GRAPH NEURAL NETWORKS & ROTATIONAL EQUIVARIANCE

University of California, Berkeley Fall 2023, CS 189/289A: Introduction to Machine Learning

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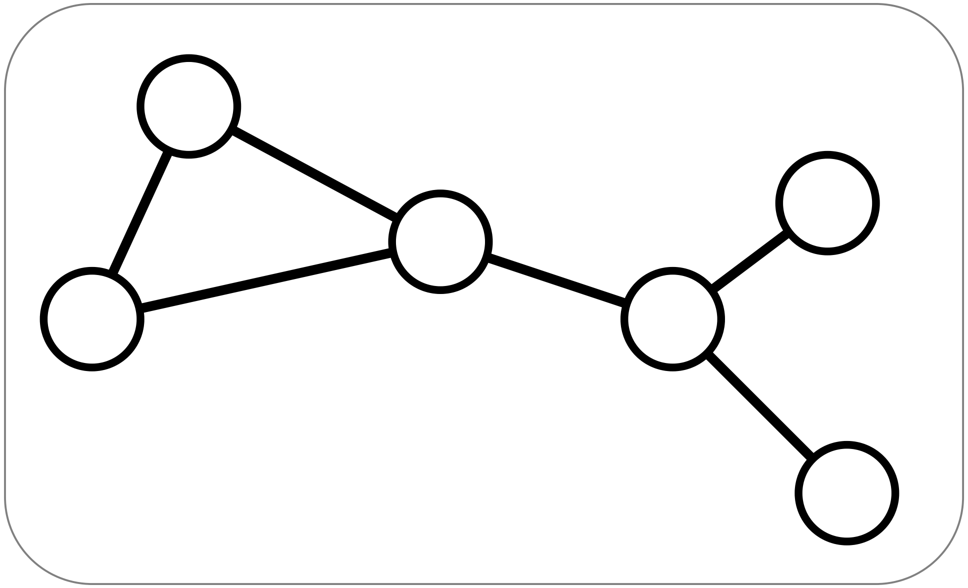
Building on slides originally made by Daniel Rothchild

OUTLINE

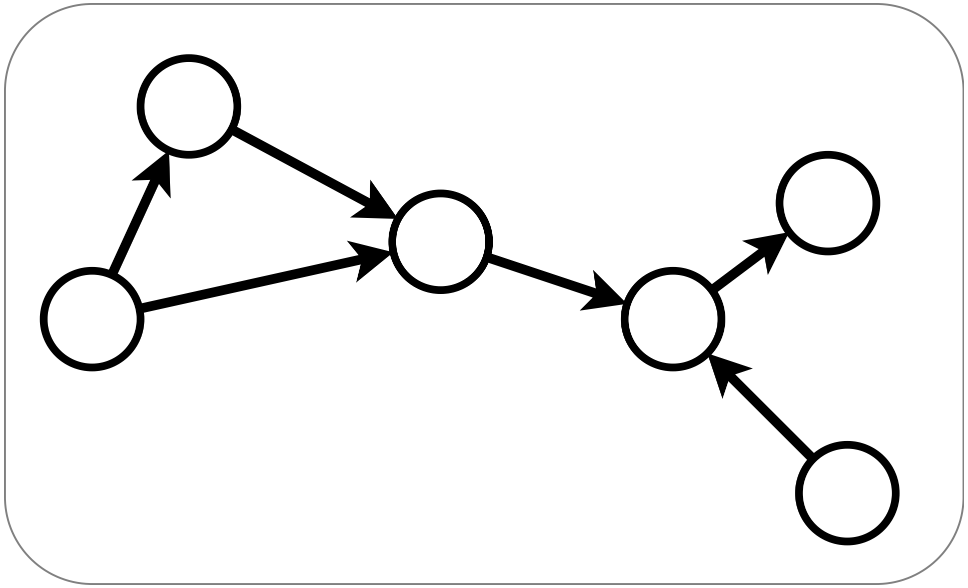
- Lecture 1
  - Graph data
  - Graph tasks
  - Invariance and equivariance
  - Message passing
- Lecture 2
  - Rotational equivariance
  - Equivariant neural networks

GRAPH DATA

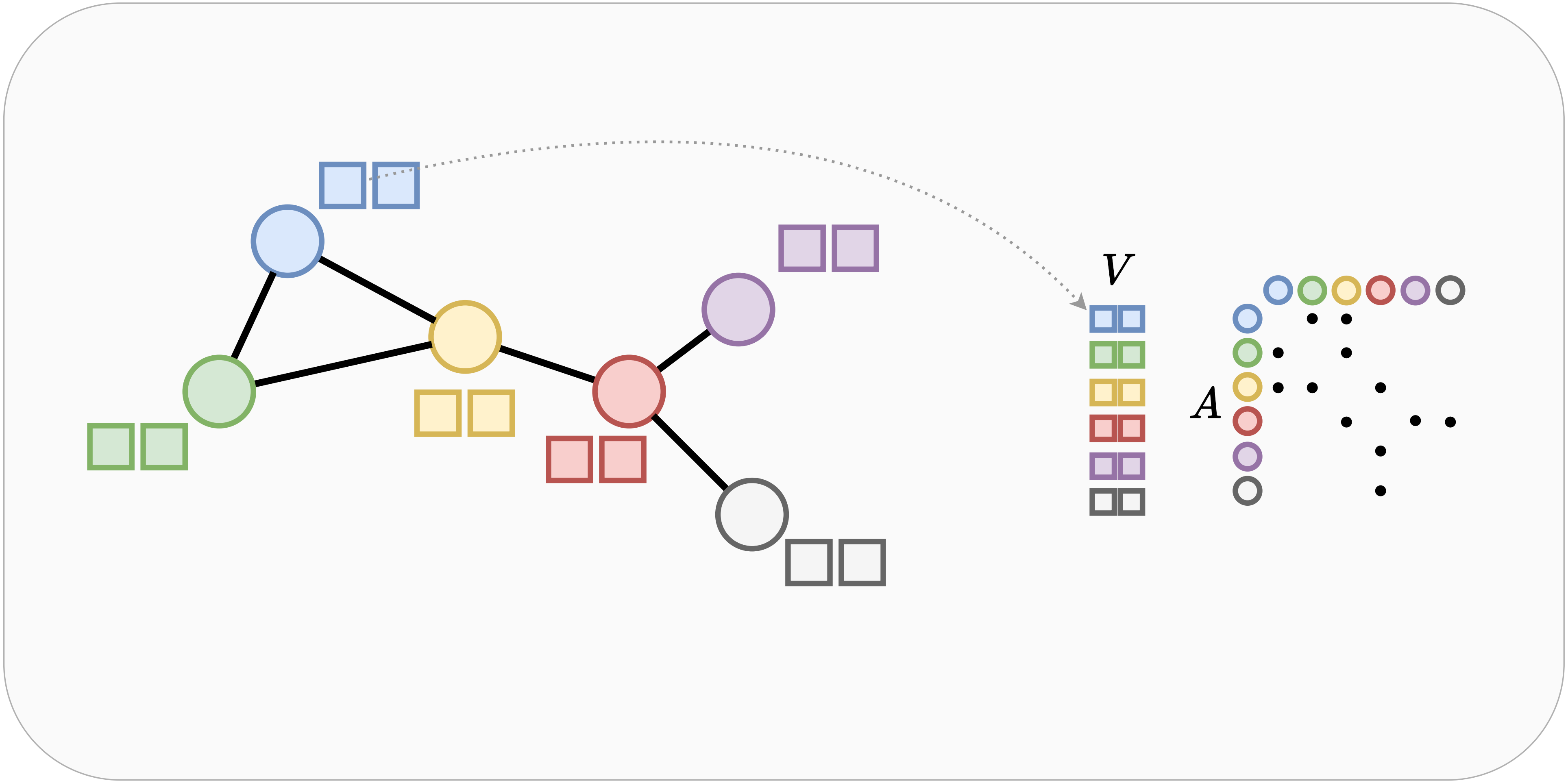
GRAPH



GRAPH



REPRESENTING A GRAPH



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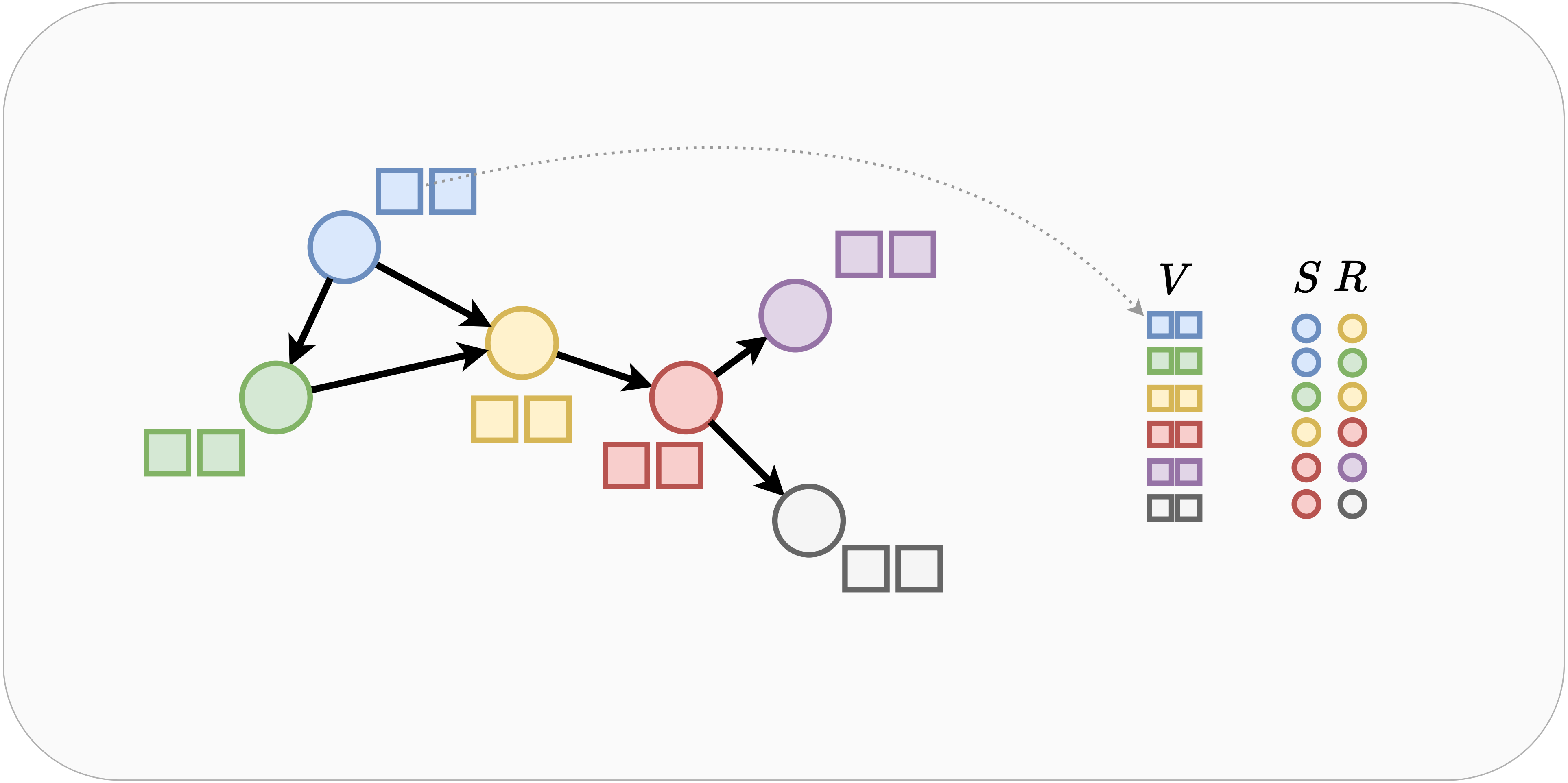

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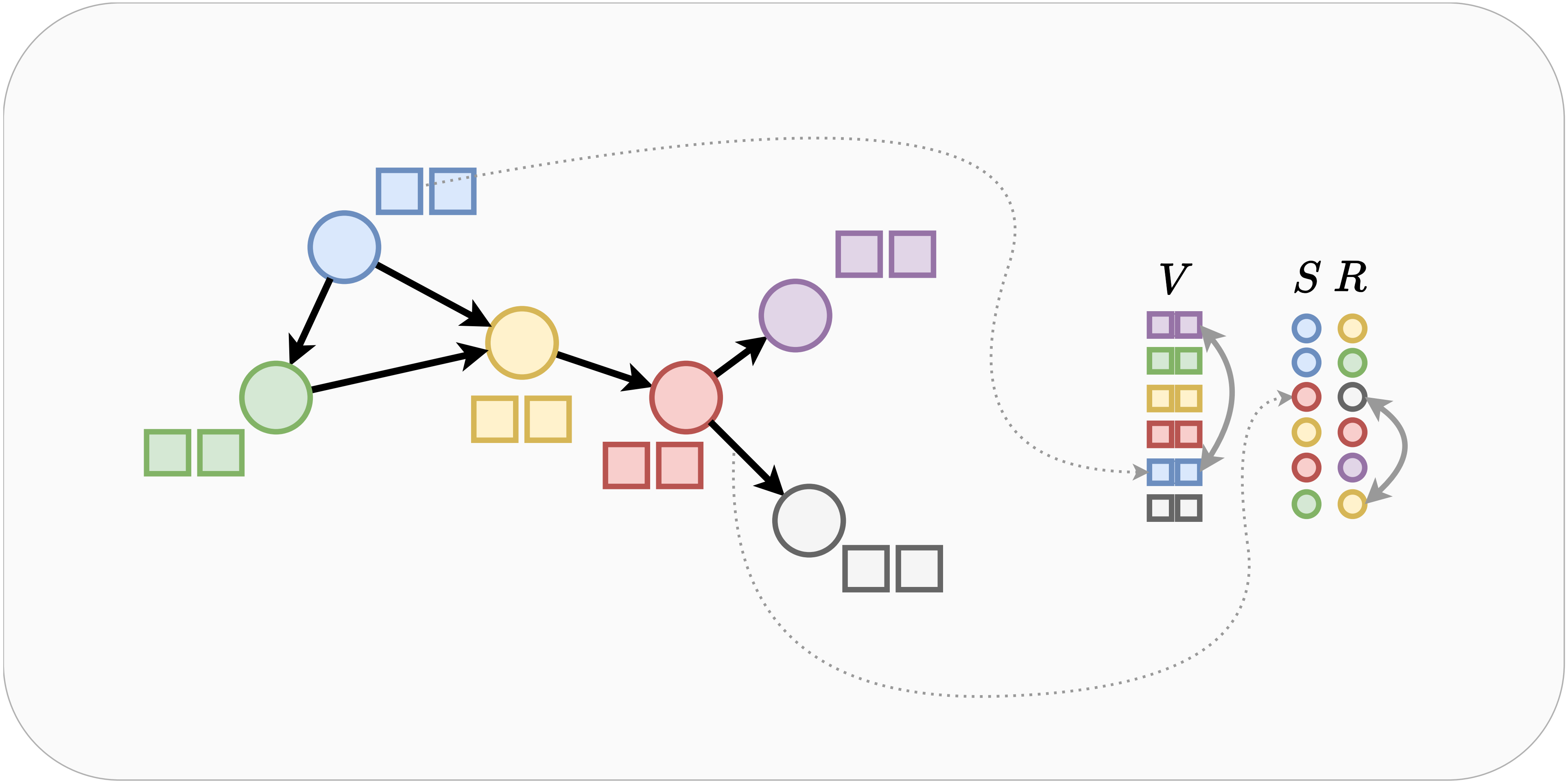

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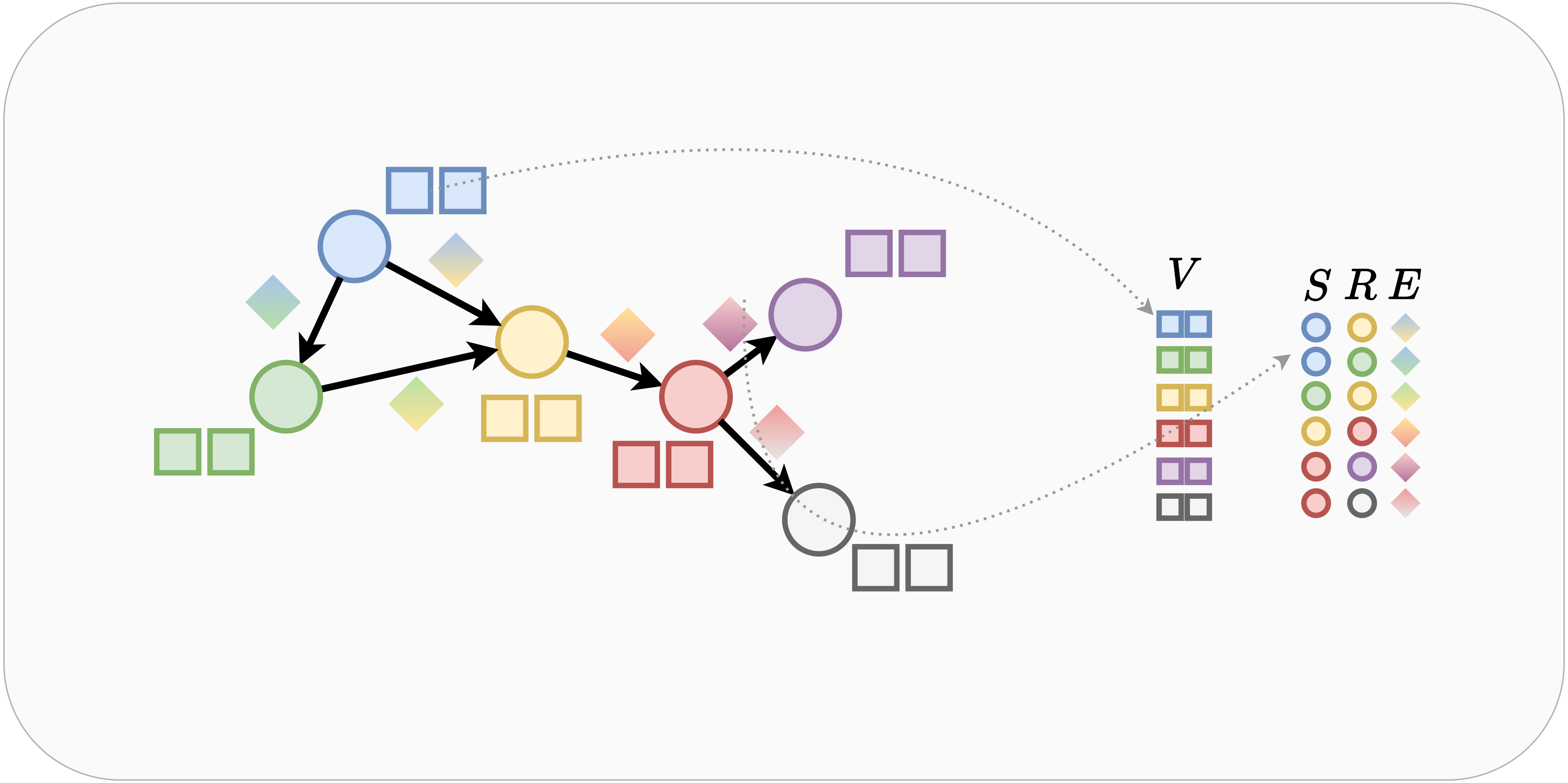

