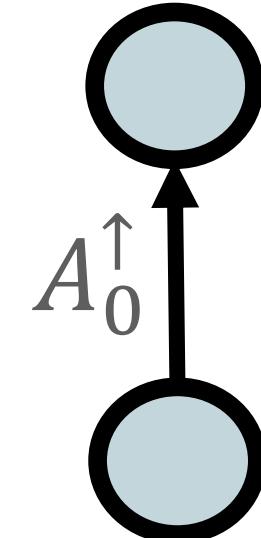
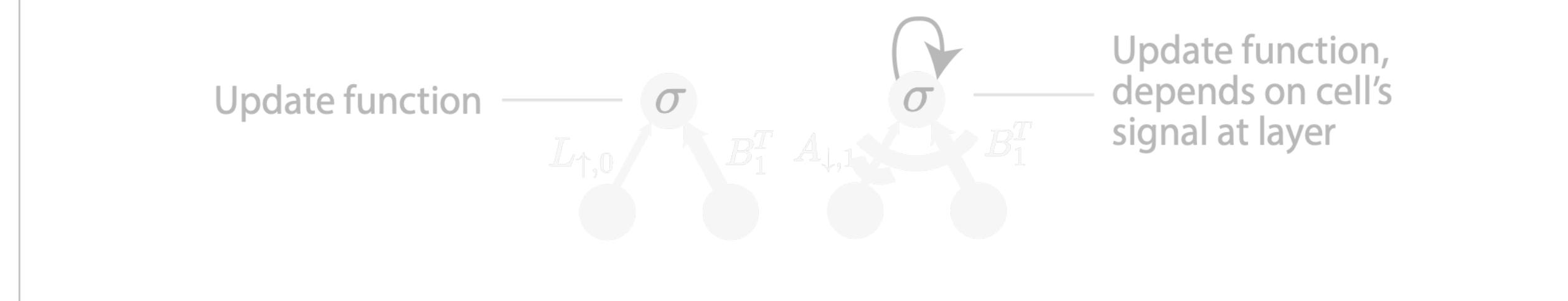
2. Aggregate intra-neighborhood



3. Aggregate inter-neighborhood



4. Update

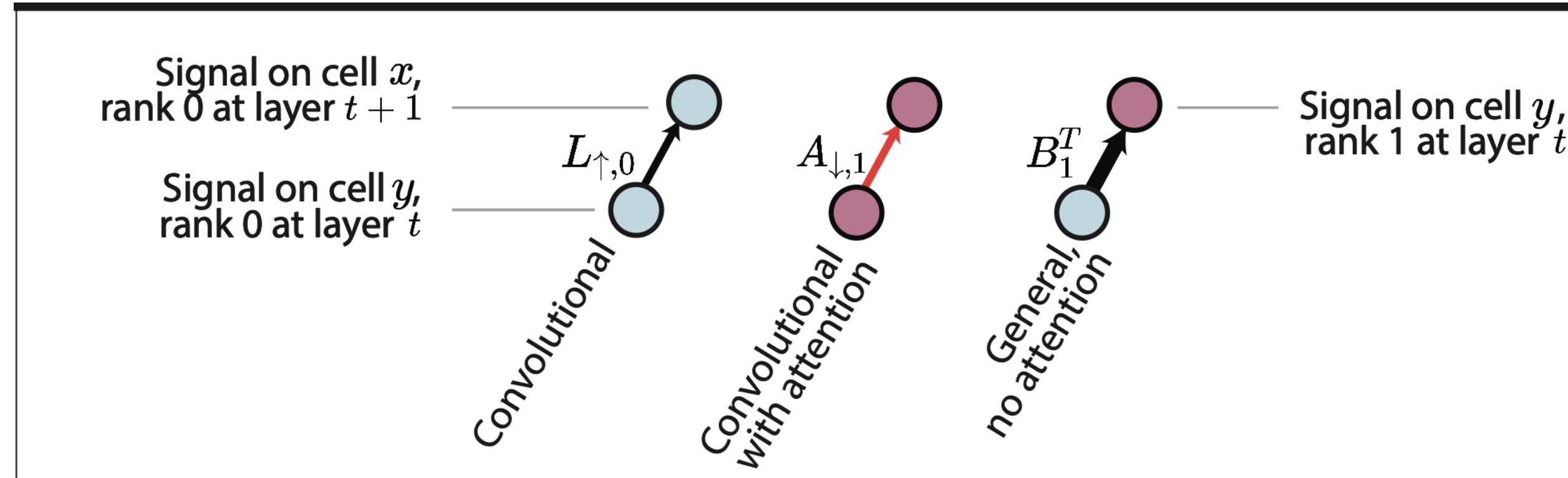


Graph Convolutional Network

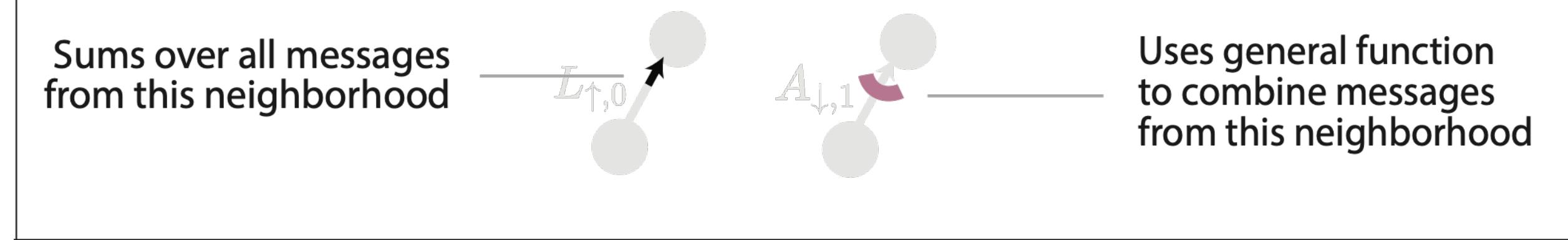
The Framework

2. Mechanism: Message passing

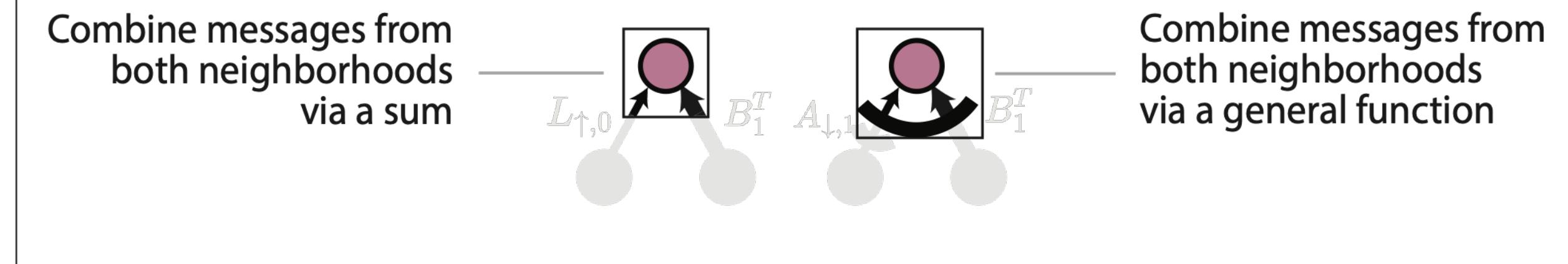
1. Define message



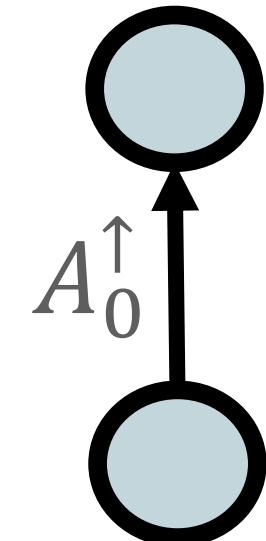
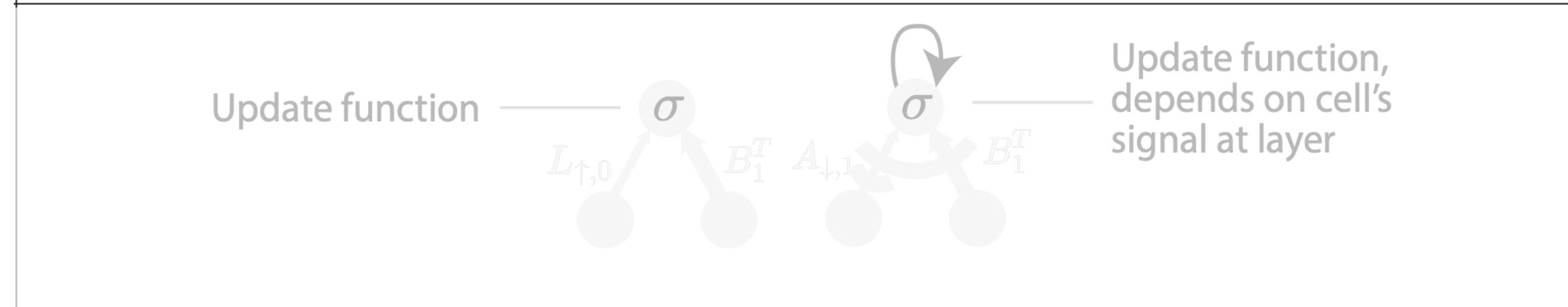
2. Aggregate intra-neighborhood



3. Aggregate inter-neighborhood



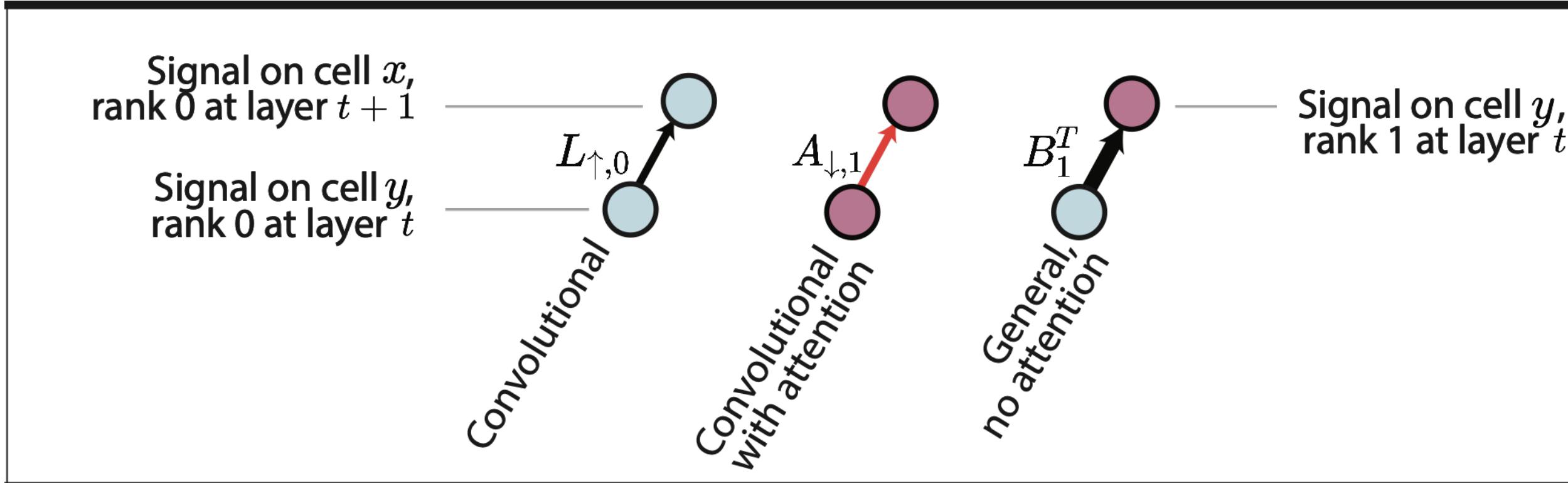
4. Update



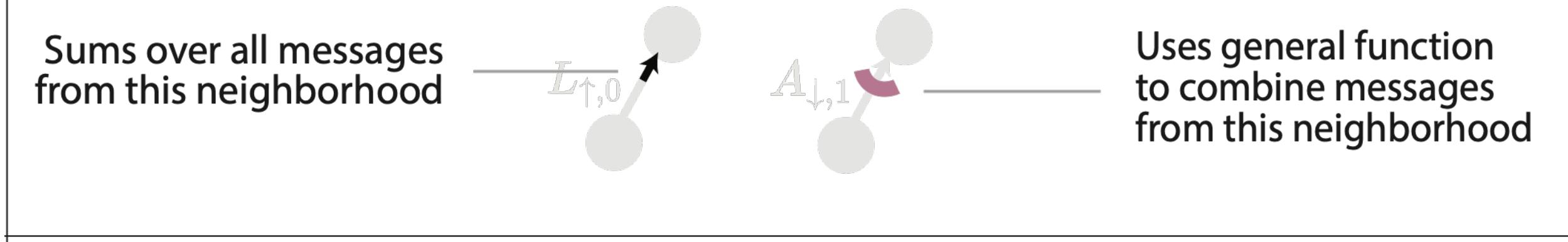
The Framework

2. Mechanism: Message passing

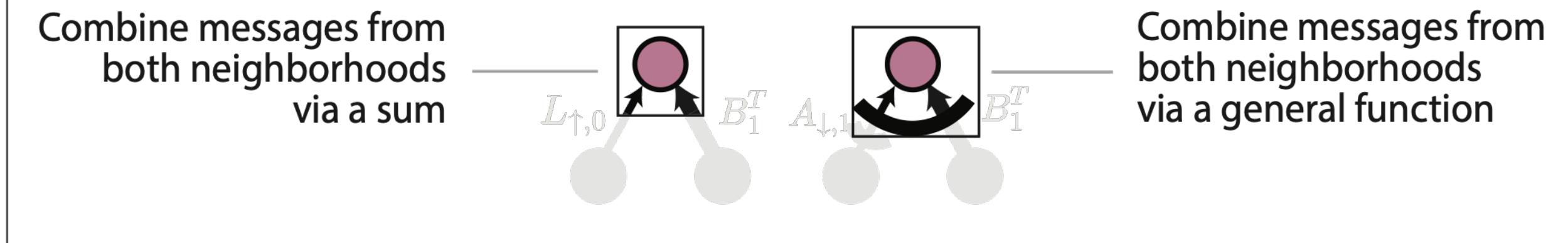
1. Define message



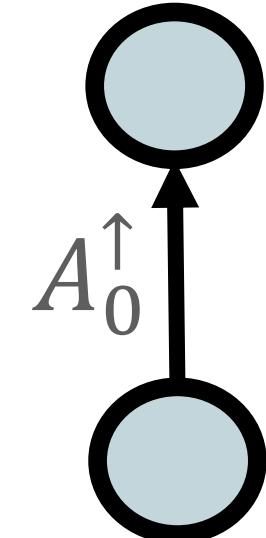
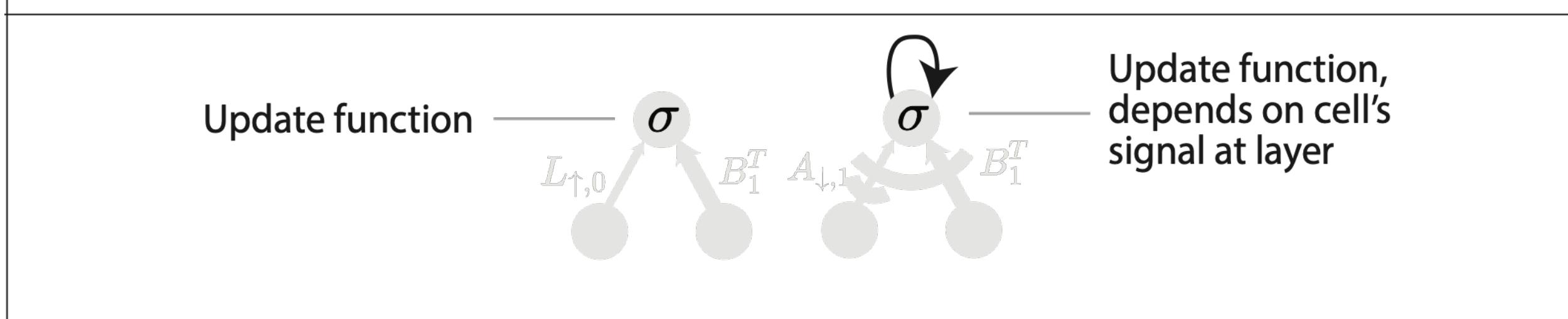
2. Aggregate intra-neighborhood