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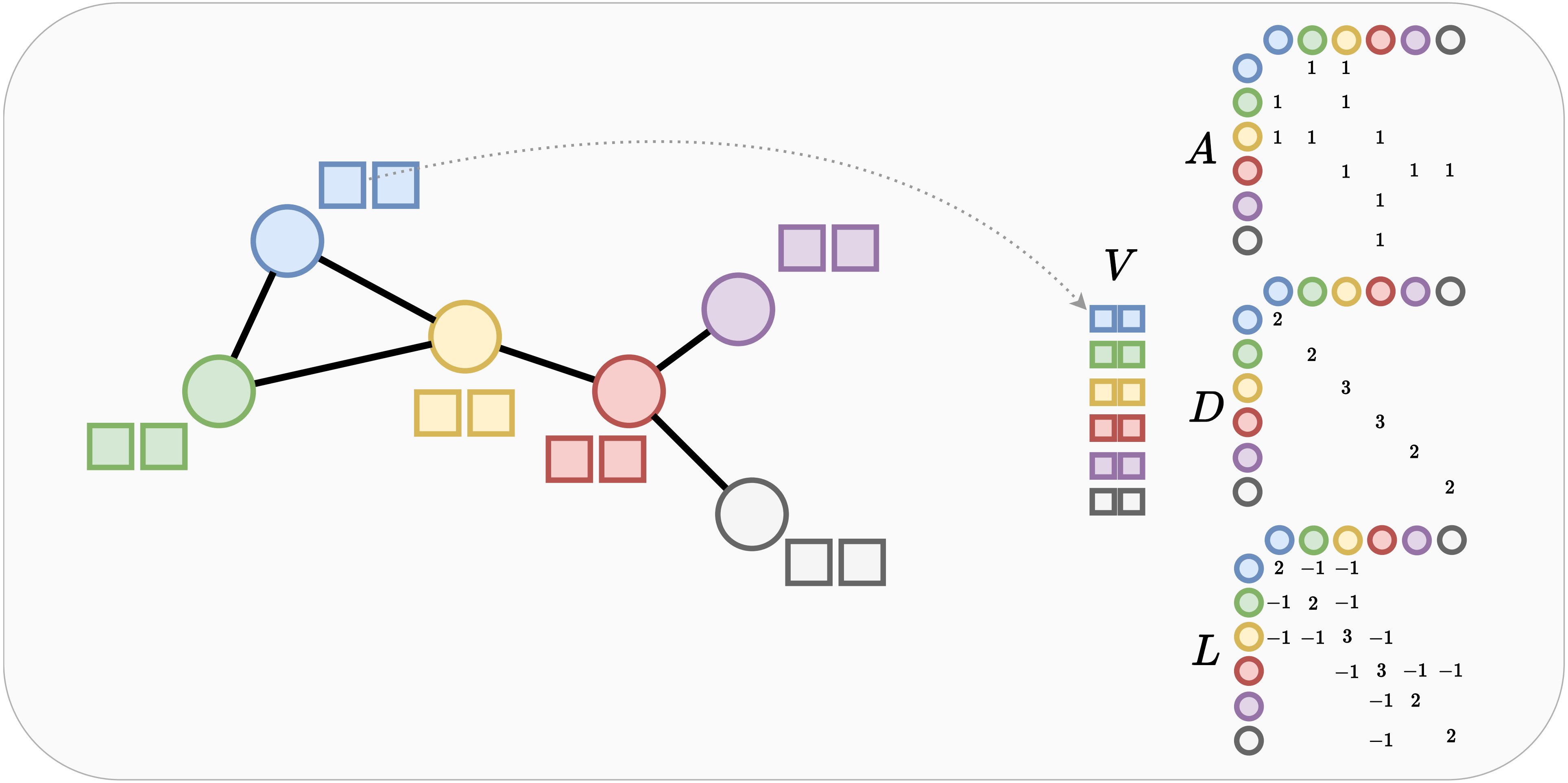
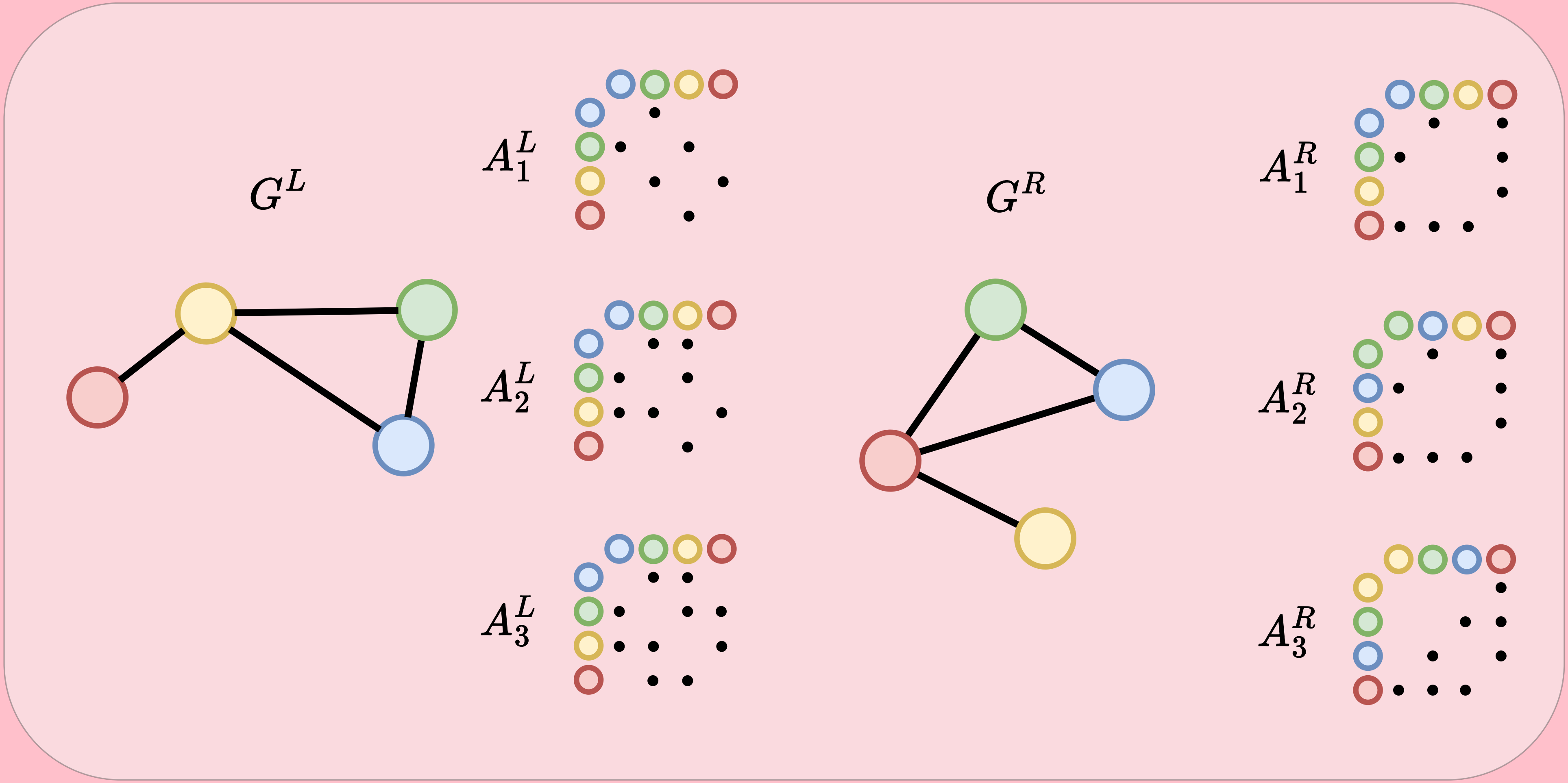
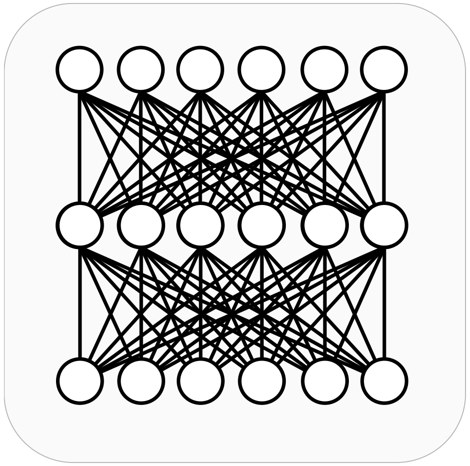
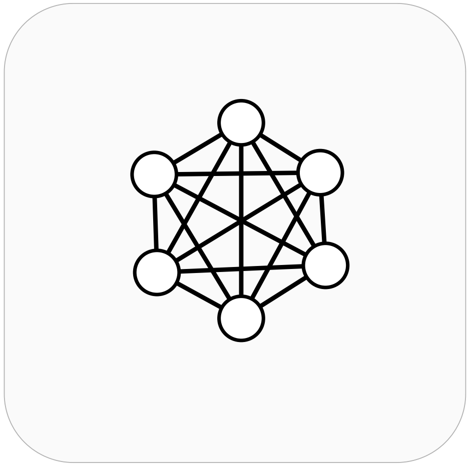


WHICH GRAPH CORRESPONDS TO THESE REPRESENTATIONS?



COMMON ARCHITECHTURES





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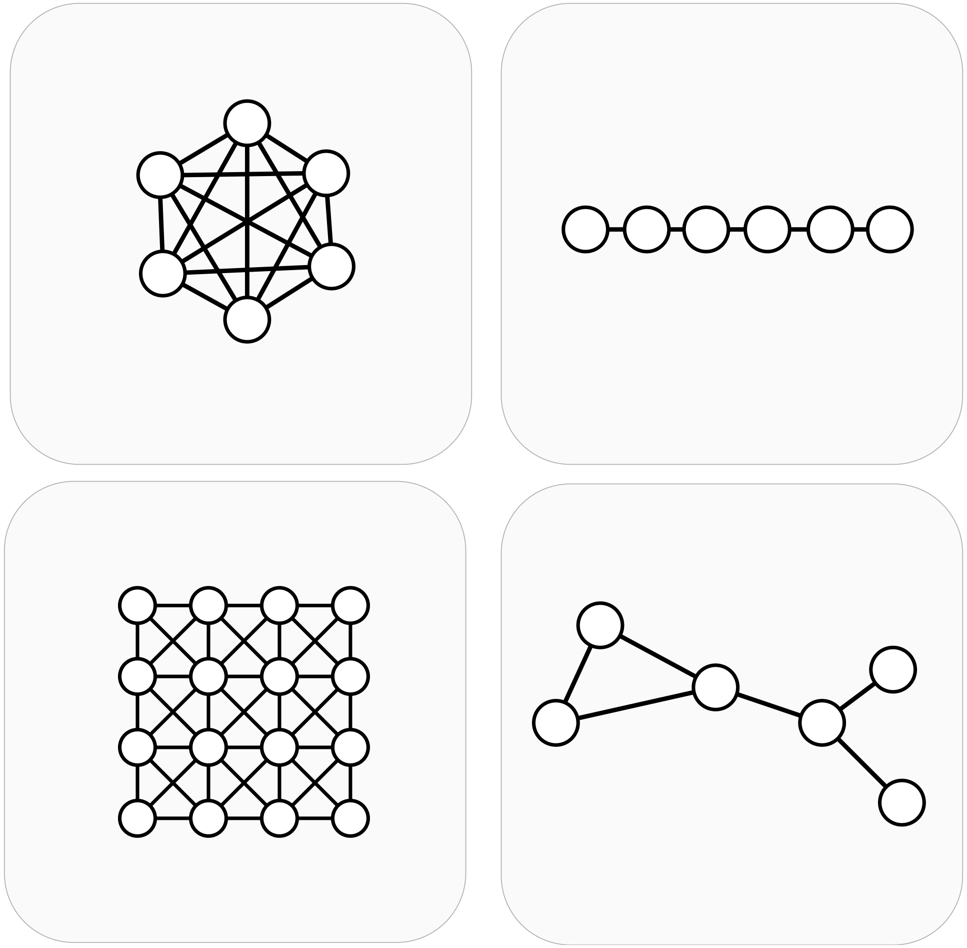
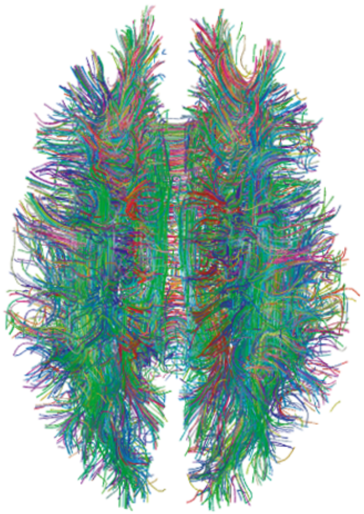
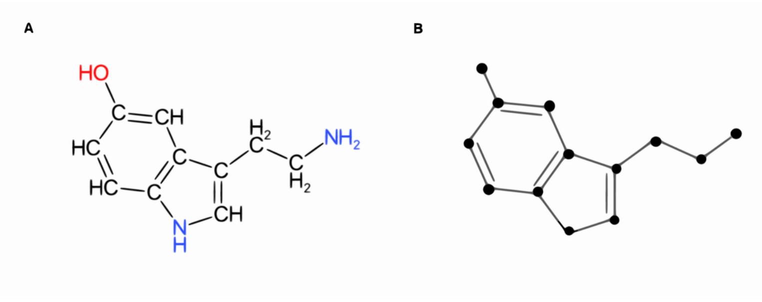
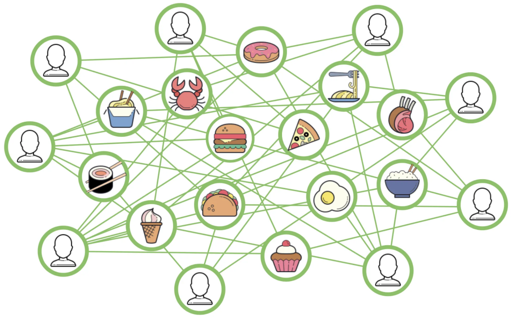
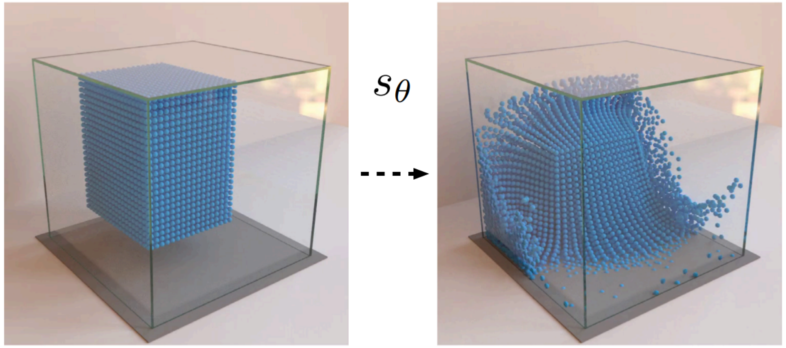


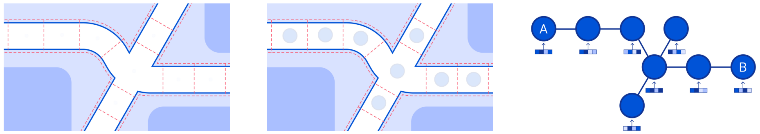
GRAPHS







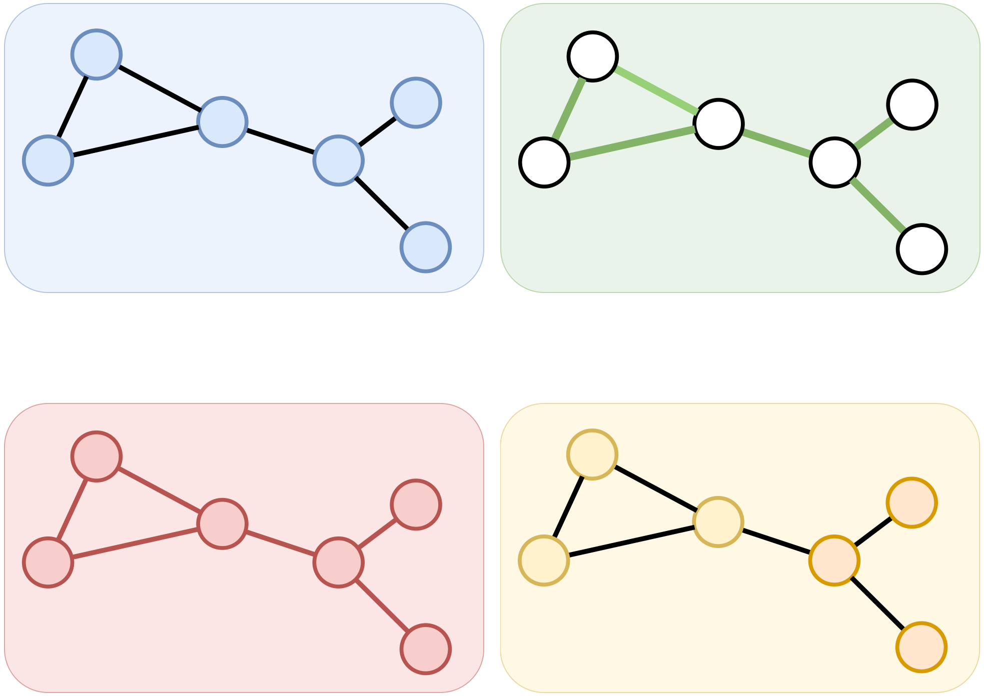




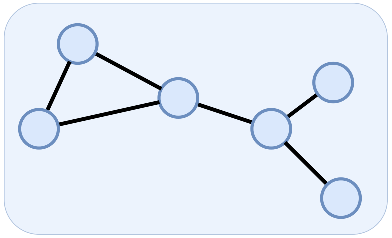
(Connectome: Gigandet X, Hagmann P, Kurant M, Cammoun L, Meuli R, et al. (2008) Estimating the Confidence Level of White Matter Connections Obtained with MRI Tractography. PLoS ONE 3(12): e4006. doi:10.1371/journal.pone.0004006.)
(Particles: Sanchez-Gonzalez, Alvaro, et al. "Learning to simulate complex physics with graph networks." International conference on machine learning. PMLR, 2020.)
(Food social network: https://www.uber.com/blog/uber-eats-graph-learning/)
(Serotonin: Yirik MA, Steinbeck C (2021) Chemical graph generators. PLoS Comput Biol 17(1): e1008504. https://doi.org/10.1371/journal.pcbi.1008504)
(Traffic: Derrow-Pinion, Austin, et al. "ETA prediction with Graph Neural Networks in Google Maps" Proceedings of the 30th ACM International Conference on Information & Knowledge Management. 2021.)

GRAPH TASKS

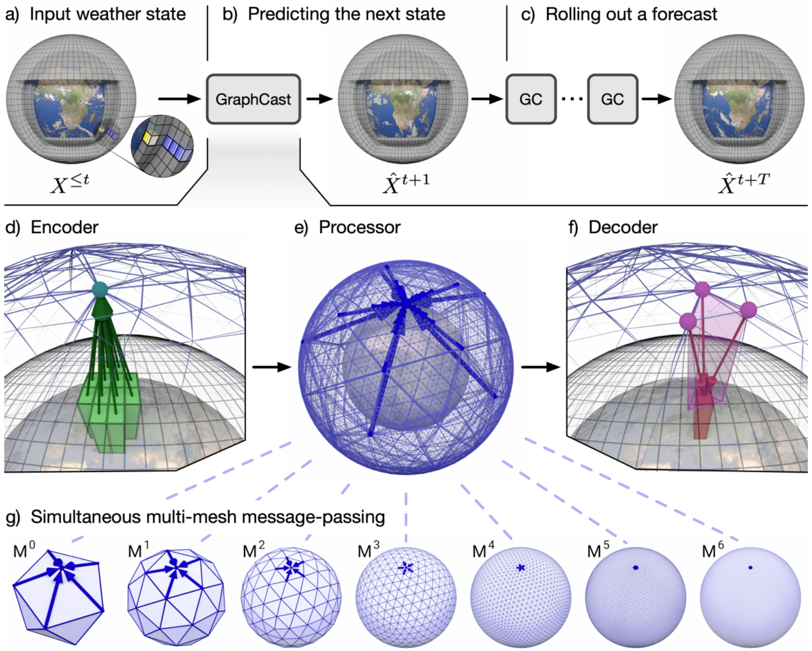
CONCEPTUAL GRAPH TASKS



NODE-LEVEL: WEATHER FORECASTING

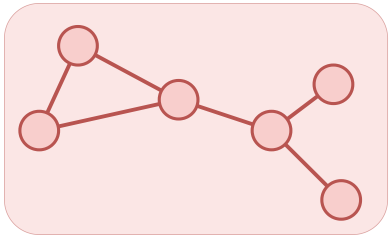


- Data: atmospheric variables like temperatures, wind speeds, pressures, etc., at diffent times, various longitude/latitudes, and levels in the atmosphere
- Represent the global weather state as a graph, model long-range dependencies with multi-mesh
- Task: predict future states of the graph, predicting future node features

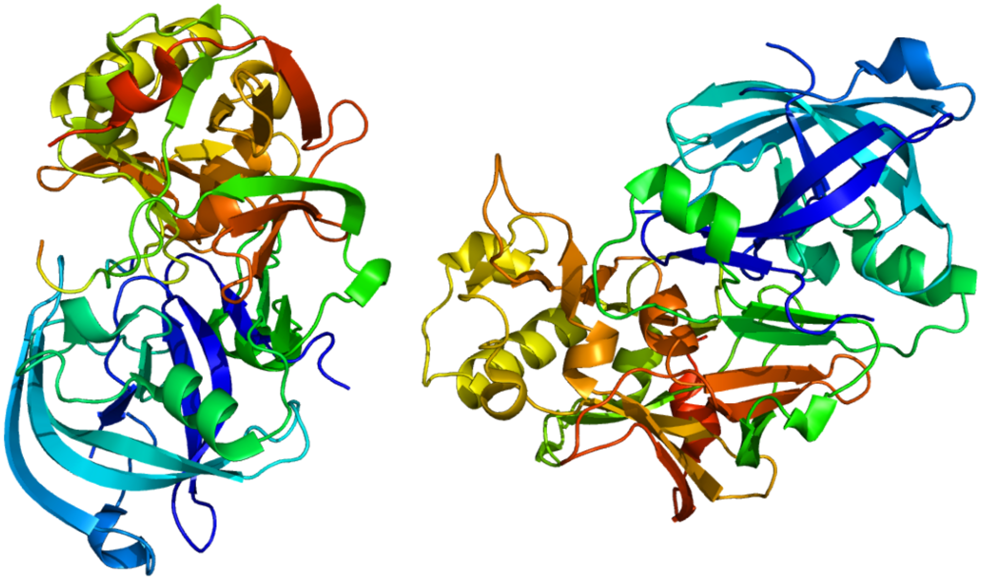


(Lam, Remi, et al. "GraphCast: Learning skillful medium-range global weather forecasting." arXiv preprint arXiv:2212.12794 (2022).)