3. Aggregate inter-neighborhood



4. Update

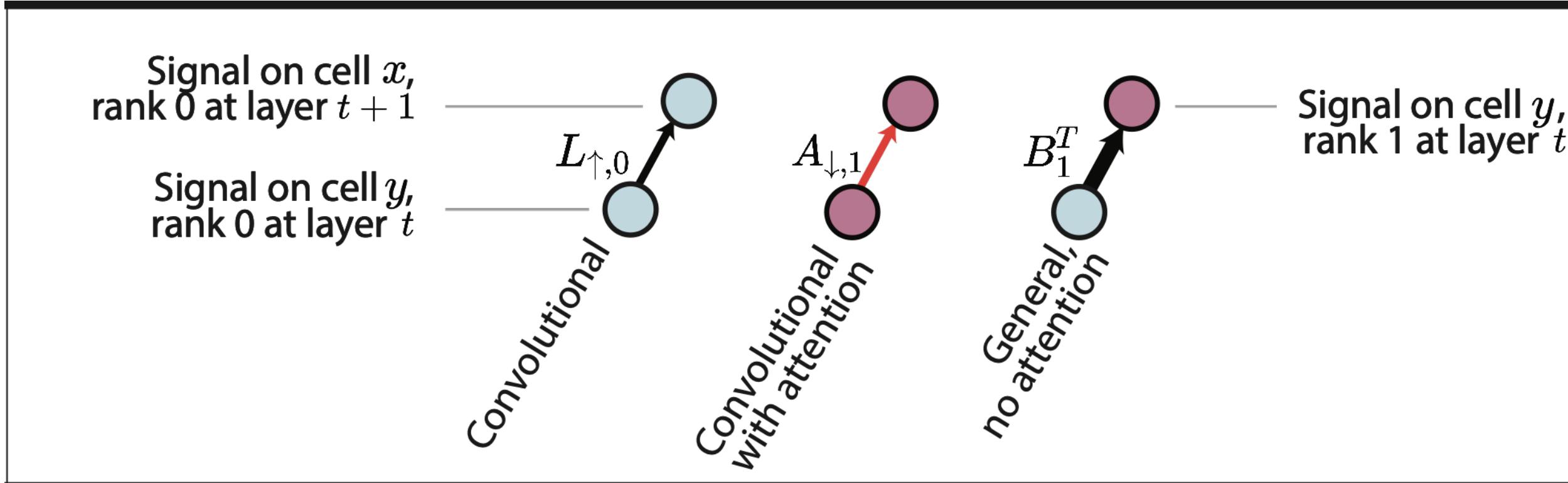


Graph Convolutional Network

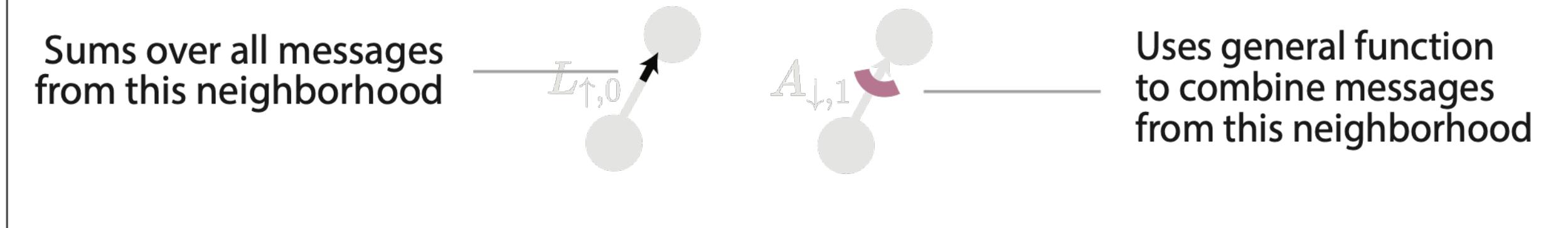
The Framework

2. Mechanism: Message passing

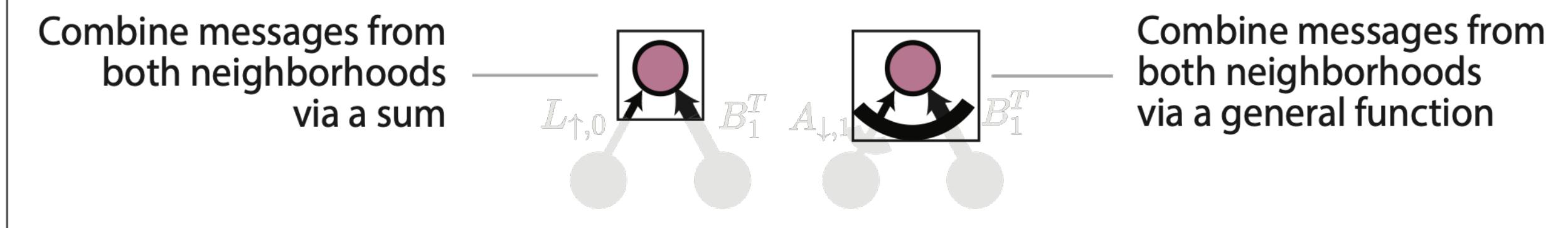
1. Define message



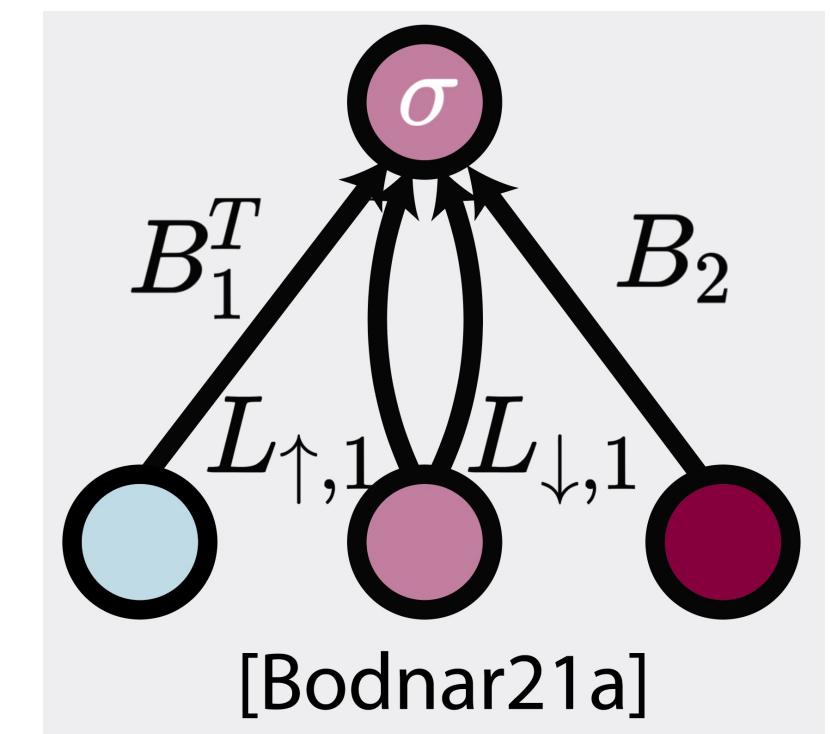
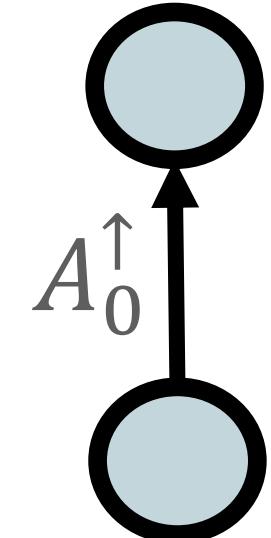
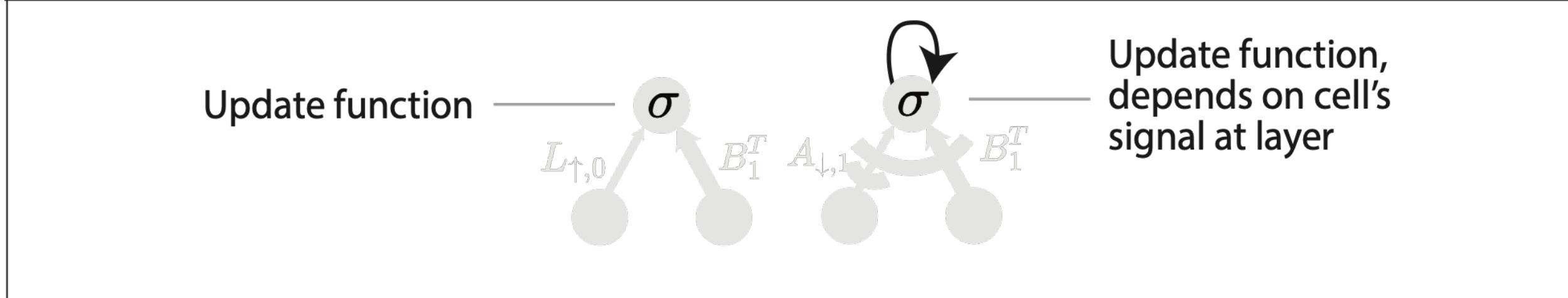
2. Aggregate intra-neighborhood



3. Aggregate inter-neighborhood



4. Update

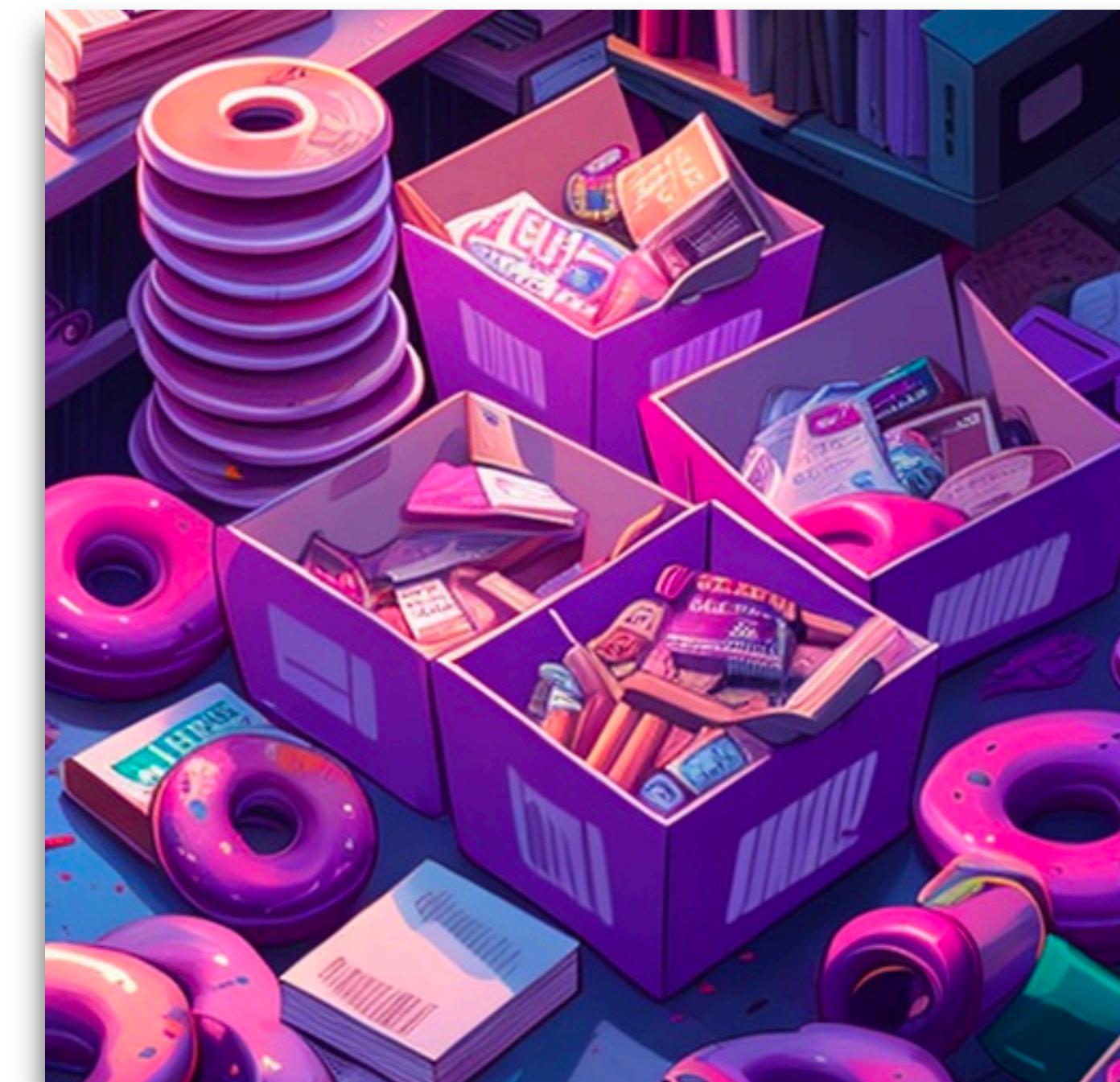


Message Passing Simplicial Network

Outline

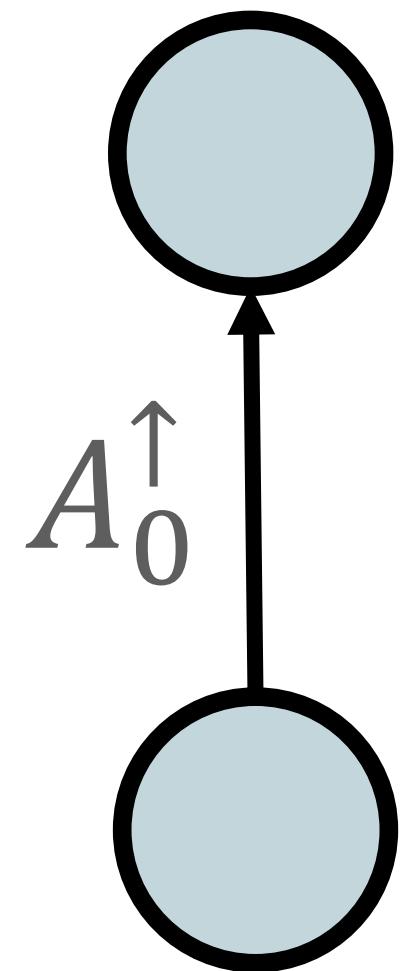


Graphical Framework



Survey of the literature

Beyond Graph Convolutional Network:

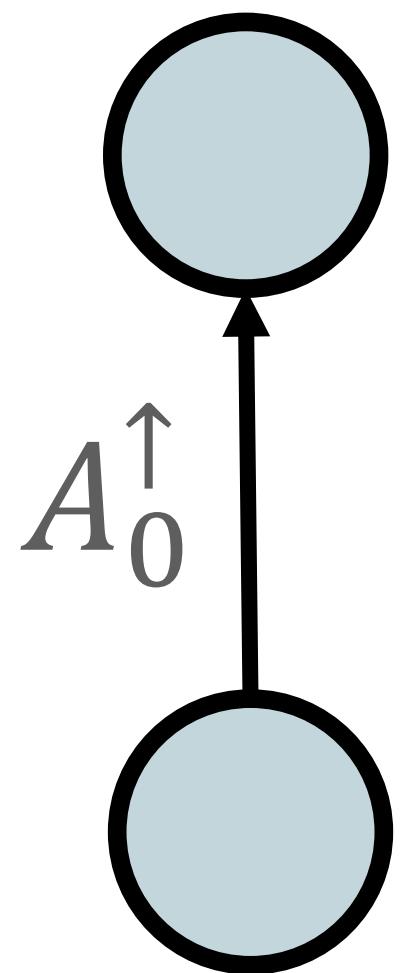


Domain ↓	← Message Passing Type →	
	Standard Convolutional	Attentional Convolutional/General
Hypergraph		
Simplicial		
Cellular		
Combinatorial		