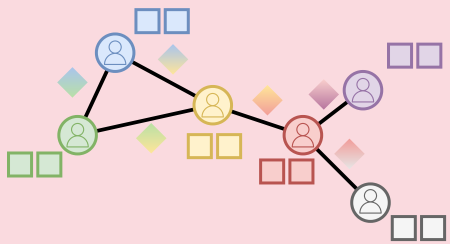
DRUG DISCOVERY: GRAPH-LEVEL



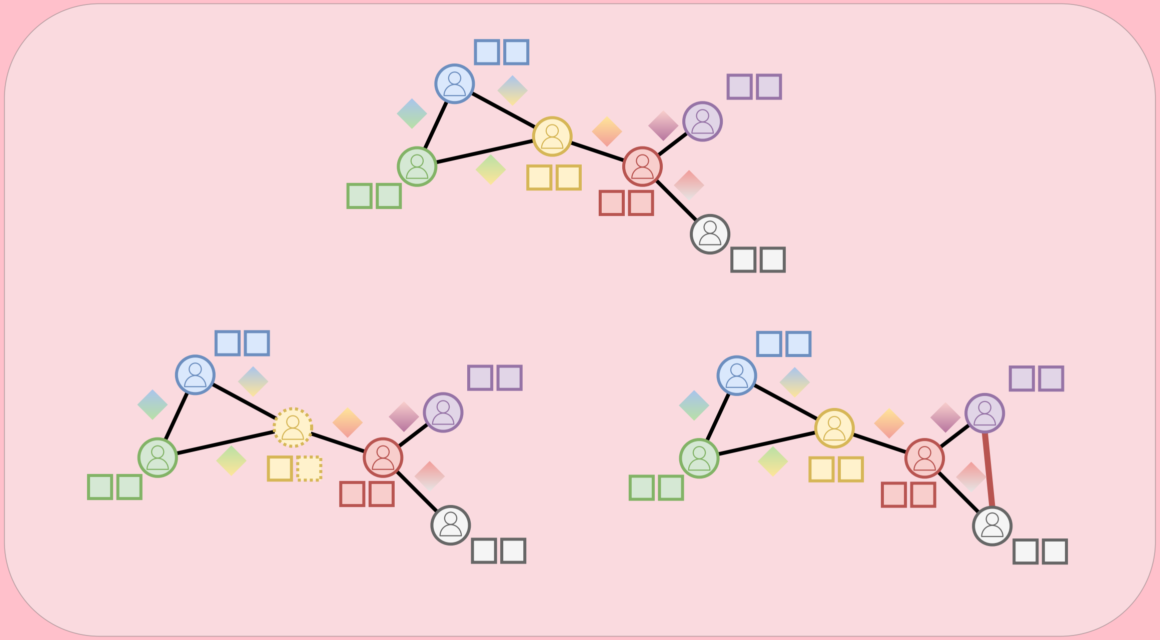
- Alzheimer's disease, Amyloid Beta plaques, beta-secretase 1 protein (BACE1)
- Inhibit BACE1: good candidate for an Alzheimer's drug
- Task: given graph predict BACE1 inhibition (IC50)

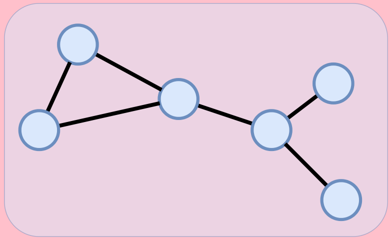


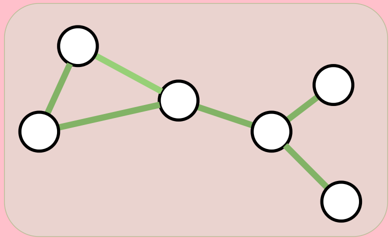
DISCUSSION: GRAPH-, NODE-, OR EDGE-LEVEL?



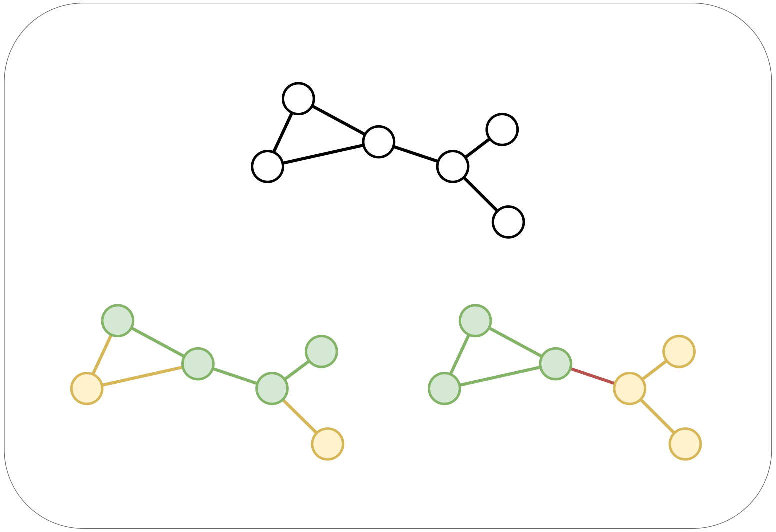
DISCUSSION: GRAPH-, NODE-, OR EDGE-LEVEL?

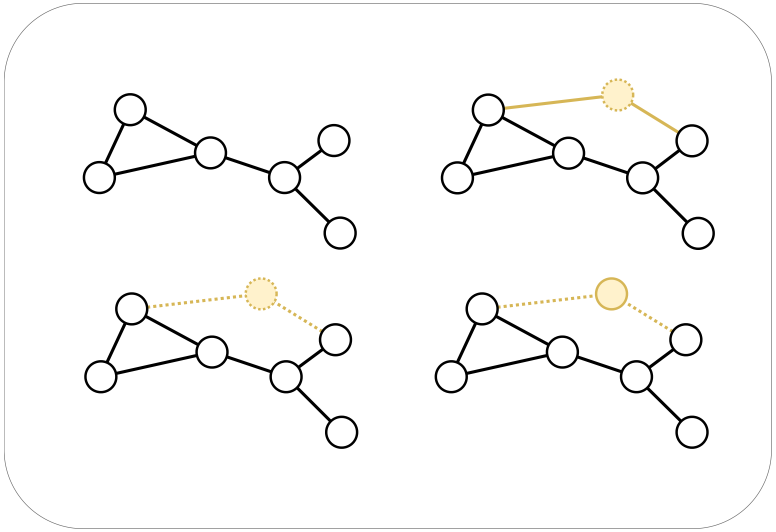






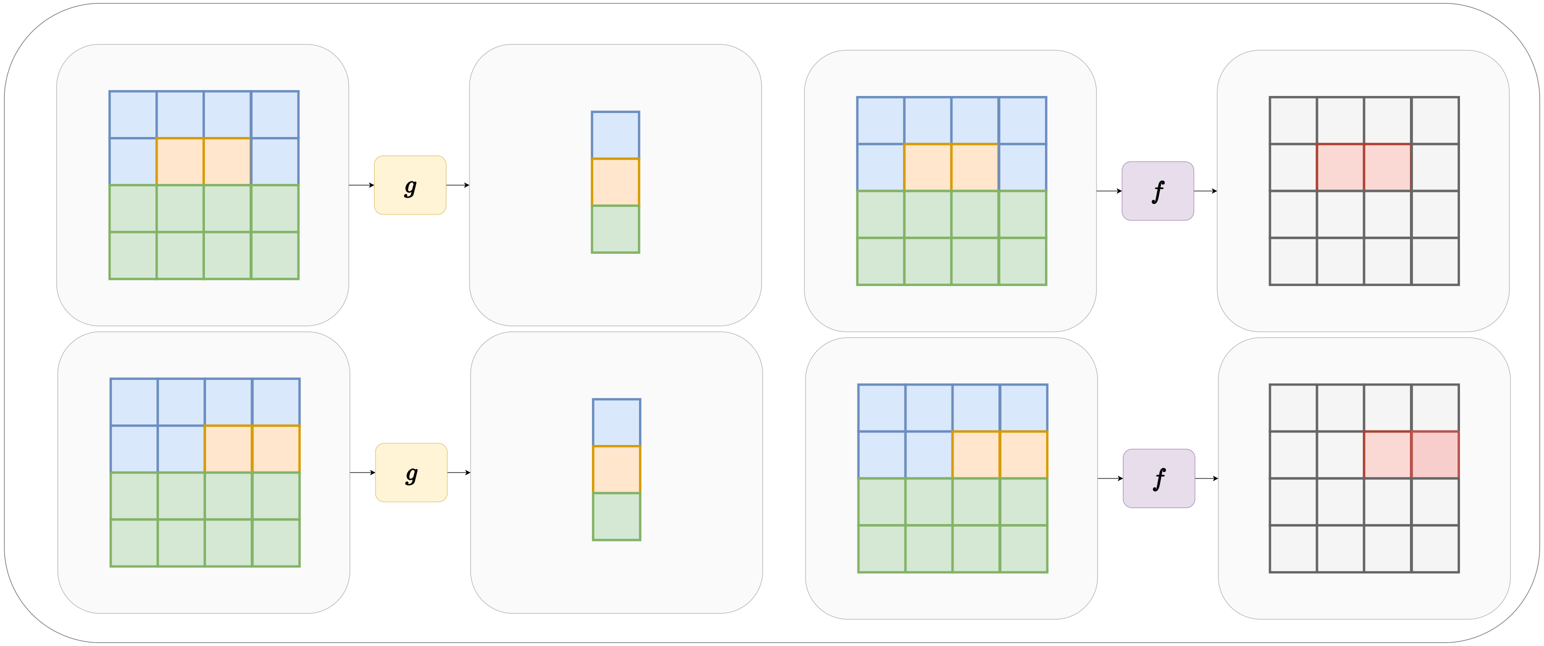
EVALUATION



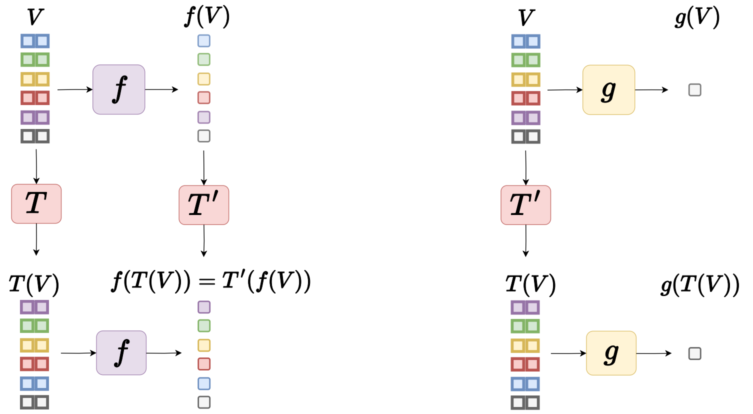


INVARIANCE AND EQUIVARIANCES

TRANSLATIONAL INVARIANCE AND EQUIVARIANCE



PERMUTATION INVARIANCE AND EQUIVARIANCE

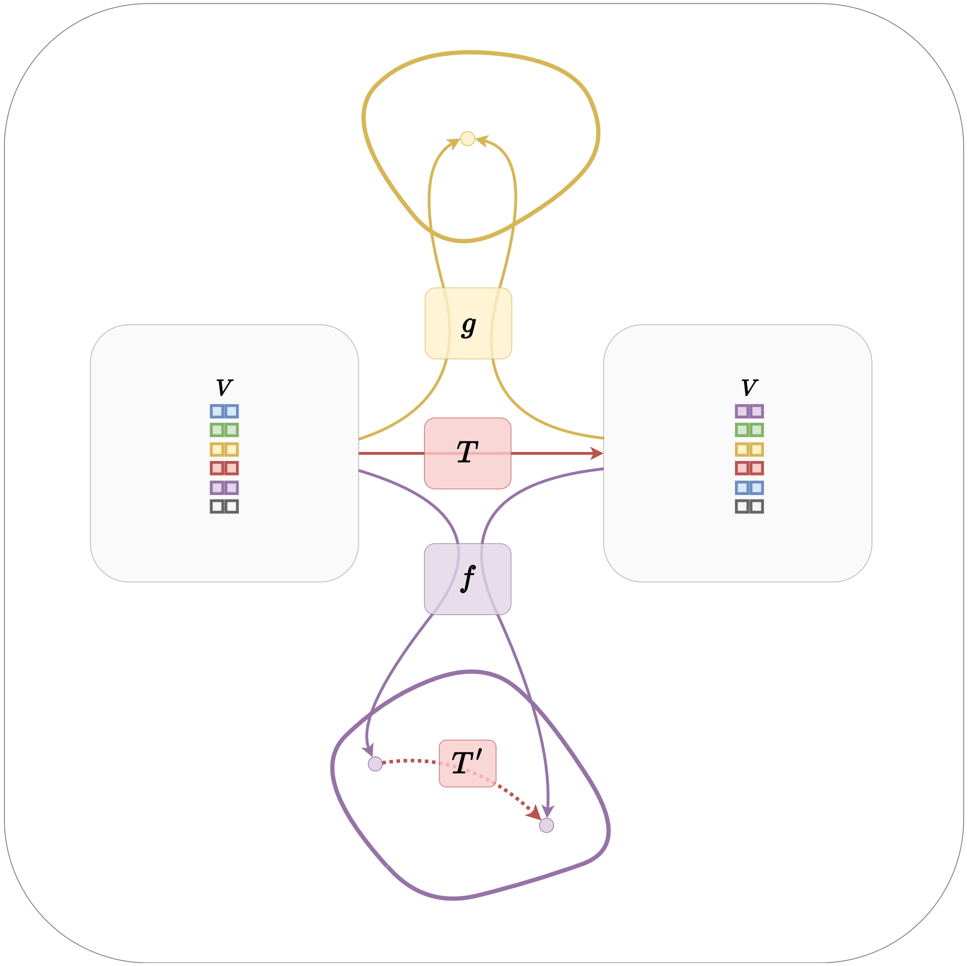


PERMUTATION INVARIANCE AND EQUIVARIANCE

$$g(\mathbf{PAP}^\top) = g(\mathbf{A})$$

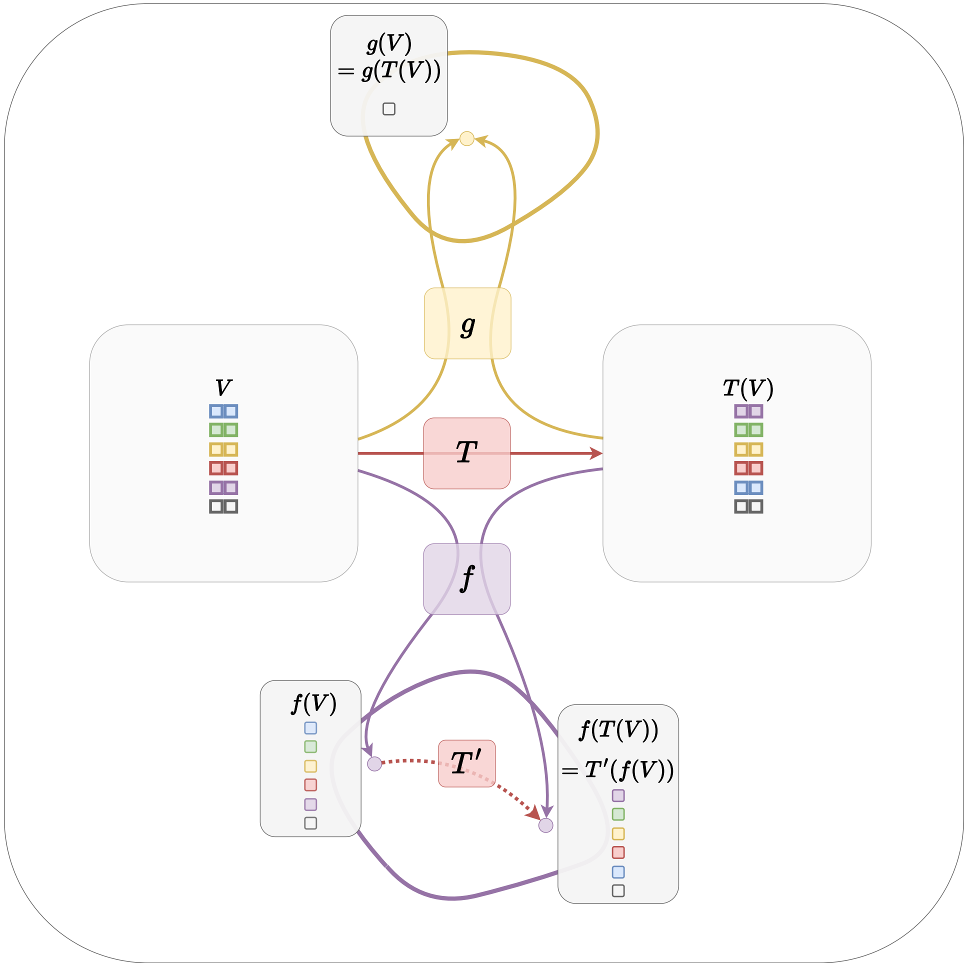
$$f(\mathbf{PAP}^\top) = \mathbf{P}f(A)$$

PERMUTATION INVARIANCE AND EQUIVARIANCE

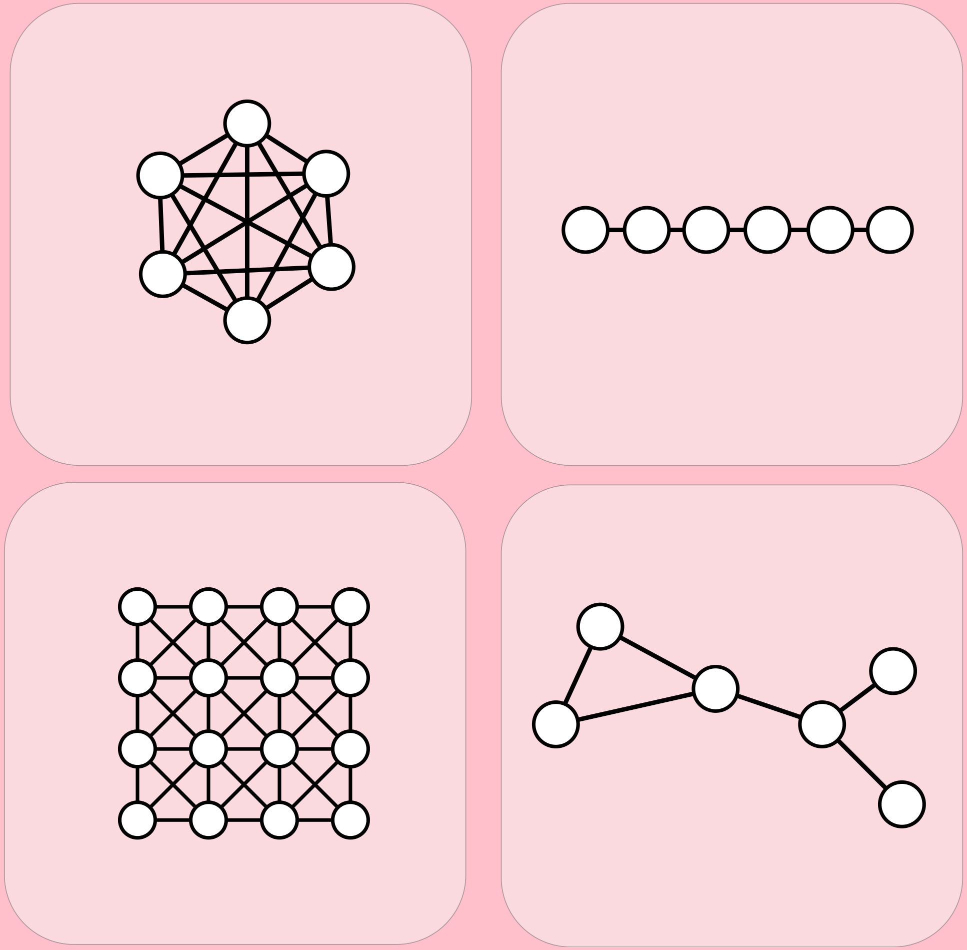


(Adapted from lecture by Mikkel Schmidt given at DTU's course (2022) "Graph Representation Learning")