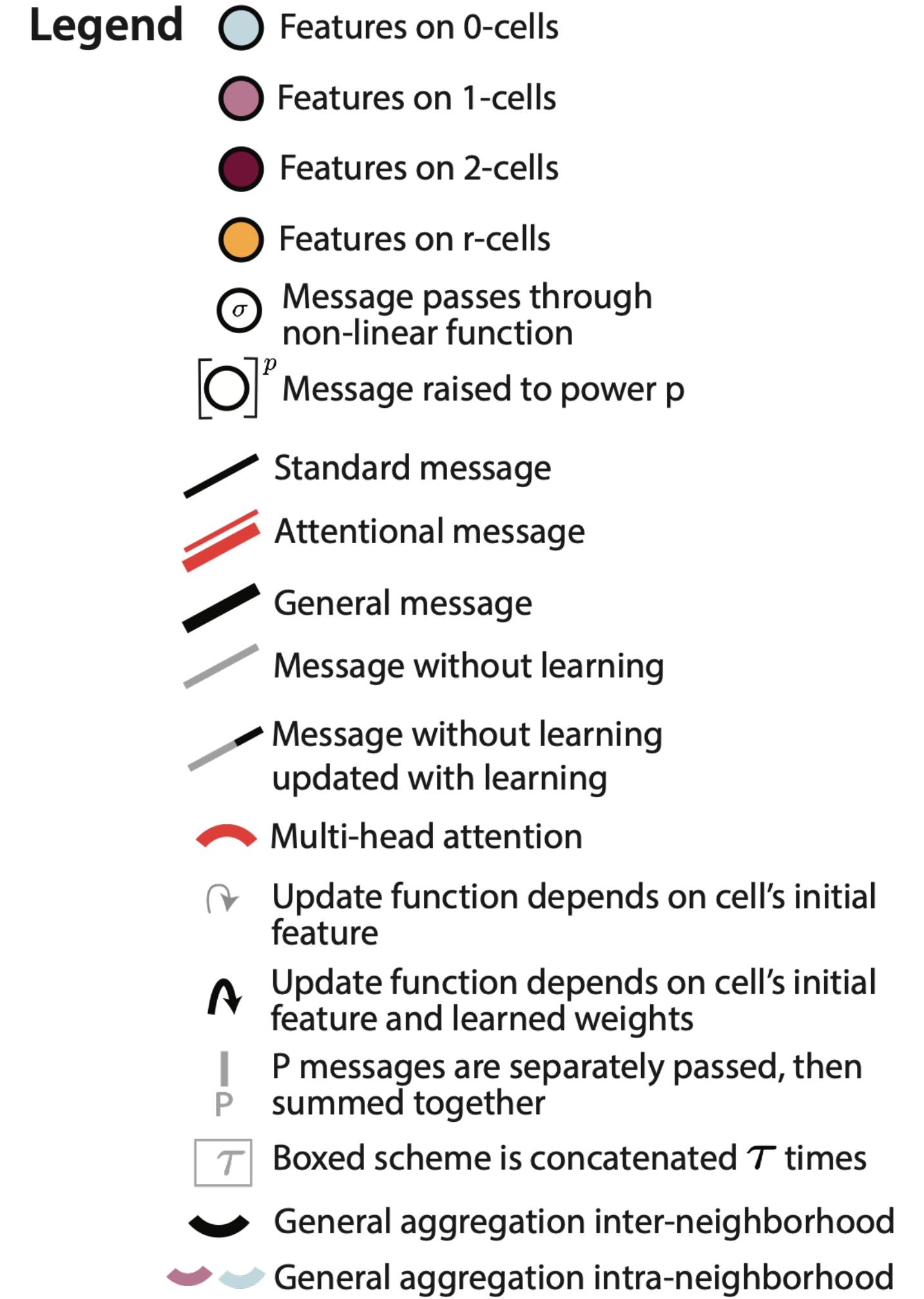
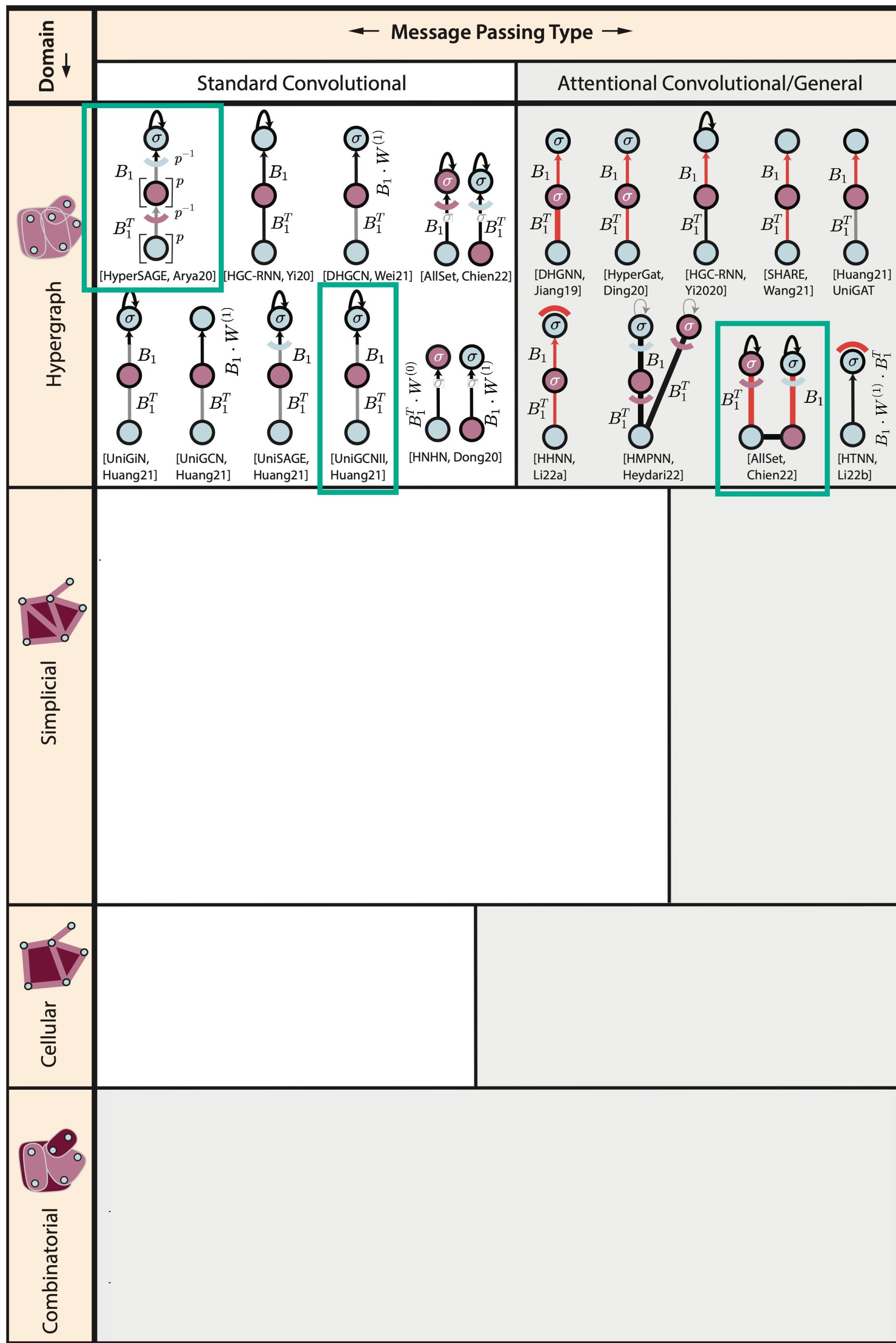
- Legend**
- Features on 0-cells
 - Features on 1-cells
 - Features on 2-cells
 - Features on r-cells
 - Message passes through non-linear function
 - [O]^p Message raised to power p
 - Standard message
 - Attentional message
 - General message
 - Message without learning
 - Message without learning updated with learning
 - Multi-head attention
 - ⟳ Update function depends on cell's initial feature
 - ⟳ Update function depends on cell's initial feature and learned weights
 - P P messages are separately passed, then summed together
 - T Boxed scheme is concatenated \mathcal{T} times
 - General aggregation inter-neighborhood
 - General aggregation intra-neighborhood

Survey of the literature

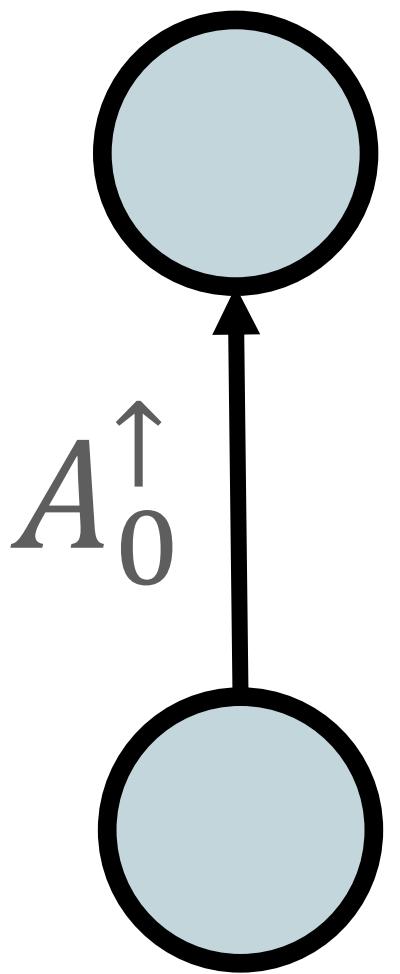
Beyond Graph Convolutional Network:



Survey of the literature



Beyond Graph Convolutional Network:

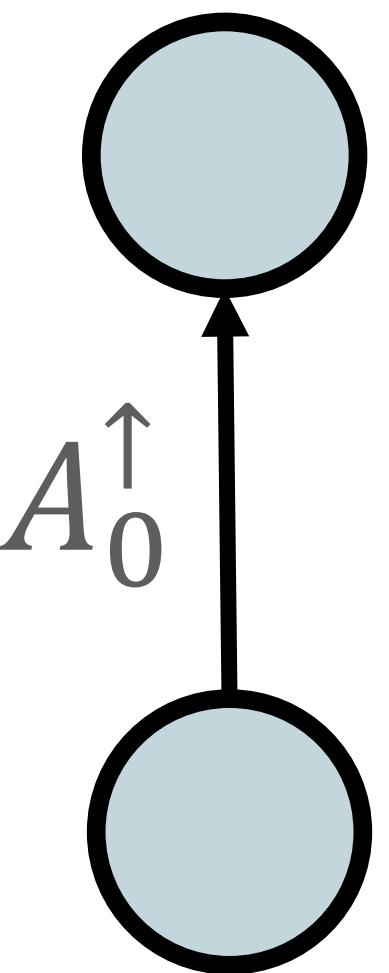


Domain ↓	← Message Passing Type →	
	Standard Convolutional	Attentional Convolutional/General
Hypergraph	<p>[HyperSAGE, Arya20] [HGC-RNN, Yi20] [DHGCN, Wei21] [AllSet, Chien22]</p> <p>[DHGNN, Jiang19] [HyperGat, Ding20] [HGC-RNN, Yi2020] [SHARE, Wang21] [UniGAT]</p>	<p>[UniGIN, Huang21] [UniGCN, Huang21] [UniSAGE, Huang21] [UniGCNII, Huang21] [HNHN, Dong20]</p> <p>[HHNN, Li22a] [HMPNN, Hevdar22] [AllSet, Chien22] [HTNN, Li22b]</p>
Simplicial	<p>[SNN, Ebli20] [SCCONV, Bunch20]</p> <p>[SCN, Yang22c] [SCN, Yang22c]</p>	<p>[SCoNe, Roddenberry21] [SCNN, Yang22b] [SCCNN, Yang23] [Dist. Cycle, Kero22] [SGCN, Chen22]</p> <p>[SAN, Giusti22a] [SAT, Goh22] [MPSN, Bodnar21a] [HSN, Hajij22b] [SCA, Hajij22c]</p>
Cellular		
Combinatorial		

- Legend**
- Features on 0-cells
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Survey of the literature

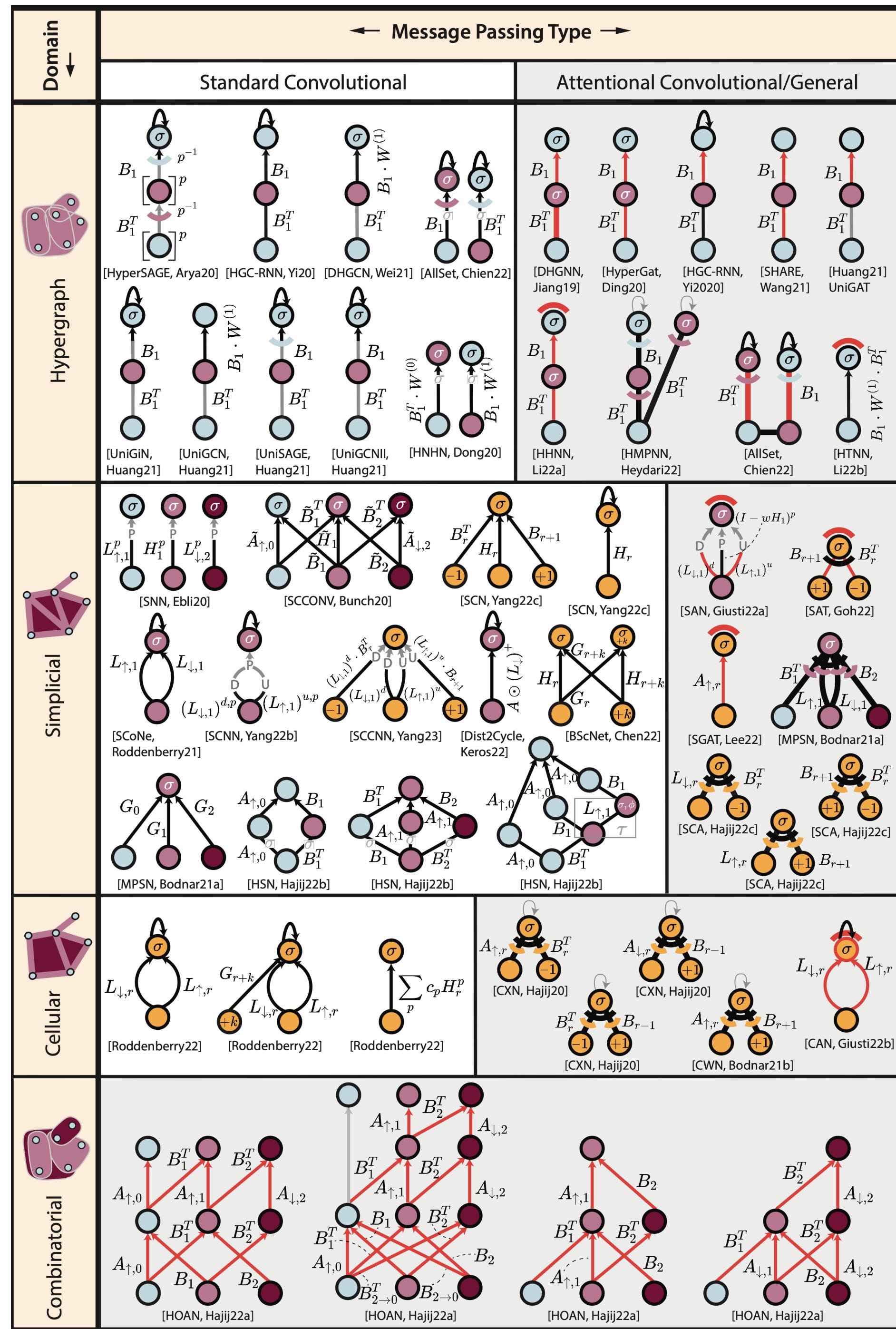
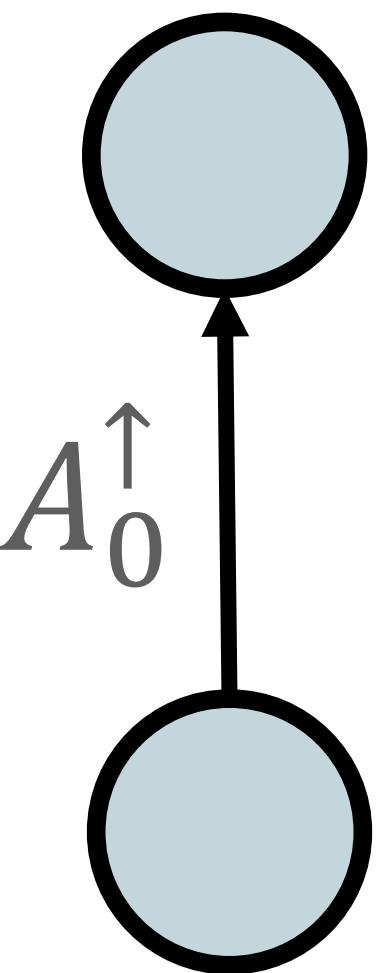
Beyond Graph Convolutional Network:



Domain ↓	← Message Passing Type →	
	Standard Convolutional	Attentional Convolutional/General
Hypergraph	<p>[HyperSAGE, Arya20] [HGC-RNN, Yi20] [DHGCN, Wei21] [AllSet, Chien22]</p> <p>[UniGIN, Huang21] [UniGCN, Huang21] [UniSAGE, Huang21] [UniGCNII, Huang21]</p> <p>[HNHN, Dong20]</p> <p>[HHNN, Li22a]</p> <p>[DHGNN, Jiang19]</p> <p>[HyperGat, Ding20]</p> <p>[HGC-RNN, Yi2020]</p> <p>[SHARE, Wang21]</p> <p>[Huang21]</p> <p>[UniGAT]</p>	<p>[AllSet, Chien22]</p> <p>[HTNN, Li22b]</p>
Simplicial	<p>[SNN, Eidi20]</p> <p>[SCCONV, Bunch20]</p> <p>[SCN, Yang22c]</p> <p>[SAN, Giusti22a]</p> <p>[SAT, Goh22]</p> <p>[SCoNe, Roddenberry21]</p> <p>[CNN, Yang22b]</p> <p>[SCCNN, Yang23]</p> <p>[Dist2Cycle, Keros22]</p> <p>[BScNet, Chen22]</p> <p>[SGAT, Lee22]</p> <p>[MPSN, Bodnar21a]</p> <p>[SCA, Hajij22c]</p> <p>[SCA, Hajij22c]</p> <p>[SCA, Hajij22c]</p> <p>[SCA, Hajij22c]</p>	<p>[HSN, Hajij22b]</p> <p>[HSN, Hajij22b]</p> <p>[HSN, Hajij22b]</p>
Cellular	<p>[Roddenberry22]</p> <p>[Roddenberry22]</p> <p>Roddenberry22</p>	<p>[CXN, Hajij20]</p> <p>[CXN, Hajij20]</p> <p>[CWN, Bodnar21a]</p> <p>[CAN, Giusti22b]</p>
Combinatorial		

- Legend**
- Features on 0-cells
 - Features on 1-cells
 - Features on 2-cells
 - Features on r-cells
 - Message passes through non-linear function
 - \square^p Message raised to power p
 - Standard message
 - Attentional message
 - General message
 - Message without learning
 - Message without learning updated with learning
 - Multi-head attention
 - Update function depends on cell's initial feature
 - Update function depends on cell's initial feature and learned weights
 - P messages are separately passed, then summed together
 - \mathcal{T} Boxed scheme is concatenated \mathcal{T} times
 - General aggregation inter-neighborhood
 - General aggregation intra-neighborhood

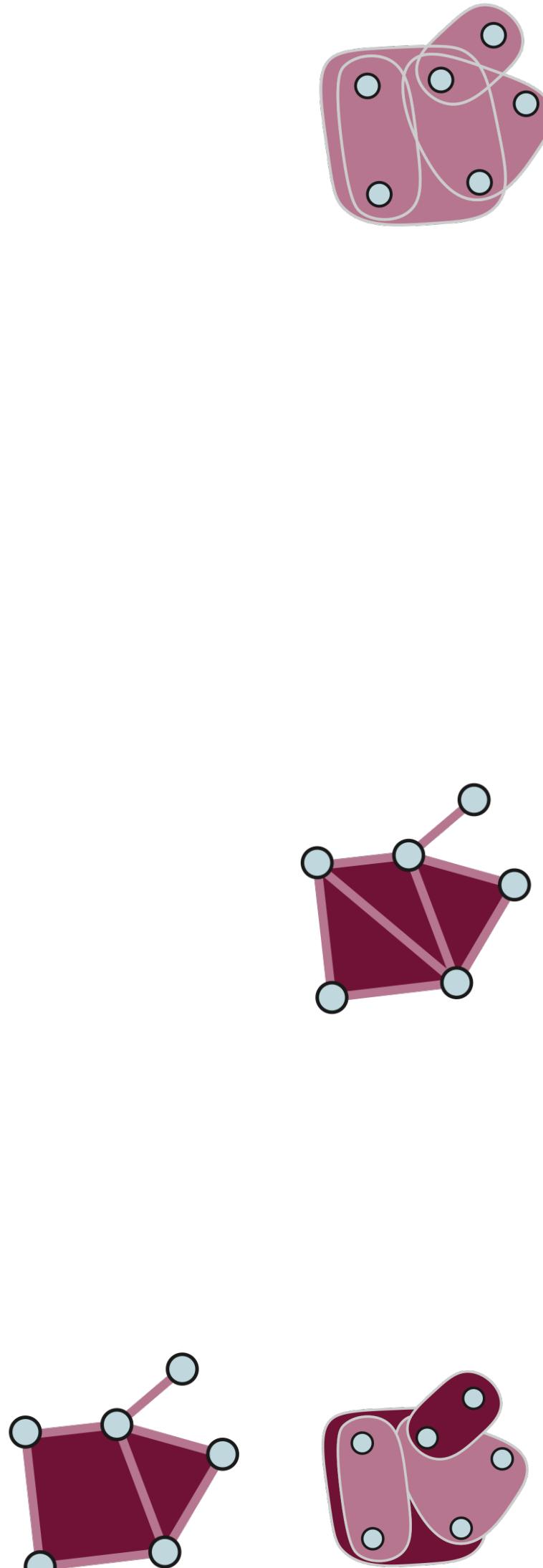
Beyond Graph Convolutional Network:



- Legend**
- Features on 0-cells
 - Features on 1-cells
 - Features on 2-cells
 - Features on r-cells
 - Message passes through non-linear function
 - ^p Message raised to power p
 - Standard message
 - Attentional message
 - General message
 - Message without learning
 - Message without learning updated with learning
 - Multi-head attention
 - Update function depends on cell's initial feature
 - Update function depends on cell's initial feature and learned weights
 - P messages are separately passed, then summed together
 - \mathcal{T} Boxed scheme is concatenated \mathcal{T} times
 - General aggregation inter-neighborhood
 - General aggregation intra-neighborhood

Survey of the literature

How Do These Models Compare?