PERMUTATION INVARIANCE AND EQUIVARIANCE

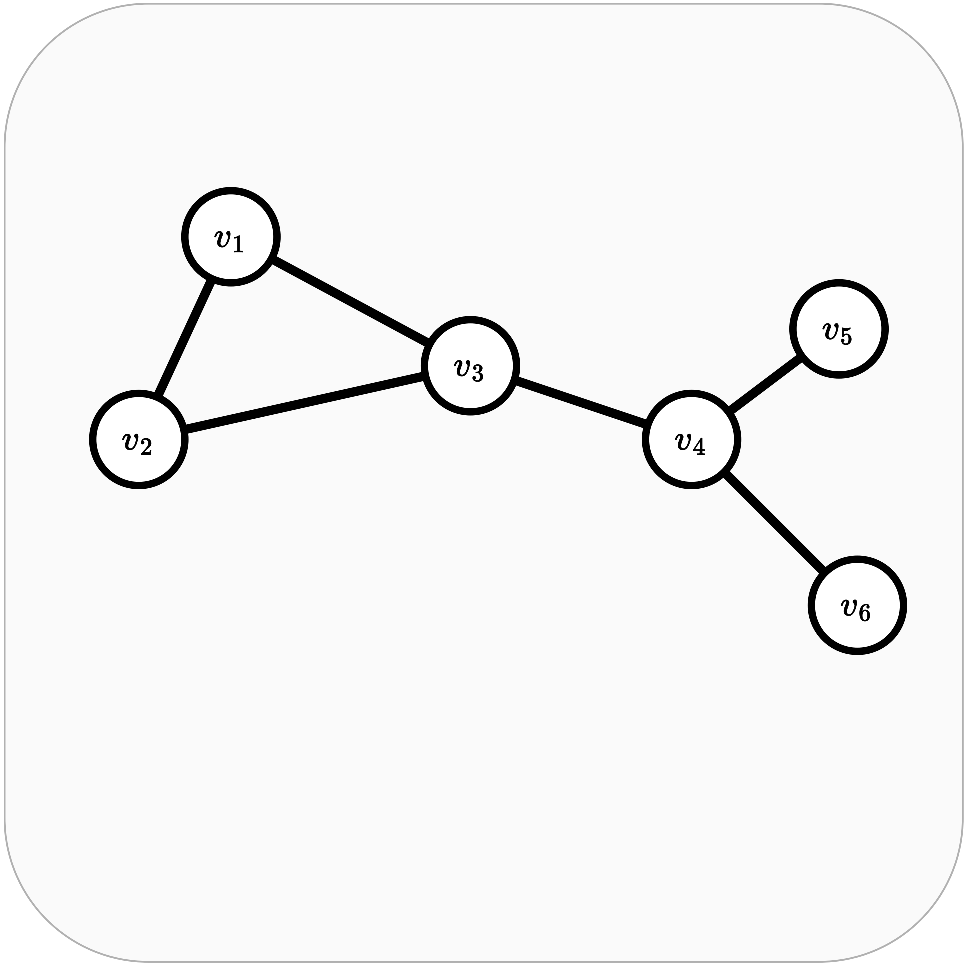


DISCUSSION: IN- AND EQUIVARIANCES OF MLPS, CNNS, RNNS, GNNS?

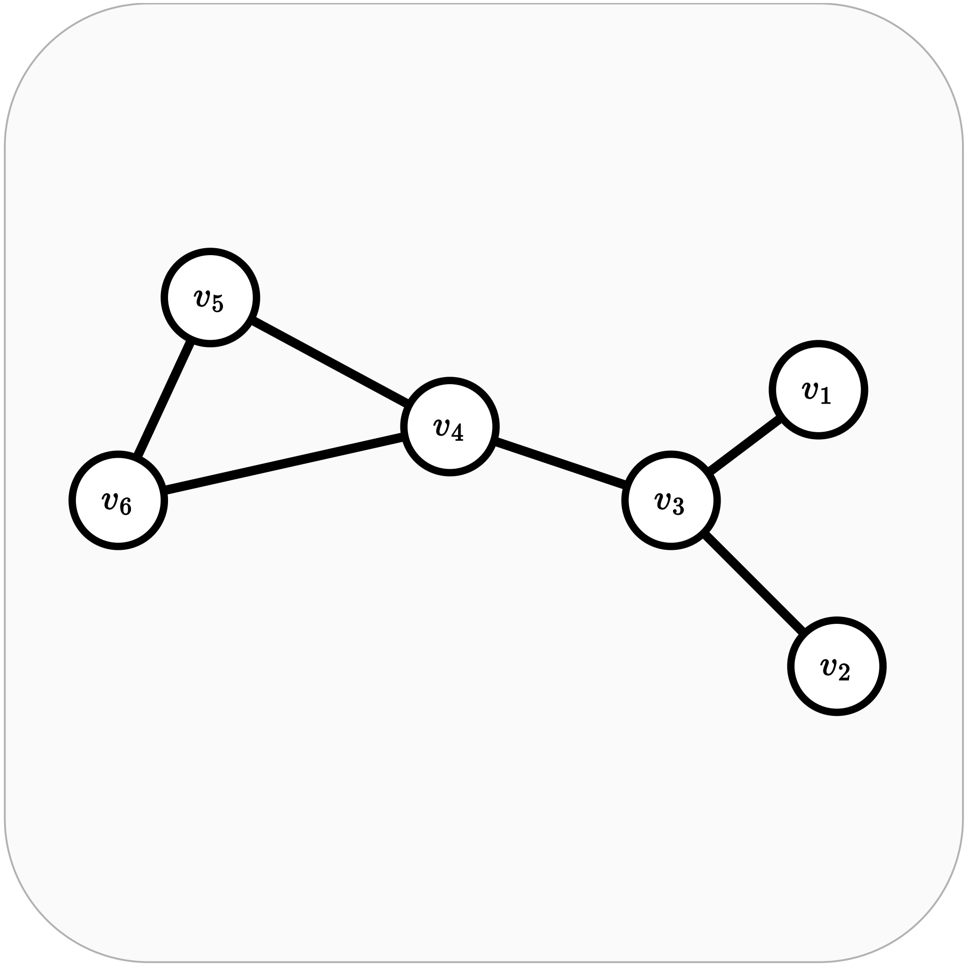


MESSAGE PASSING

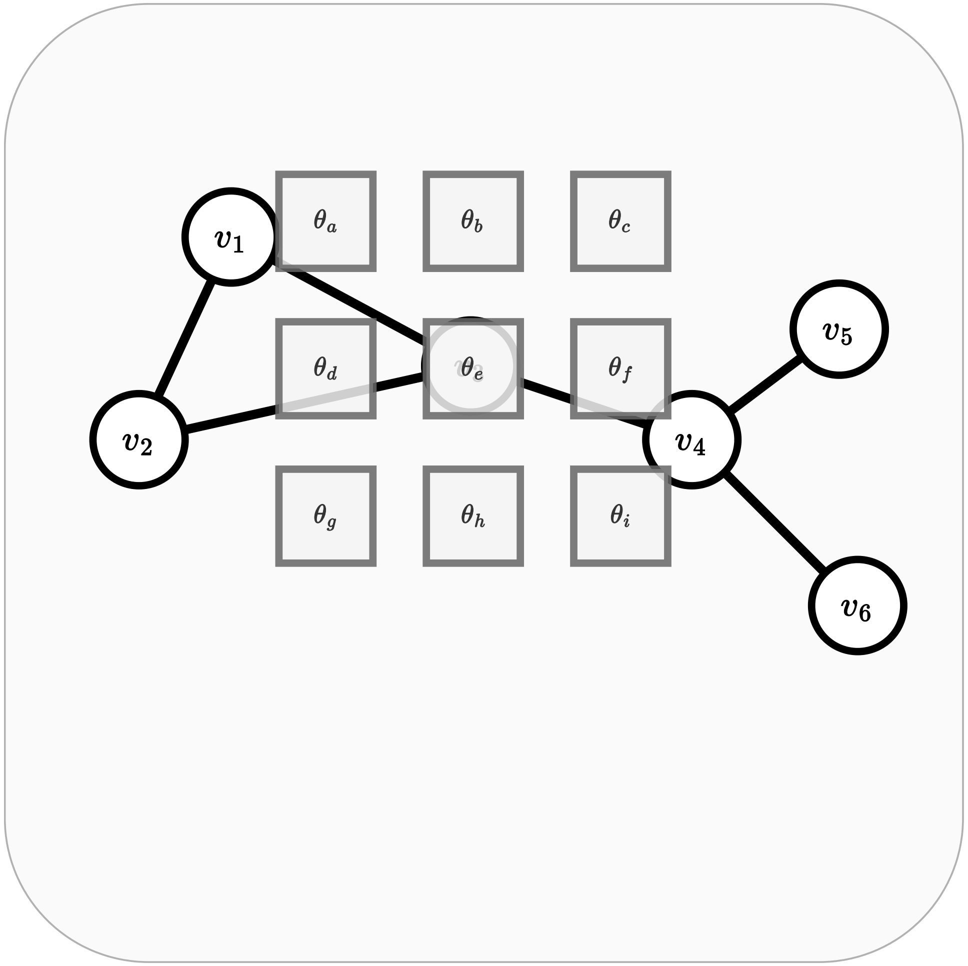
GRAPH WITH ORDERING



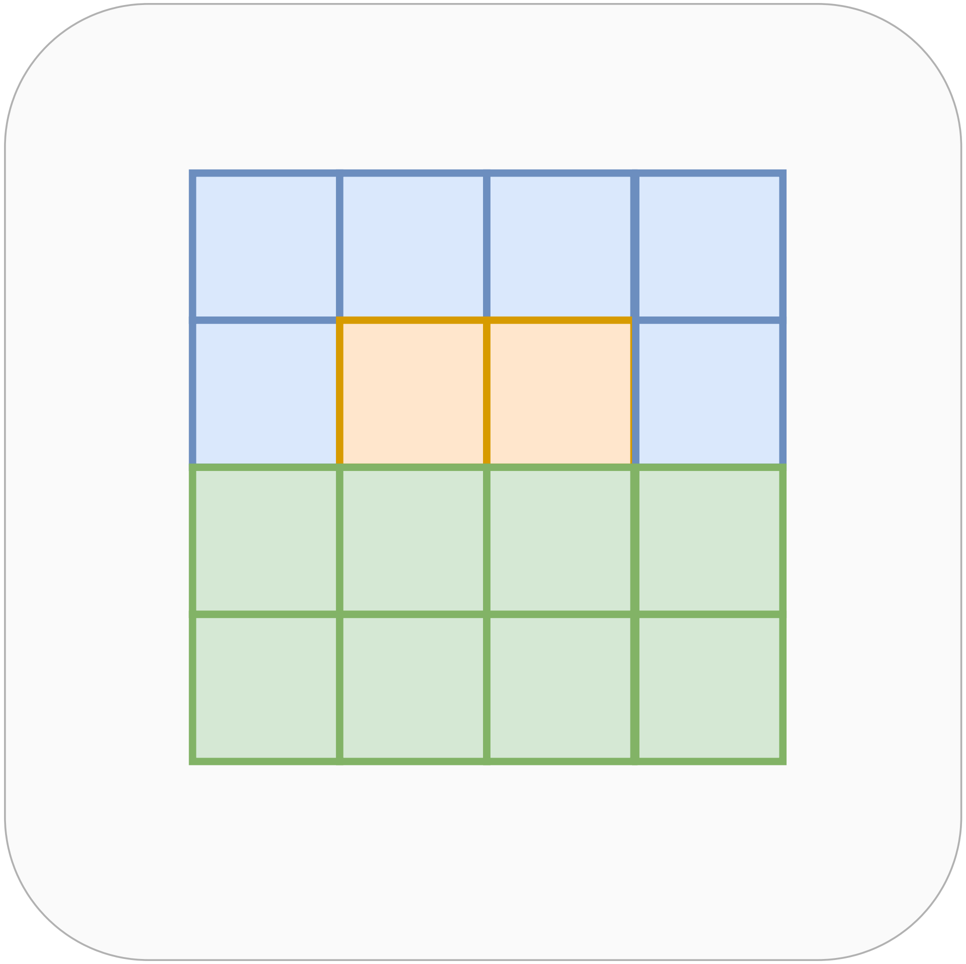
GRAPH WITH ORDERING



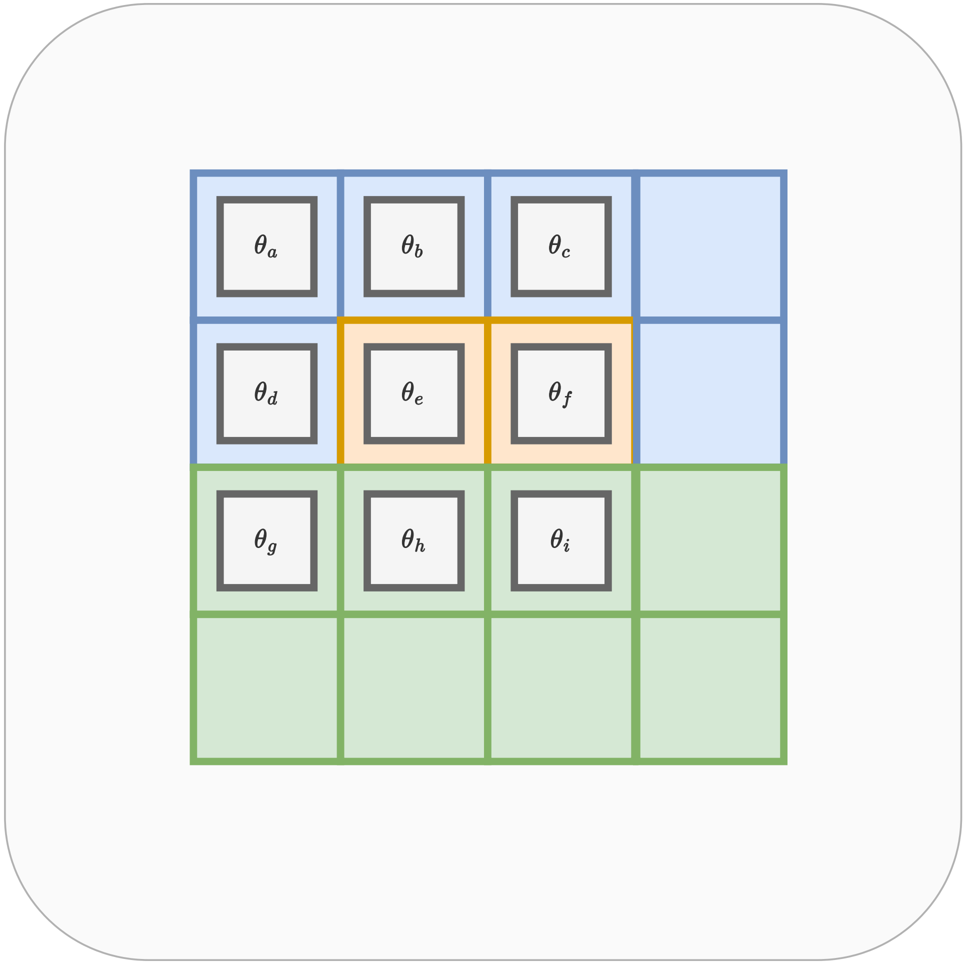
APPLYING CONVOLUTIONAL FILTER?



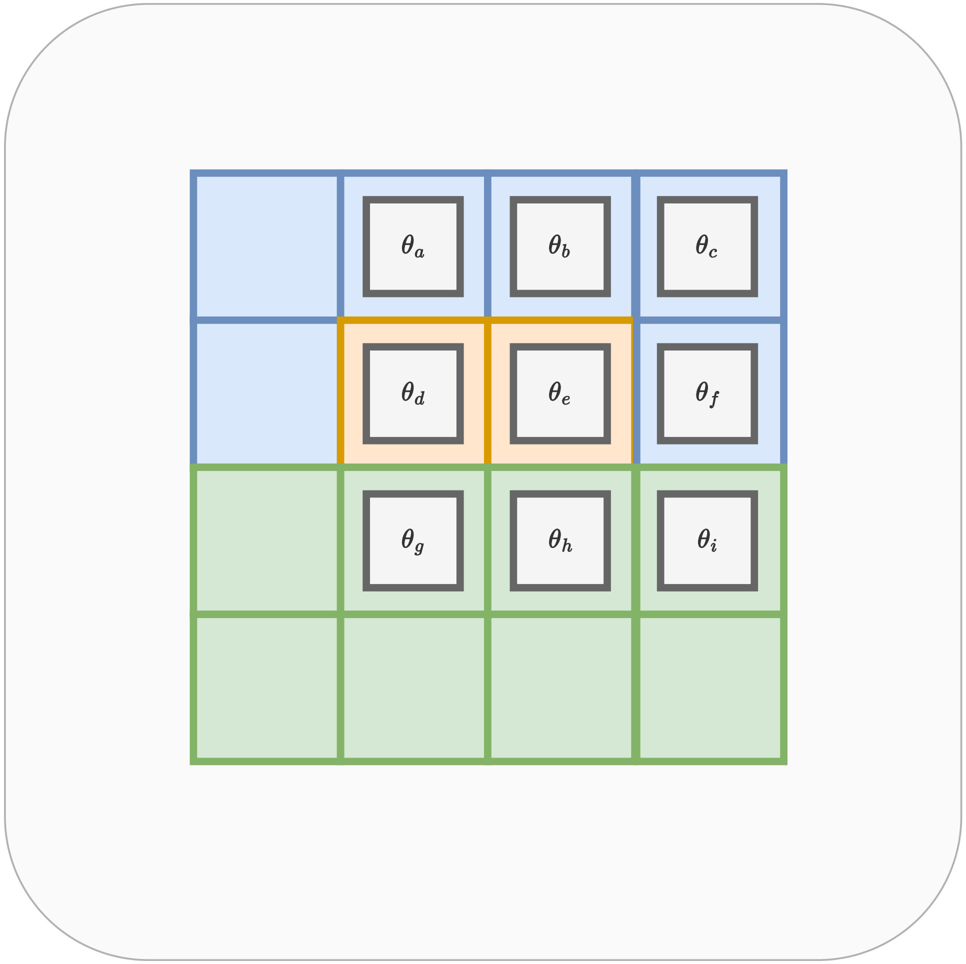
CONVOLUTION AS MESSAGE PASSING



CONVOLUTION AS MESSAGE PASSING



CONVOLUTION AS MESSAGE PASSING



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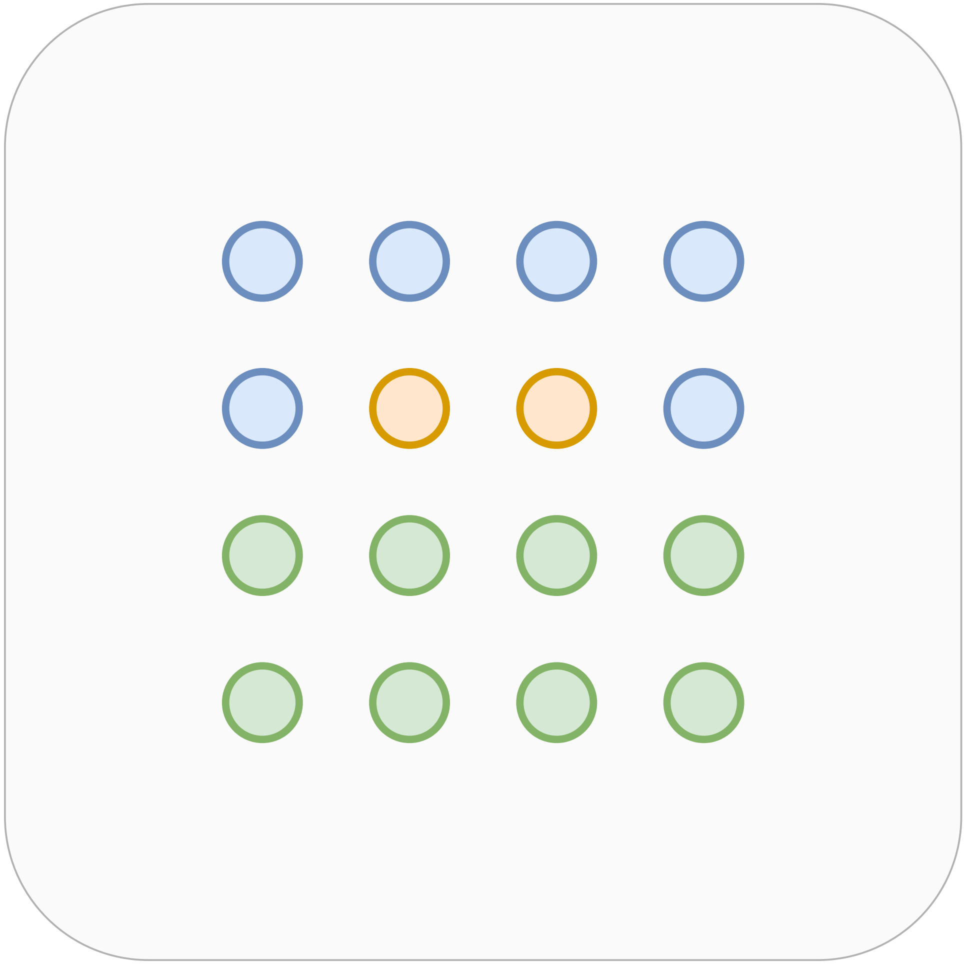
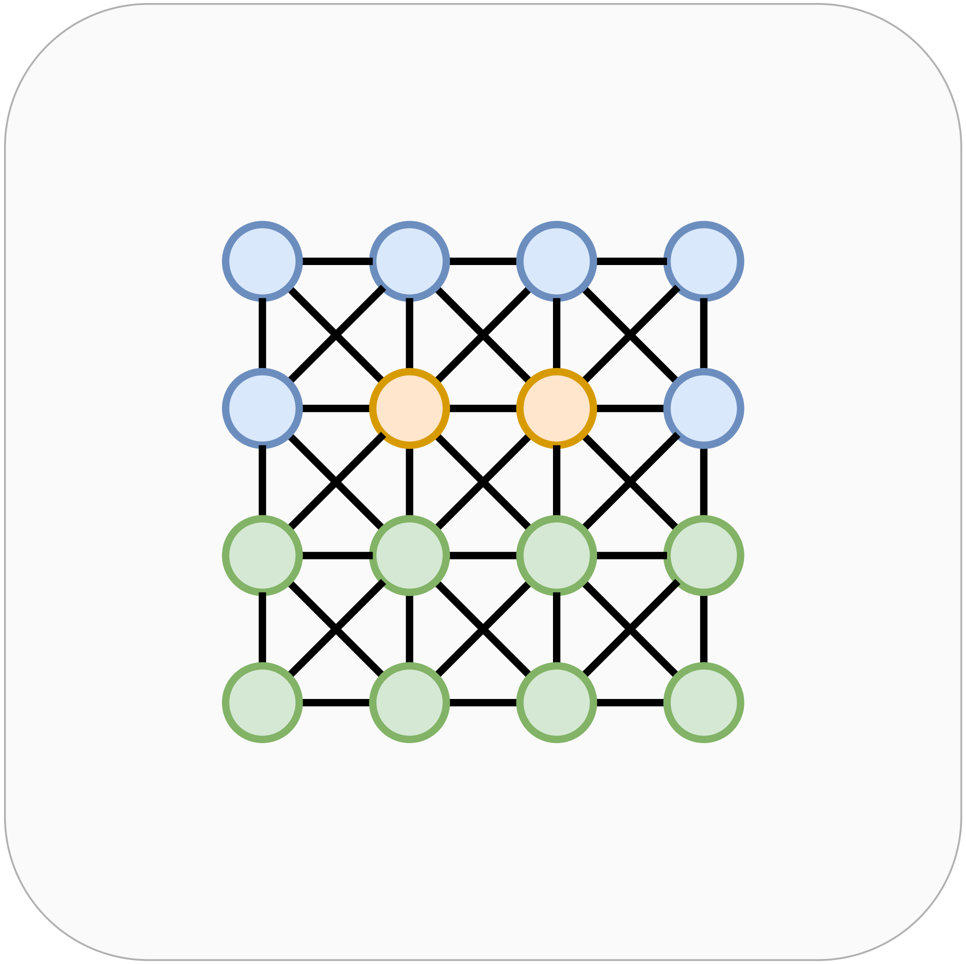
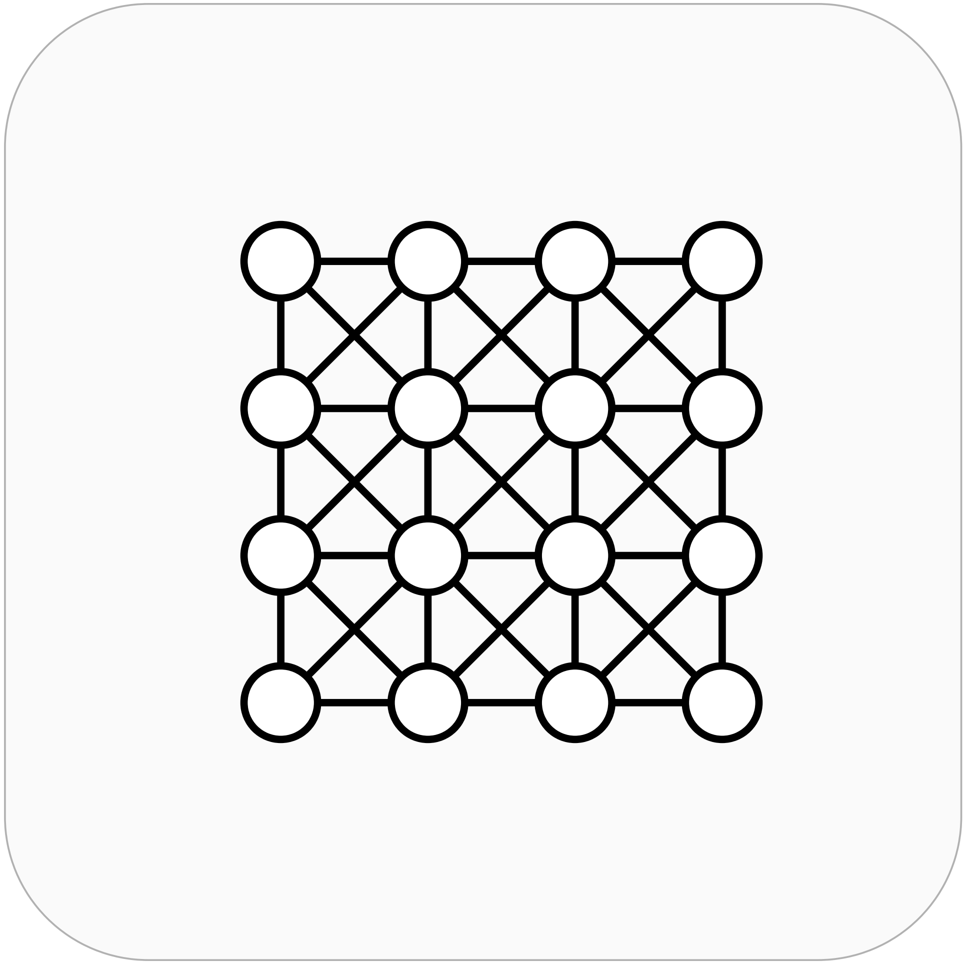


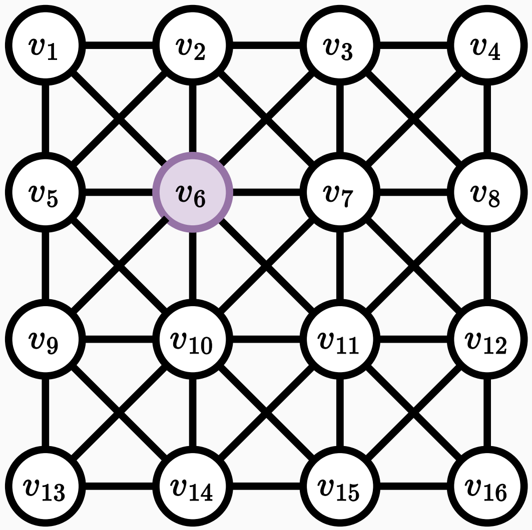
CONVOLUTION AS MESSAGE PASSING



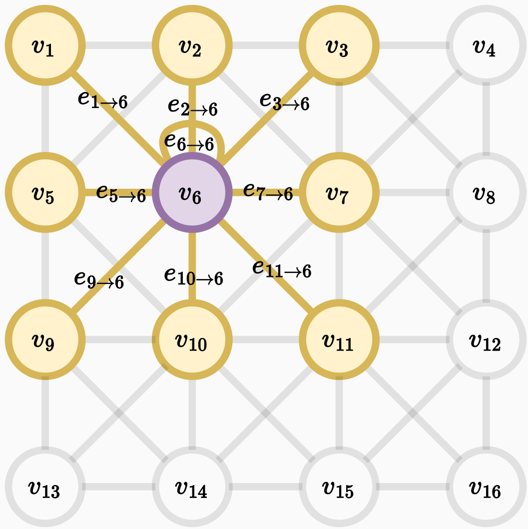
CONVOLUTION AS MESSAGE PASSING



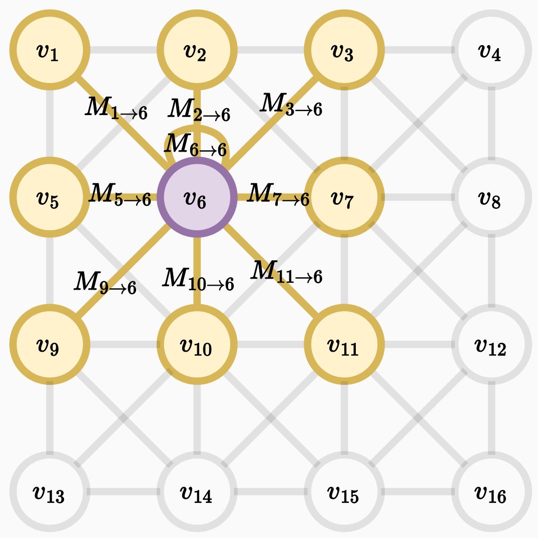
CONVOLUTION AS MESSAGE PASSING



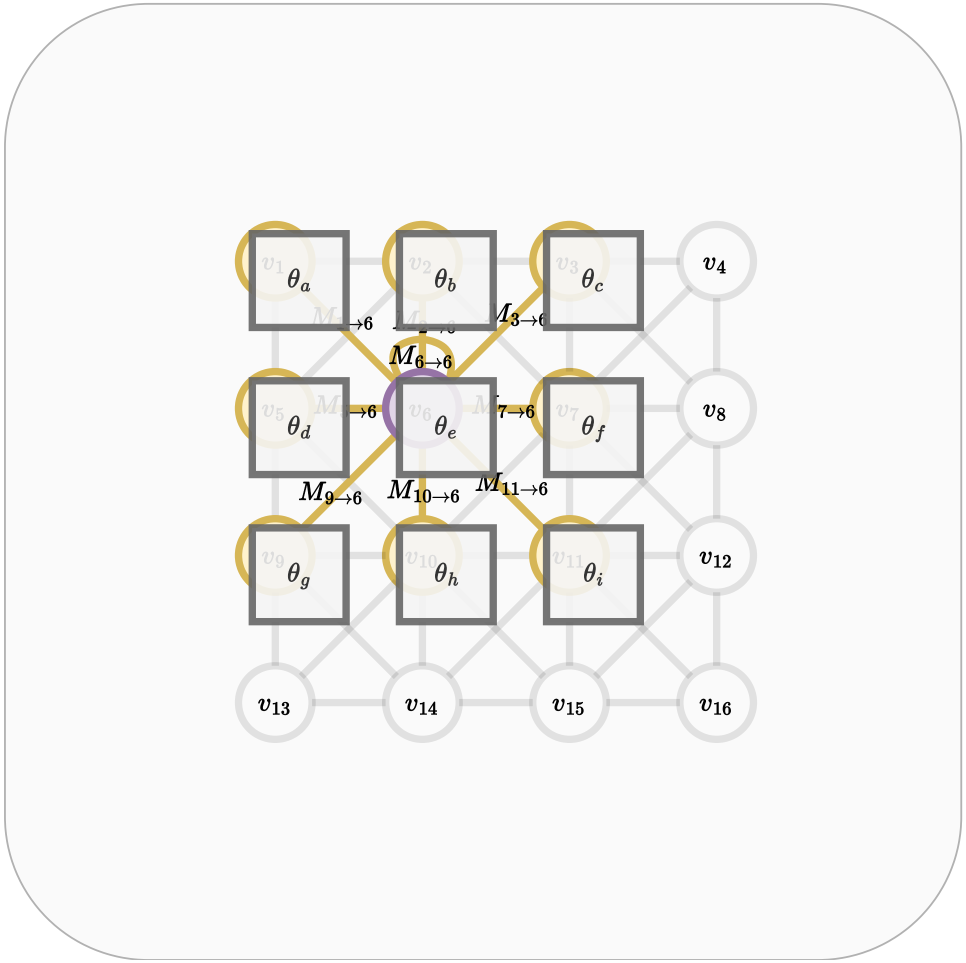
CONVOLUTION AS MESSAGE PASSING



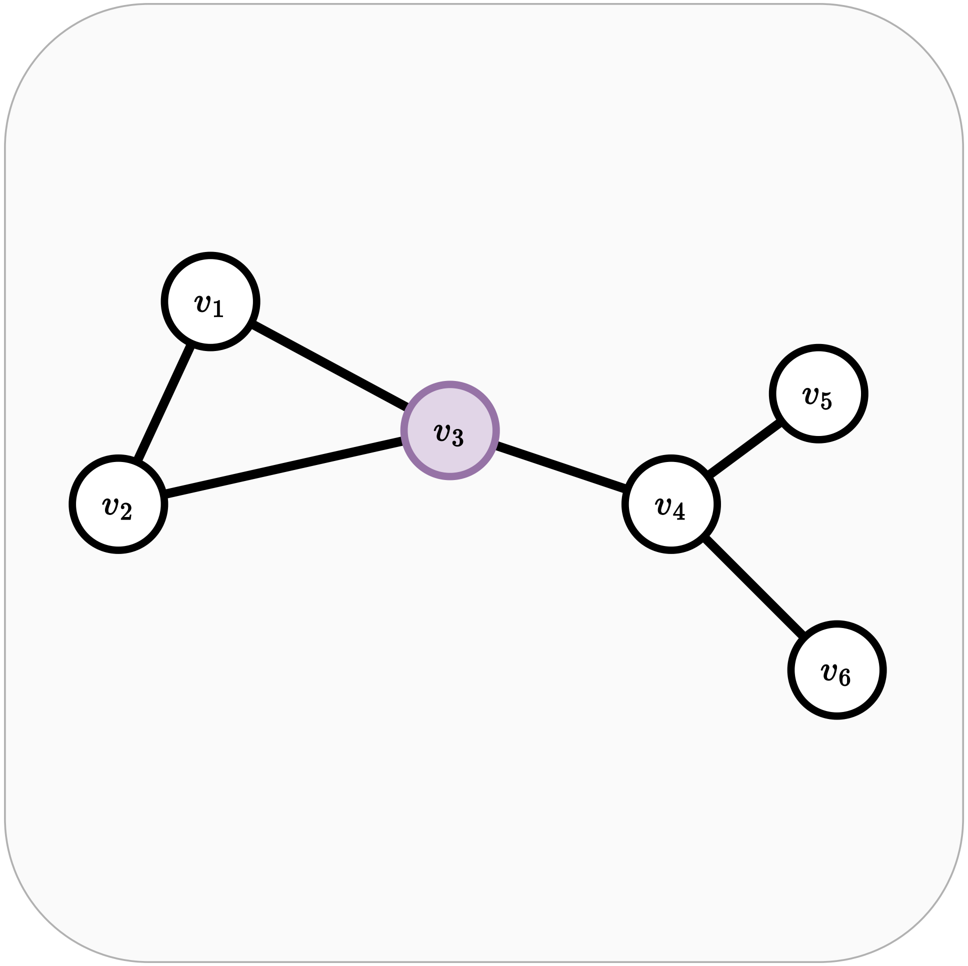
CONVOLUTION AS MESSAGE PASSING



CONVOLUTION AS MESSAGE PASSING



MESSAGE PASSING ON GRAPH



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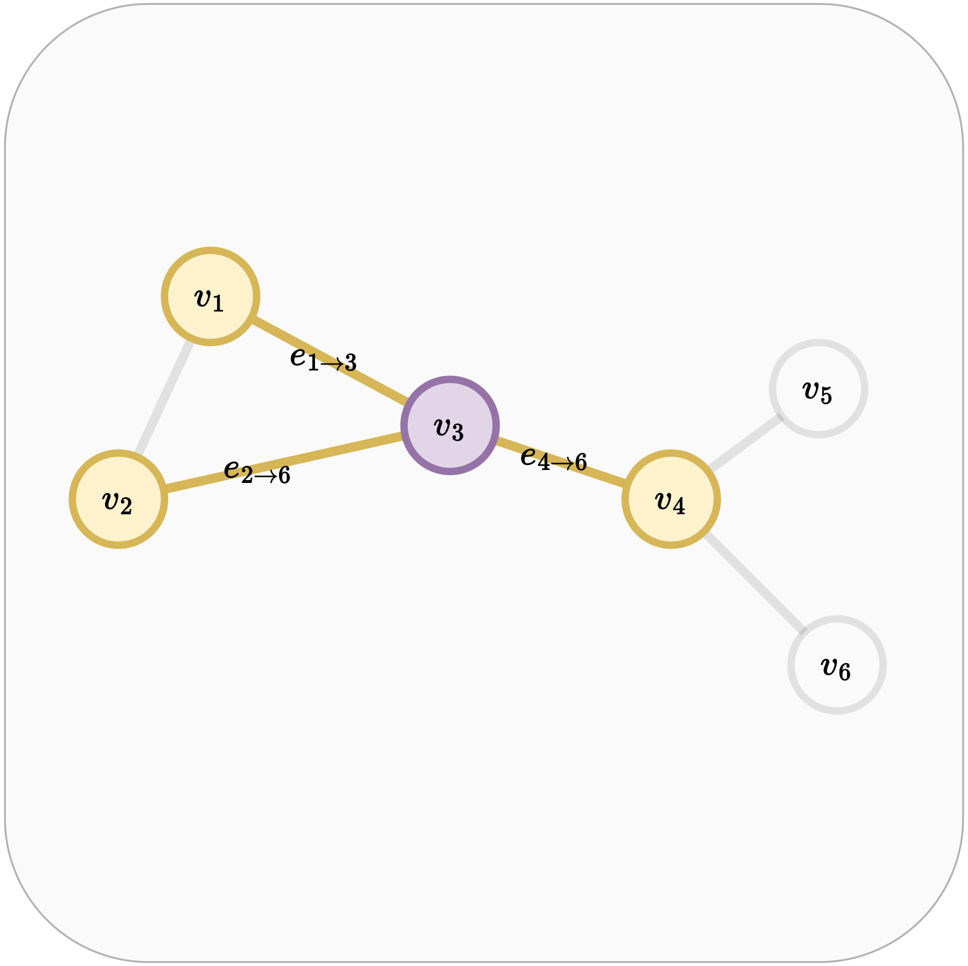