Domain	Model	Task Level	Task Purpose	Comparisons
SC	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
	MPSN Bodnar et al. (2021a)	✓ ✓	Classification, Trajectory Classification	GNN SOTA
	SCCONV Bunch et al. (2020)	✓	Classification	Graph
CC	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
	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:

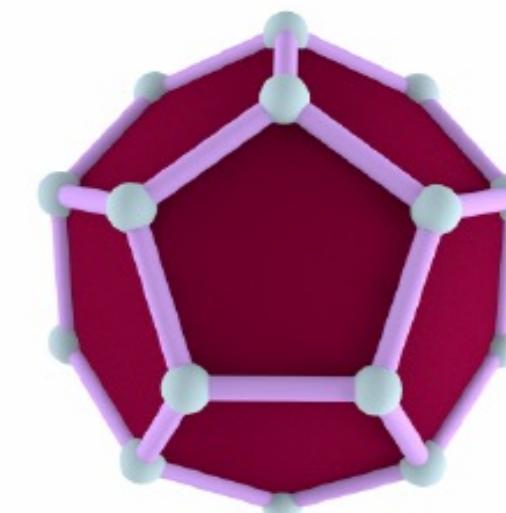
Outperform GNNs

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

Outperform other TNNs

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

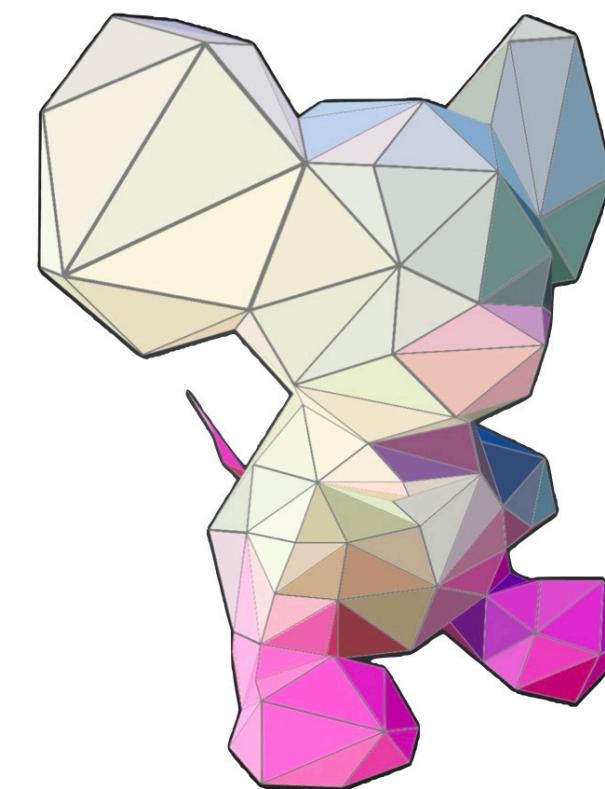
How Do These Models Compare?



PyT

github.com/pyt-team

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



TopoBench

geometric-intelligence/TopoBench

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?

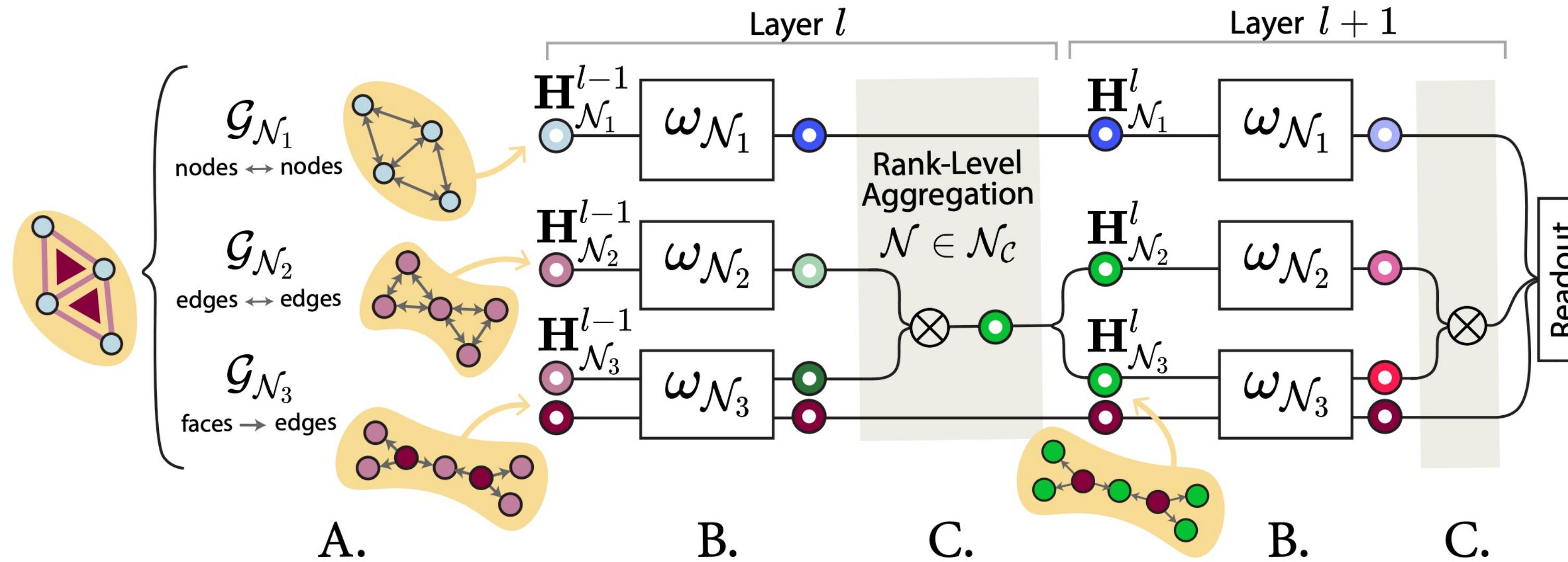


Figure 1. Generalized Combinatorial Complex Network (GCCN). The input complex \mathcal{C} has neighborhoods $\mathcal{N}_C = \{\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3\}$. **A.** The complex is expanded into three augmented Hasse graphs $\mathcal{G}_{\mathcal{N}_i}$, $i = \{1, 2, 3\}$, each with features $H_{\mathcal{N}_i}$ 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!

Mathilde Papillon



Sophia Sanborn



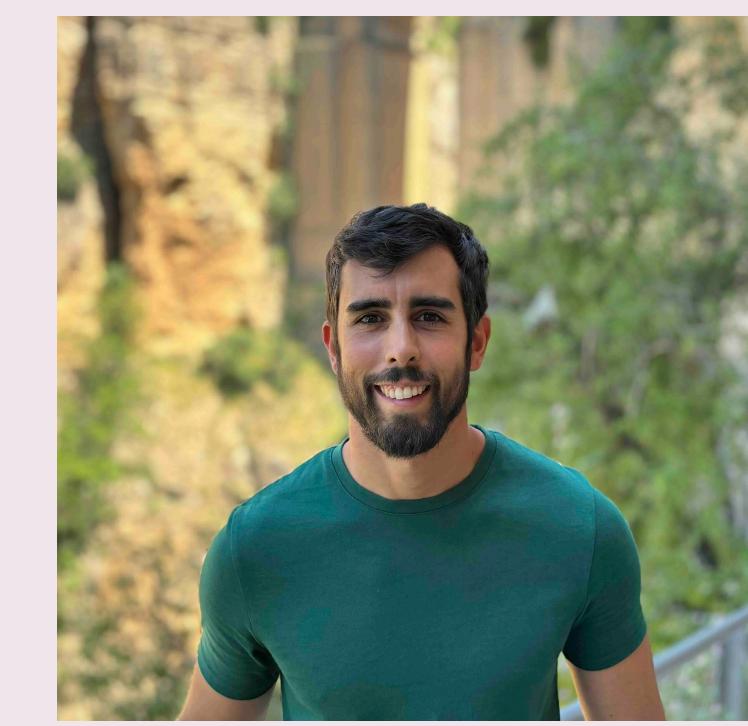
Mustafa Hajij



Lev Telyanikov



Guillermo Bernárdez



Claudio Battiloro



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Hajij et al. (2023). Topological Deep Learning: Going Beyond Graph Data.

Hajij et al. (2024). TopoX: a suite of Python packages for machine learning on topological domains. Journal of Machine Learning Research.

Papillon et al. (2024). TopoTune: A Framework for Generalized Combinatorial Complex Neural Networks.

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



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