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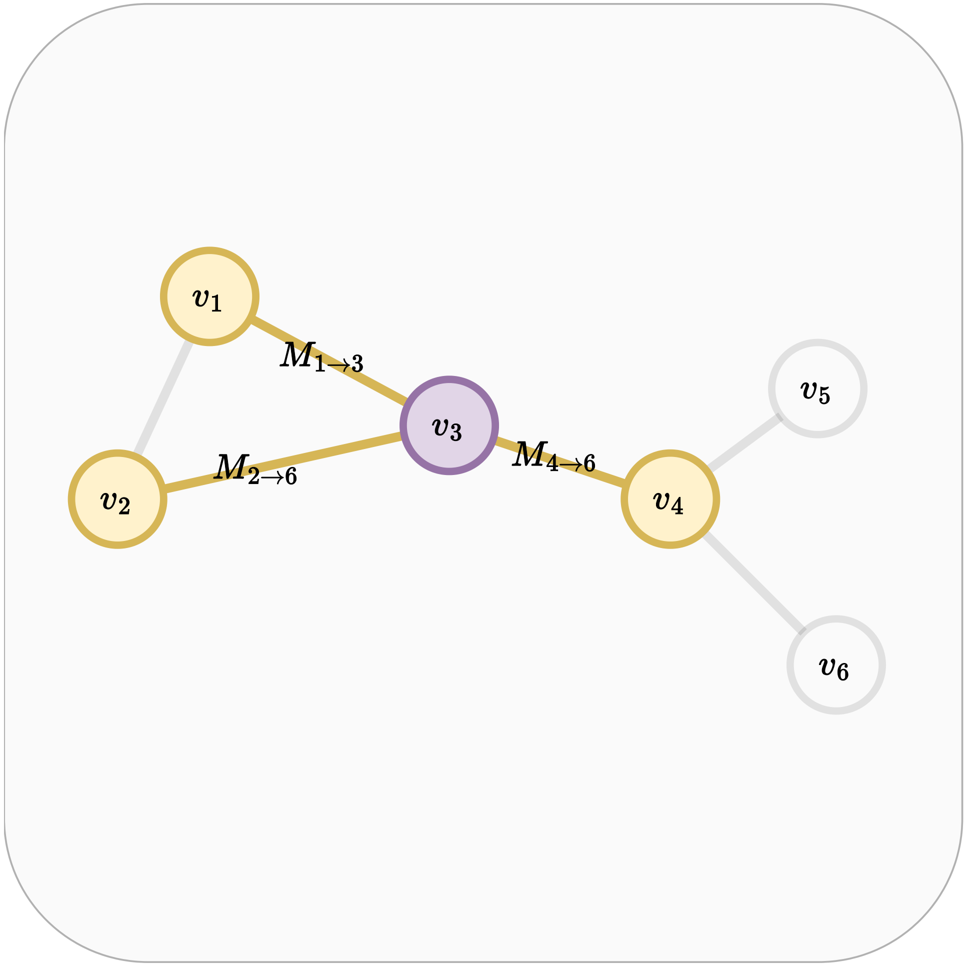

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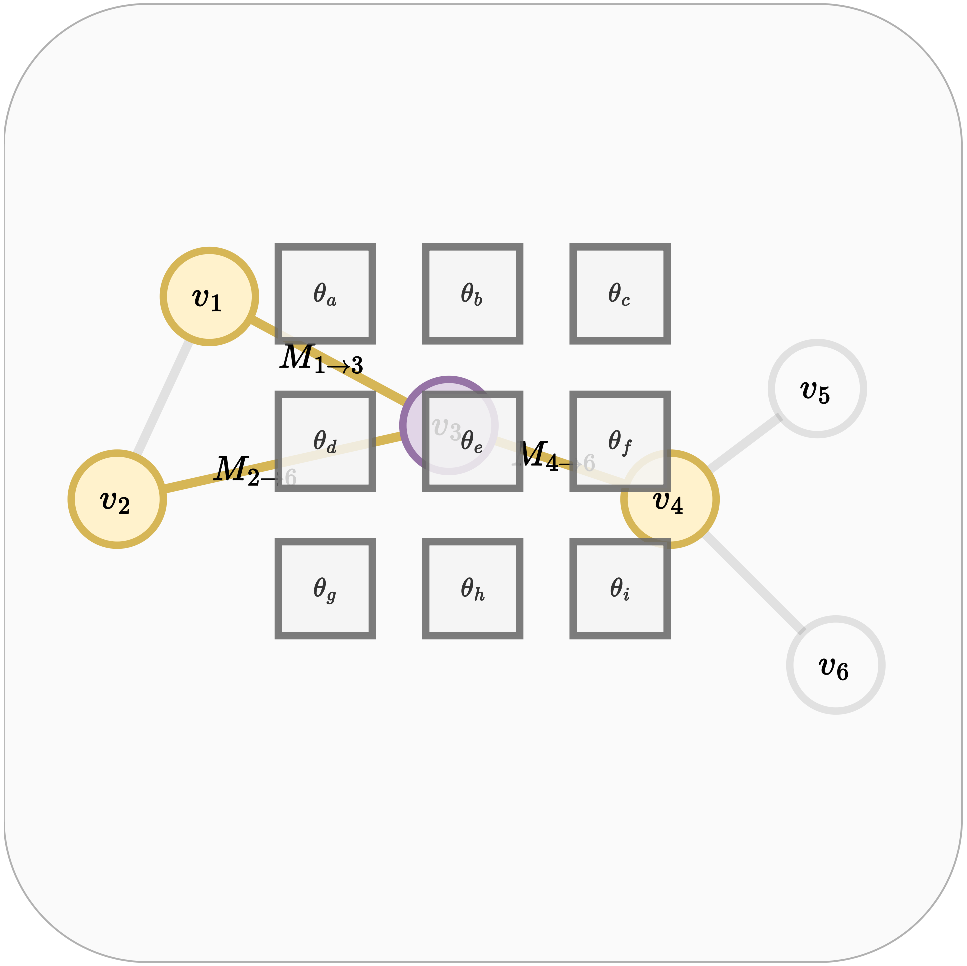


ABSTRACT MESSAGE PASSING

$$\mathbf{M}_{\mathcal{N}(u)}^{(k)} = \mathrm{AGGREGATE}^{(k)}\left(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\}\right)$$

$$\mathbf{h}_u^{k+1} = \mathrm{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{M}_{\mathcal{N}(u)}^{(k)}\right)$$

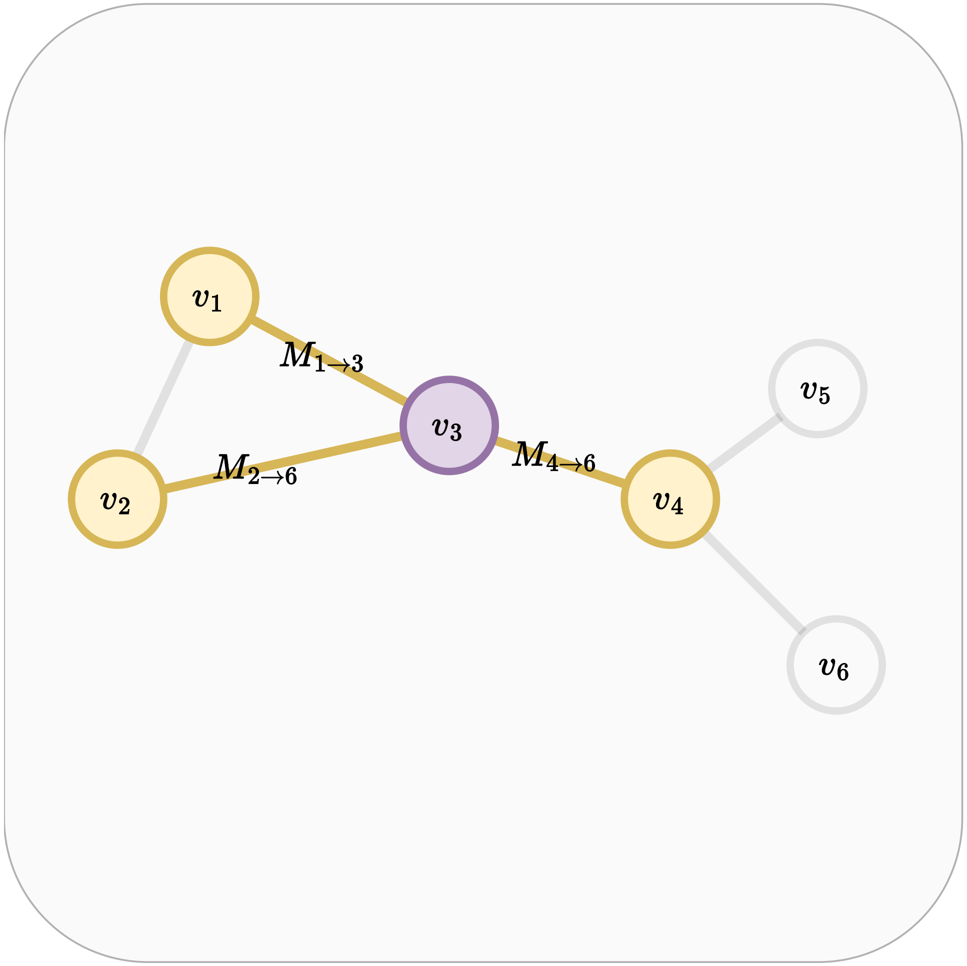
(Based on Chap. 5 in: Hamilton, William L. Graph representation learning. Morgan & Claypool Publishers, 2020.)

BASIC INSTANTIATION OF MESSAGE PASSING

$$\mathbf{h}_u^{(k)} = \sigma\left(\mathbf{W}_{\text{self}}^{(k)}\mathbf{h}_u^{(k-1)} + \mathbf{W}_{\text{neigh}}^{(k)}\sum_{v\in\mathcal{N}(u)}\left(\mathbf{h}_v^{(k-1)} + \mathbf{b}^{(k)}\right)\right)$$

(Based on Chap. 5 in: Hamilton, William L. Graph representation learning. Morgan & Claypool Publishers, 2020.)

CONVOLUTION AS MESSAGE PASSING

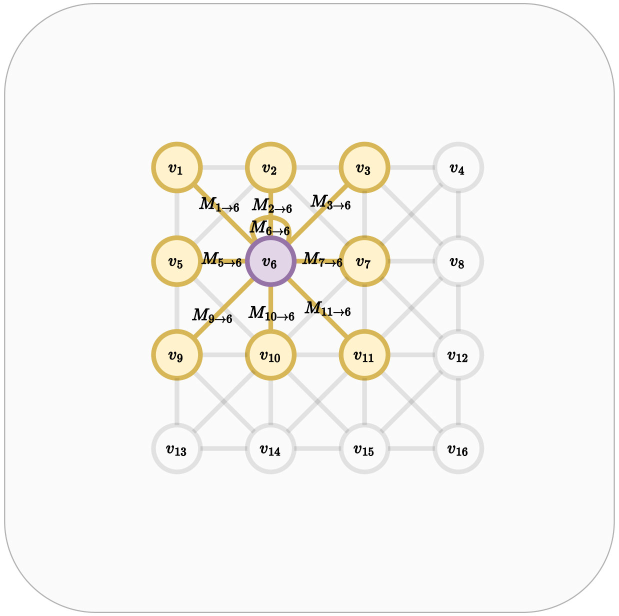


CONVOLUTION AS MESSAGE PASSING ON GRID

Algorithm 1 CNN as message passing

Input: Weight matrix, $\mathbf{W}$, with parameters $\theta_{u \to v}$, neighborhood function, $\mathcal{N}$.
Input: Graph, $\mathcal{G}$ with nodes $\mathcal{V} = \{v_i\}_{i=0}^{V}$ and edges $\mathcal{E} = \{e_{u \to v} | u, v \in \mathcal{V}\}$.
Output: Updated node features $\mathbf{h}_u^{(1)}$ for all nodes u

Initialize $\mathbf{h}_u^{(0)}$ as v_u
for $k \in [0]$ **do**
  for $u \in \mathcal{V}$ **do**
    for $v \in \mathcal{N}(u) \cup \{u\}$ **do**
      Compute messages : $\mathbf{M}_{v \to u} = \theta_{v \to u} \cdot \mathbf{h}_v^{(k)}$
    end for
    Compute total message: $\mathbf{M}_u = \sum_{v \in \mathcal{N}(u)} \mathbf{M}_{v \to u}$
    Update node: $\mathbf{h}_u^{(k+1)} \leftarrow \sigma(\mathbf{M}_u)$
  end for
end for



MESSAGE PASSING ON GRAPH

Algorithm 2 Basic graph message passing

Input: Weight matrices, $\mathbf{W}_{\text{self}}$, $\mathbf{W}_{\text{neigh}}$, and bias, $\mathbf{b}$, neighborhood function, $\mathcal{N}$.

Input: Graph, $\mathcal{G}$ with nodes $\mathcal{V} = \{v_i\}_{i=0}^{V}$ and edges $\mathcal{E} = \{e_{u \to v} | u, v \in \mathcal{V}\}$, and a specified K number of rounds of message passing.

Output: Updated node features $\mathbf{h}_u^{(K+1)}$ for all nodes u

Initialize $\mathbf{h}_u^{(0)}$ as v_u for all nodes u

for $k \in [0, 1, \ldots, K]$ **do**

  for $u \in \mathcal{V}$ **do**

    for $v \in \mathcal{N}(u)$ **do**

      Compute messages : $\mathbf{M}_{v \to u} = \mathbf{W}_{\text{neighbors}} \mathbf{h}_v^{(k)} + \mathbf{b}$

    end for

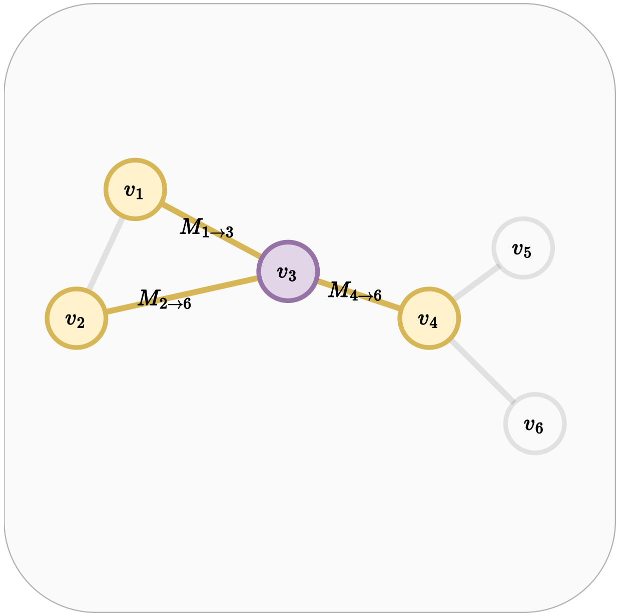
    Compute self message: $\mathbf{M}_{\text{self}} = \mathbf{W}_{\text{self}} \mathbf{h}_u^k$

    Compute total message: $\mathbf{M}_u = \mathbf{M}_{\text{self}} + \sum_{v \in \mathcal{N}(u)} \mathbf{M}_{v \to u}$

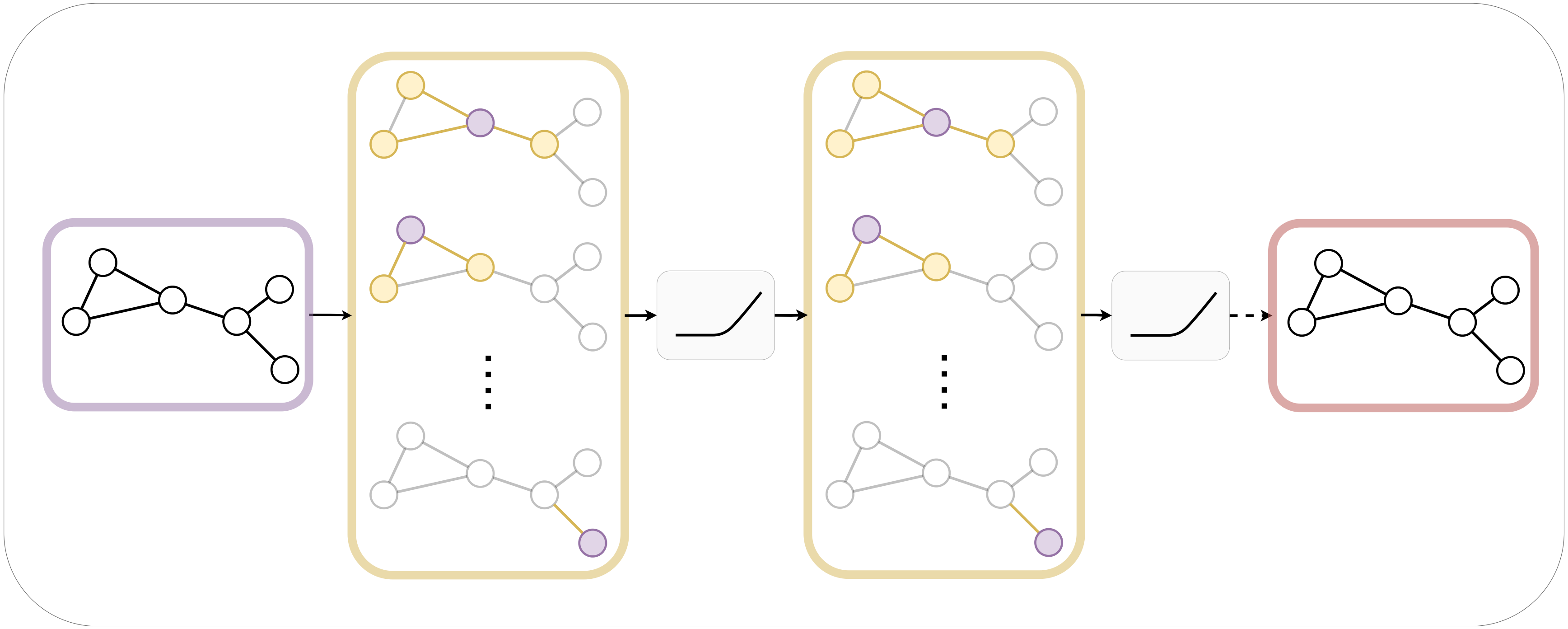
    Update node: $\mathbf{h}_u^{(k+1)} \leftarrow \sigma(\mathbf{M}_u)$

  end for

end for

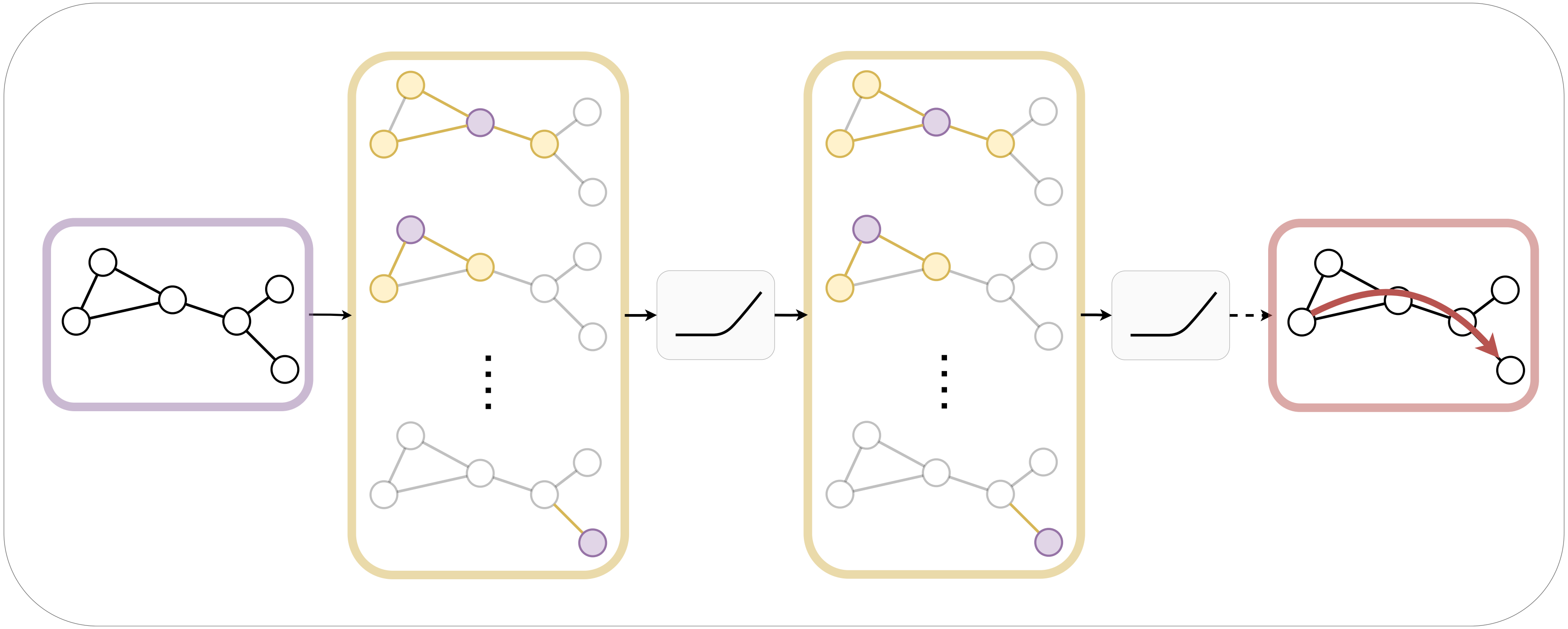


GRAPH MESSAGE PASSING NETWORKS



(Adapted from Thomas Kipf, https://tkipf.github.io/graph-convolutional-networks/)

GRAPH MESSAGE PASSING NETWORKS



DISCUSSION: WHAT ISSUES MIGHT A NAIVE IMPLEMENTATION RUN INTO?

DISCUSSION: WHAT ISSUES MIGHT A NAIVE IMPLEMENTATION RUN INTO?

Graph-level:

$$\mathbf{H}^{(t)} = \sigma\left(\mathbf{A}\mathbf{H}^{(k-1)}\mathbf{W}^{(k)}_{\text{neigh}} + \mathbf{H}^{(k-1)}\mathbf{W}^{k}_{\text{self}}\right)$$

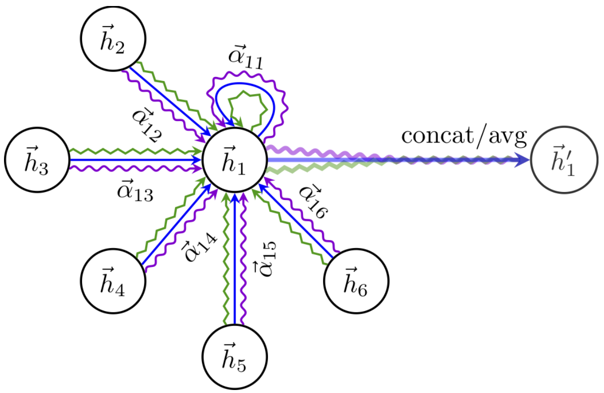
Normalization:

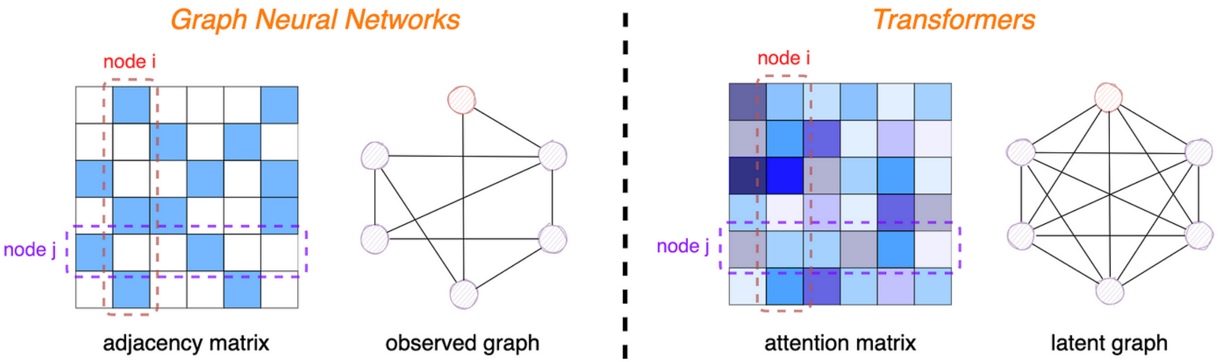
$$\mathbf{h}^{k}_{u} = \sigma\left(\mathbf{W}^{(k)} \sum_{v\in\mathcal{N}(u)\cup\{u\}} \frac{\mathbf{h}_v}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}\right)$$

GRAPH ATTENTION NETWORKS AND TRANSFORMERS

$$\mathbf{M}_{\mathcal{N}(u)} = \sum_{v \in \mathcal{N}(u)} \alpha_{u,v} \mathbf{h}_v$$

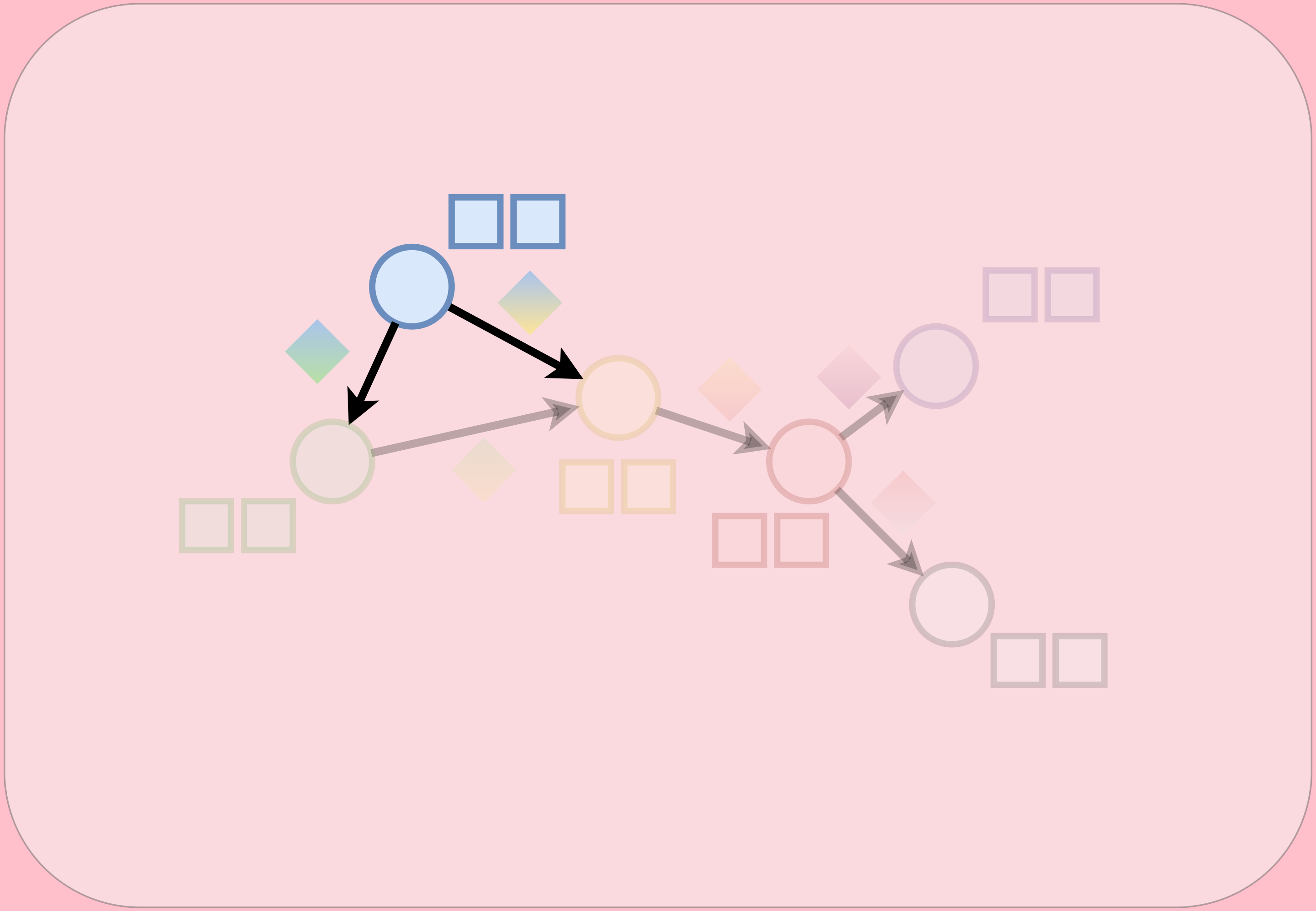
$$\alpha_{u,v} = \frac{\exp\left(\mathbf{a}^\top [\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_v]\right)}{\sum_{v' \in \mathcal{N}(u)} \exp\left(\mathbf{a}^\top [\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_{v'}]\right)}$$



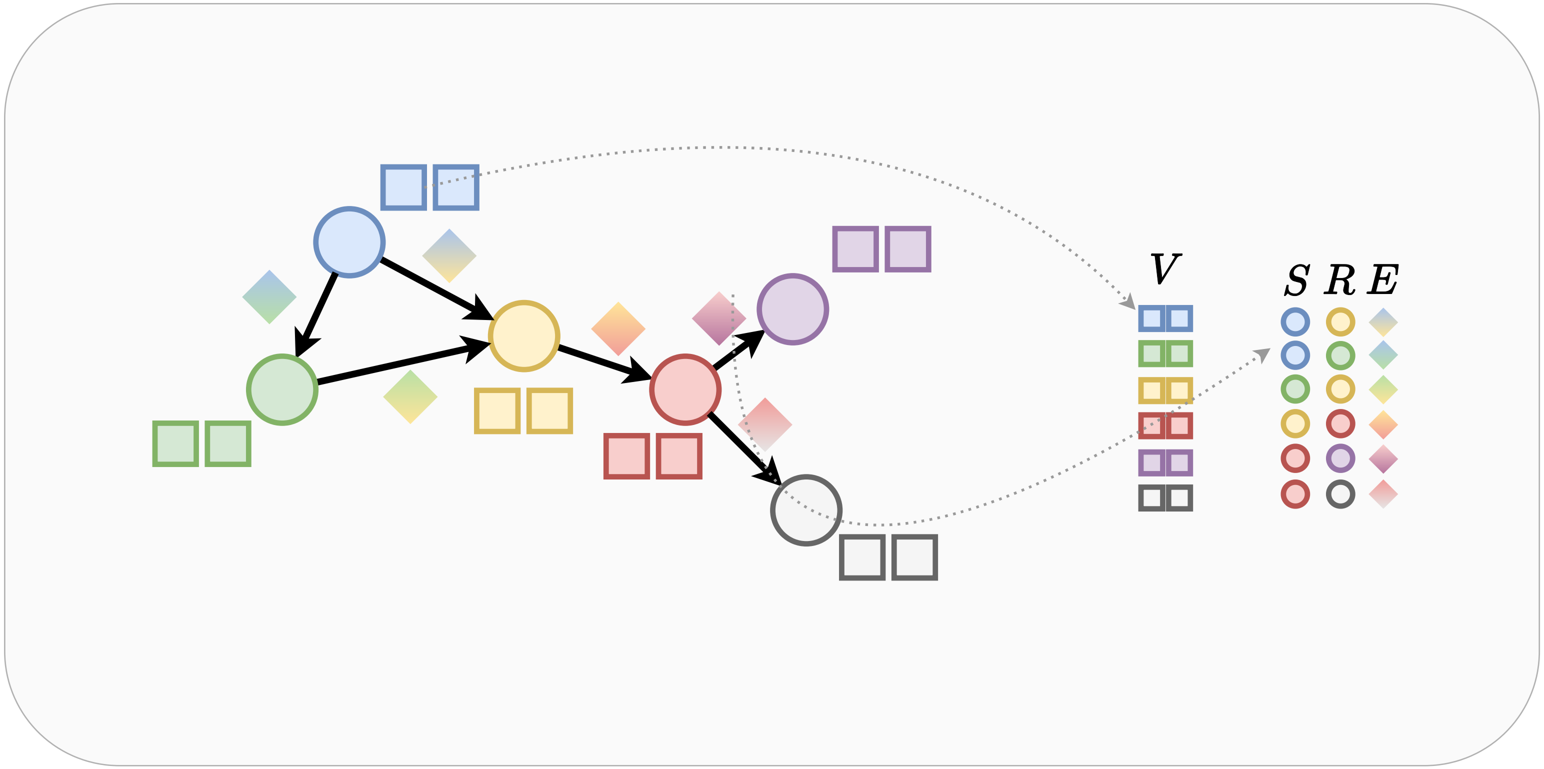


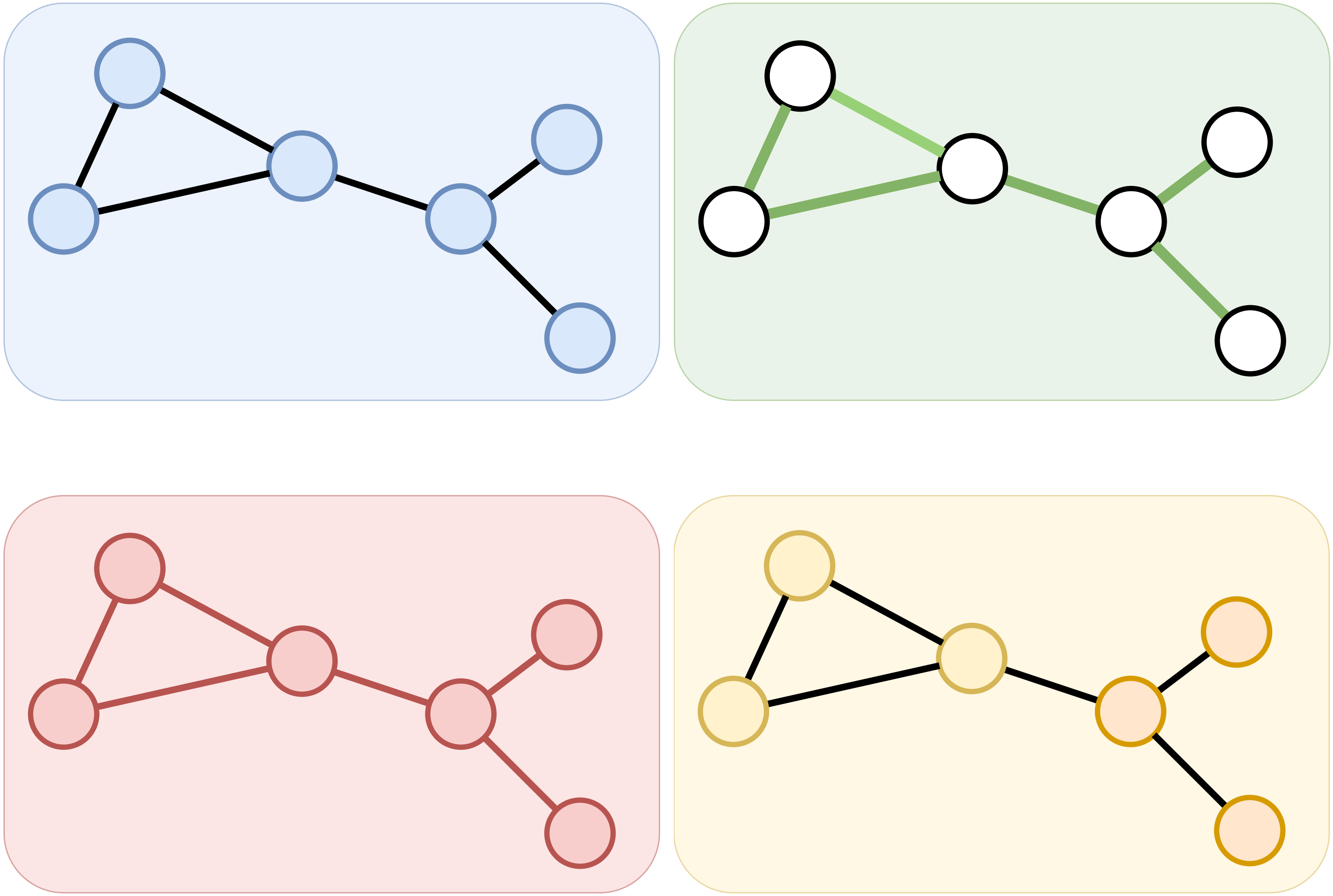
(left: Veličković, Petar, et al. "Graph Attention Networks." arXiv preprint arXiv:1710.10903 (2017))
(right: How to Build Graph Transformers with O(N) Complexity by Qitian Wu in @TDataScience)

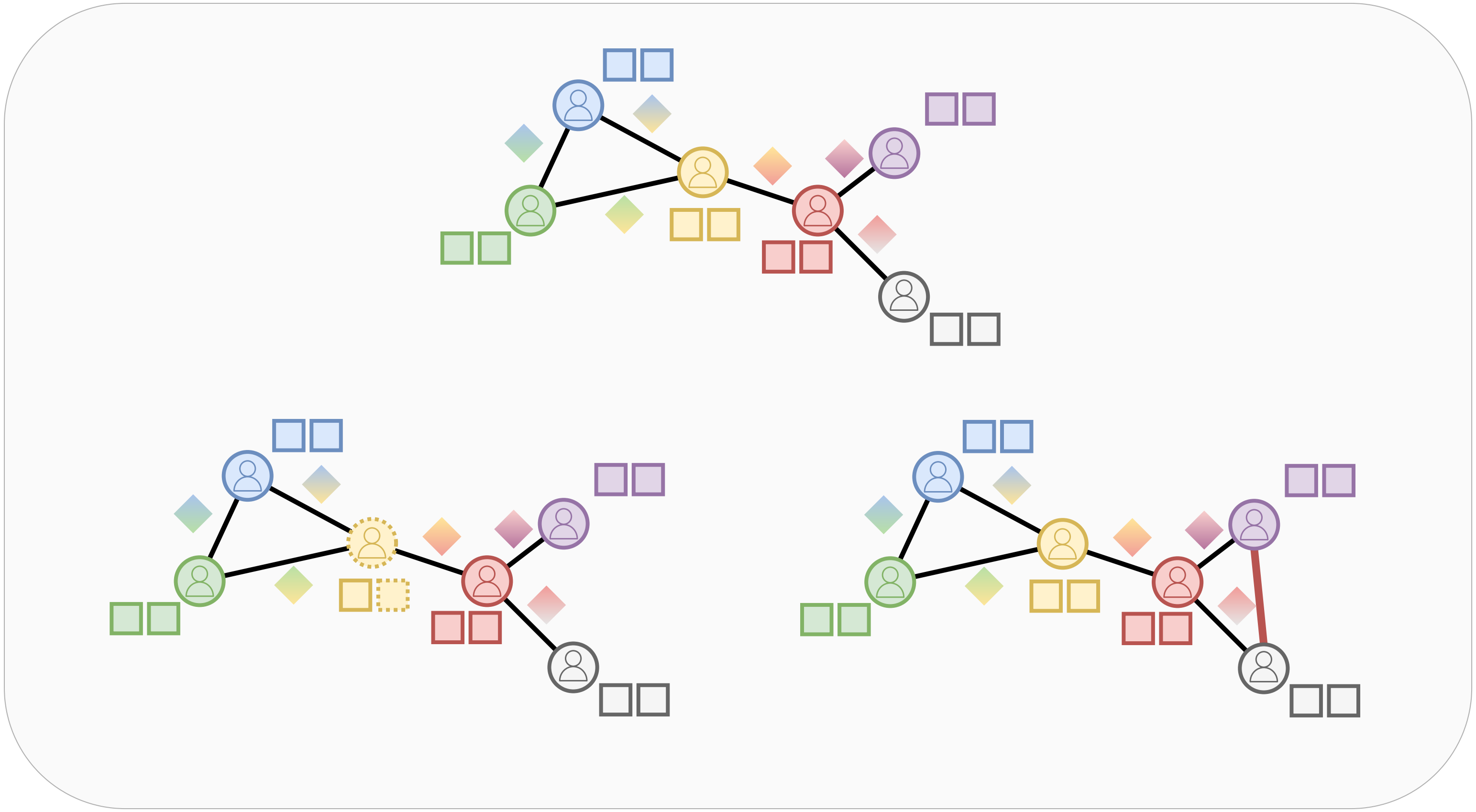
DISCUSSION: LIVE DEMO

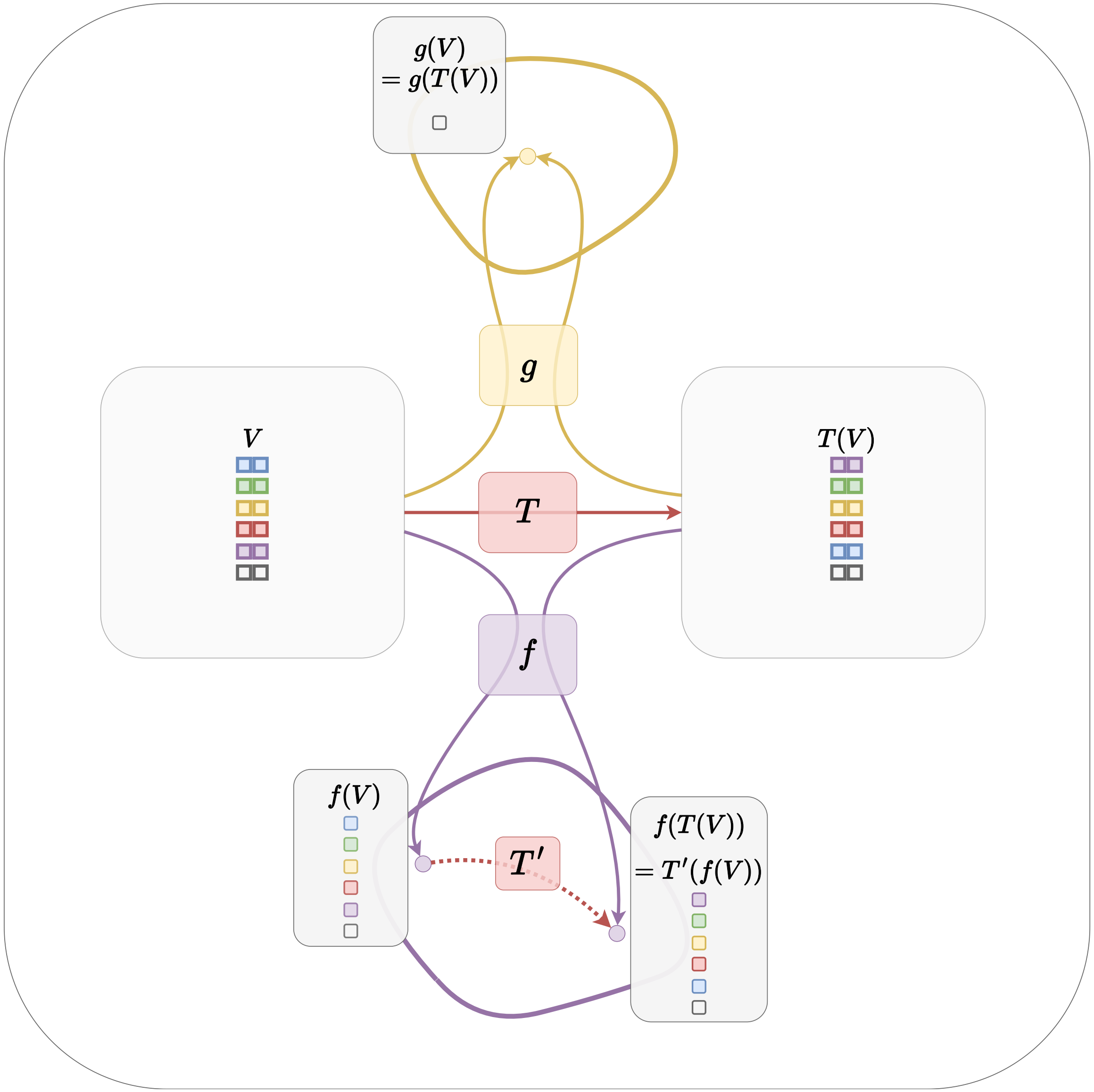


RECAP LECTURE 1

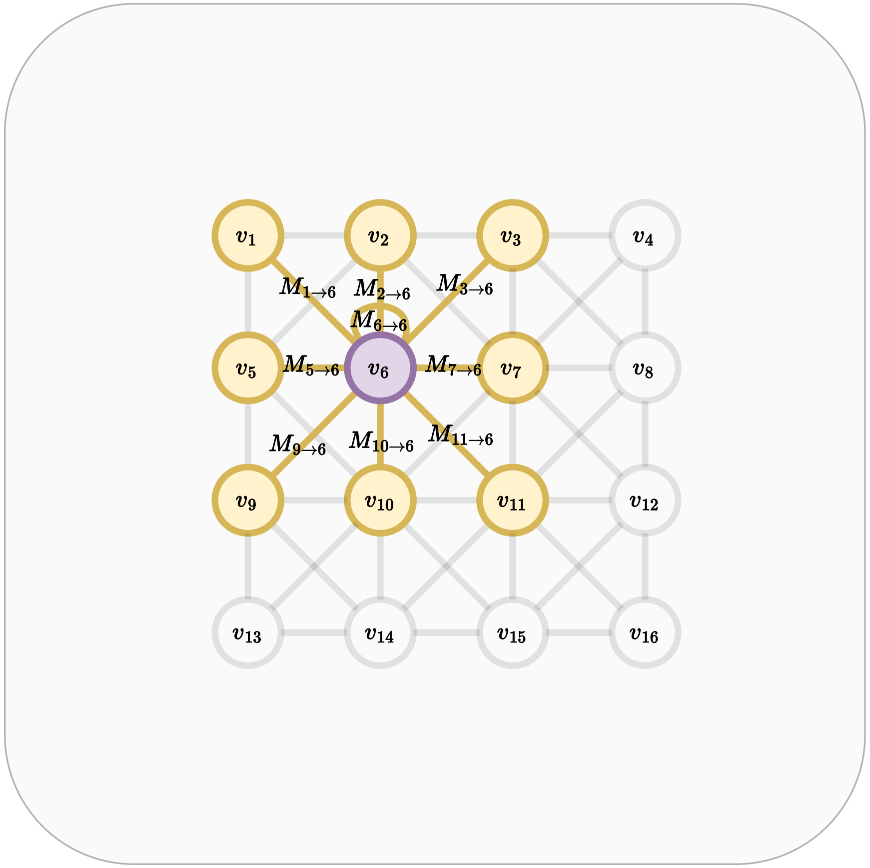

V
S R E

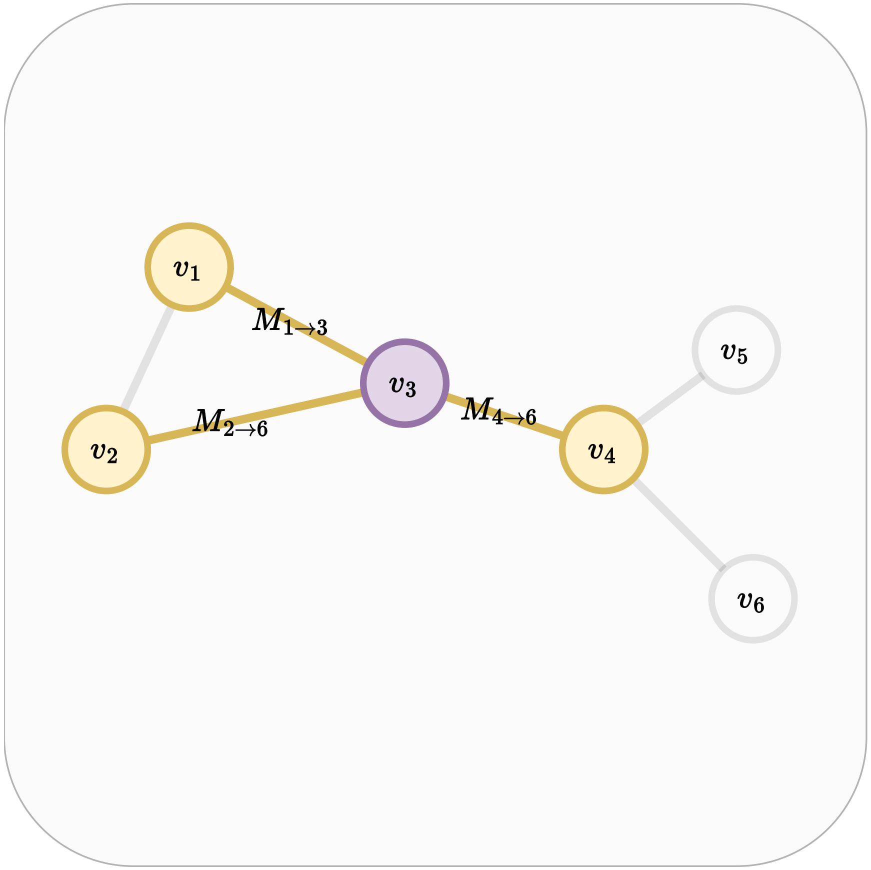


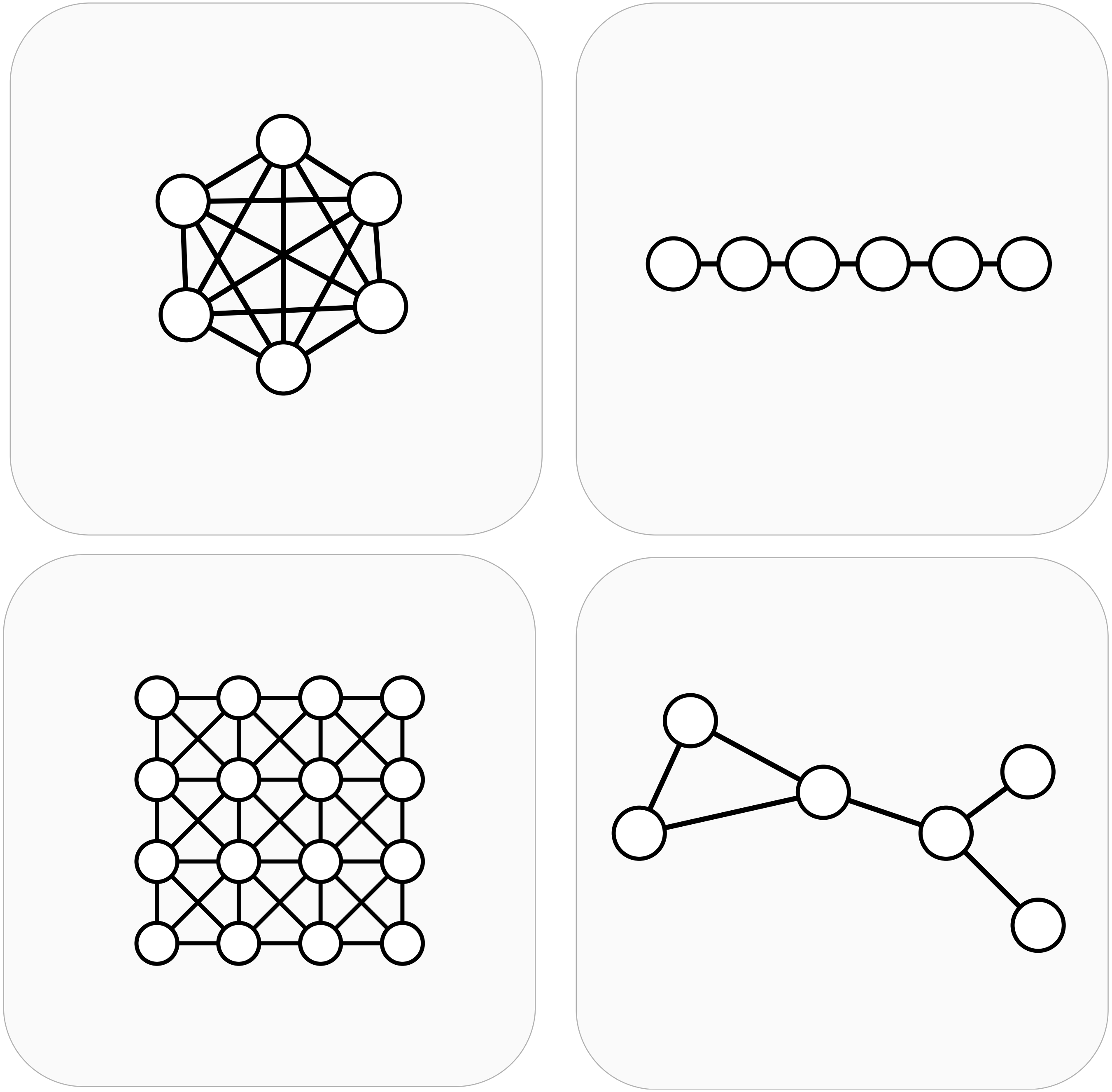




$g(V)$
$= g(T(V))$
g
V
T
$T(V)$
f
$f(V)$
T'
$f(T(V))$
$= T'(f(V))$


v_1 v_2 v_3 v_4
v_5 v_6 v_7 v_8
v_9 v_{10} v_{11} v_{12}
v_{13} v_{14} v_{15} v_{16}
$M_{1\to6}$
$M_{2\to6}$
$M_{3\to6}$
$M_{6\to6}$
$M_{5\to6}$
$M_{7\to6}$
$M_{9\to6}$
$M_{10\to6}$
$M_{11\to6}$


v_1
v_2
v_3
v_4
v_5
v_6
$M_{1\to3}$
$M_{2\to6}$
$M_{4\to6}$



MESSAGE PASSING ON GRAPH

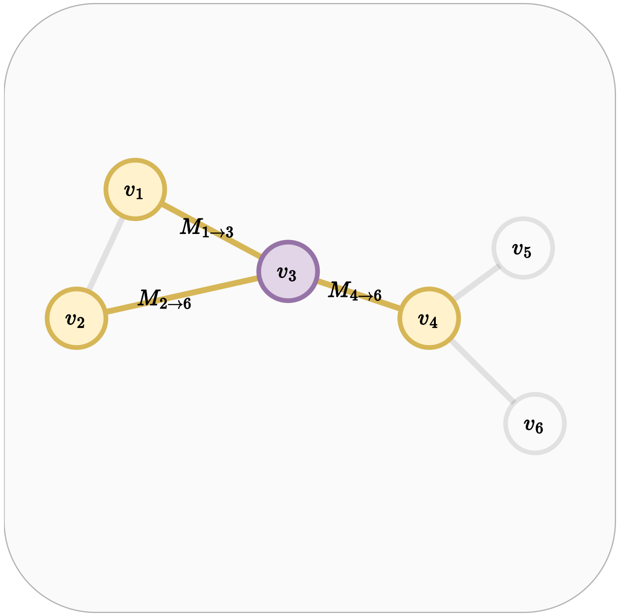
Algorithm 3 Basic graph message passing

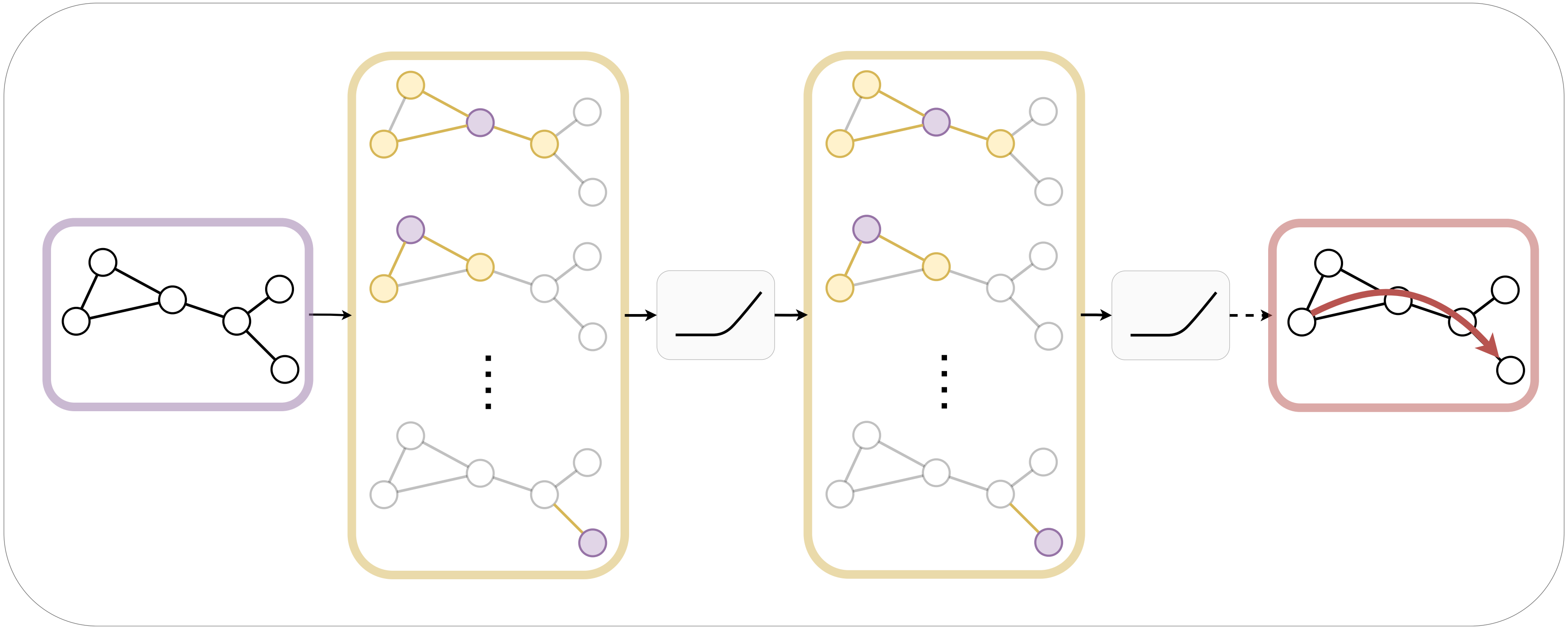
Input: Weight matrices, $\mathbf{W}_{\text{self}}$, $\mathbf{W}_{\text{neigh}}$, and bias, $\mathbf{b}$, neighborhood function, $\mathcal{N}$.

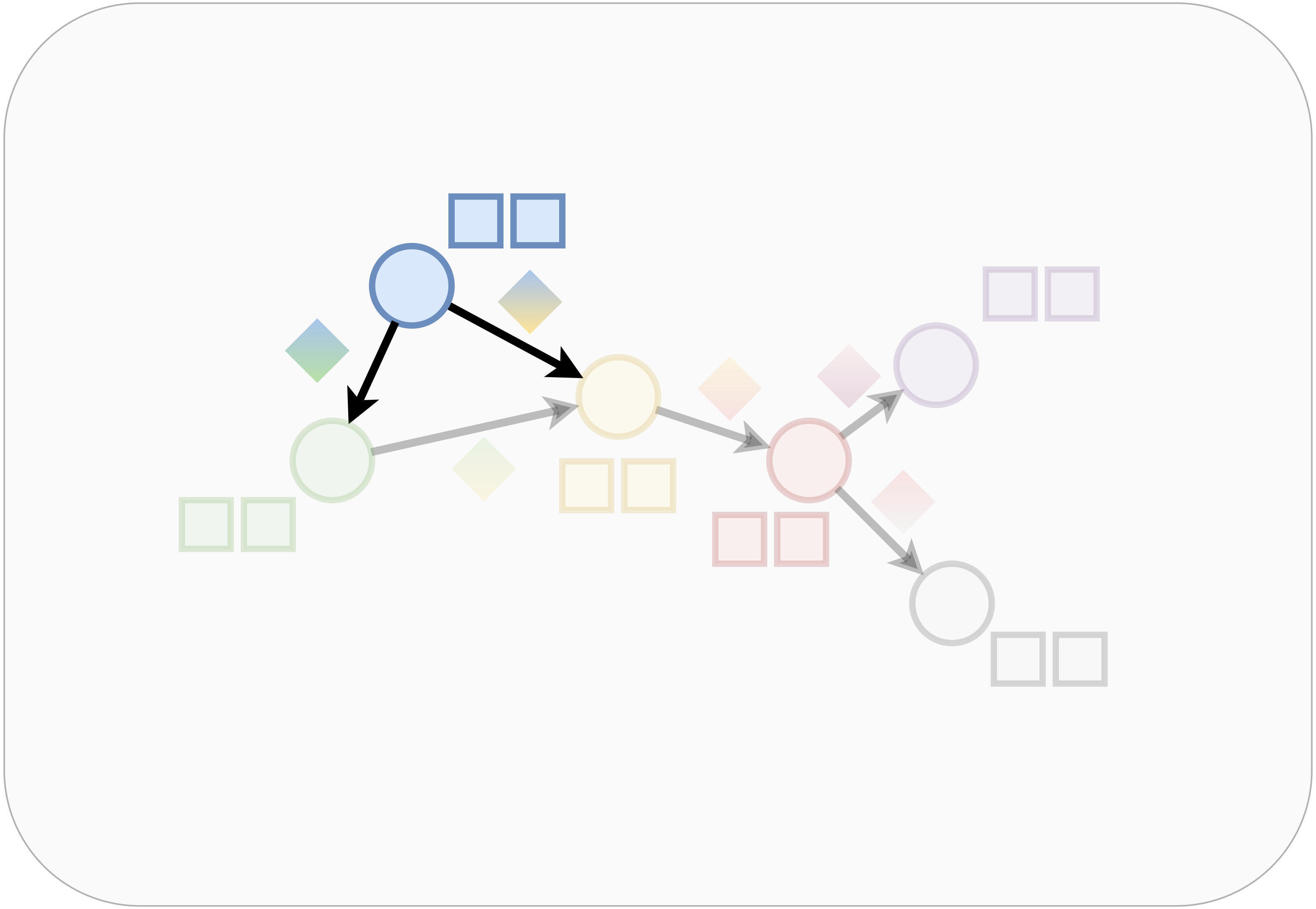
Input: Graph, $\mathcal{G}$ with nodes $\mathcal{V} = \{v_i\}_{i=0}^{V}$ and edges $\mathcal{E} = \{e_{u\to v} | u, v \in \mathcal{V}\}$, and a specified K number of rounds of message passing.

Output: Updated node features $\mathbf{h}_u^{(K+1)}$ for all nodes u

Initialize $\mathbf{h}_u^{(0)}$ as v_u for all nodes u
for $k \in [0, 1, \ldots, K]$ **do**
  for $u \in \mathcal{V}$ **do**
    for $v \in \mathcal{N}(u)$ **do**
      Compute messages : $\mathbf{M}_{v\to u} = \mathbf{W}_{\text{neighbors}} \mathbf{h}_v^{(k)} + \mathbf{b}$
    end for
    Compute self message: $\mathbf{M}_{\text{self}} = \mathbf{W}_{\text{self}} \mathbf{h}_u^{k}$
    Compute total message: $\mathbf{M}_u = \mathbf{M}_{\text{self}} + \sum_{v \in \mathcal{N}(u)} \mathbf{M}_{v\to u}$
    Update node: $\mathbf{h}_u^{(k+1)} \leftarrow \sigma(\mathbf{M}_u)$
  end for
end for

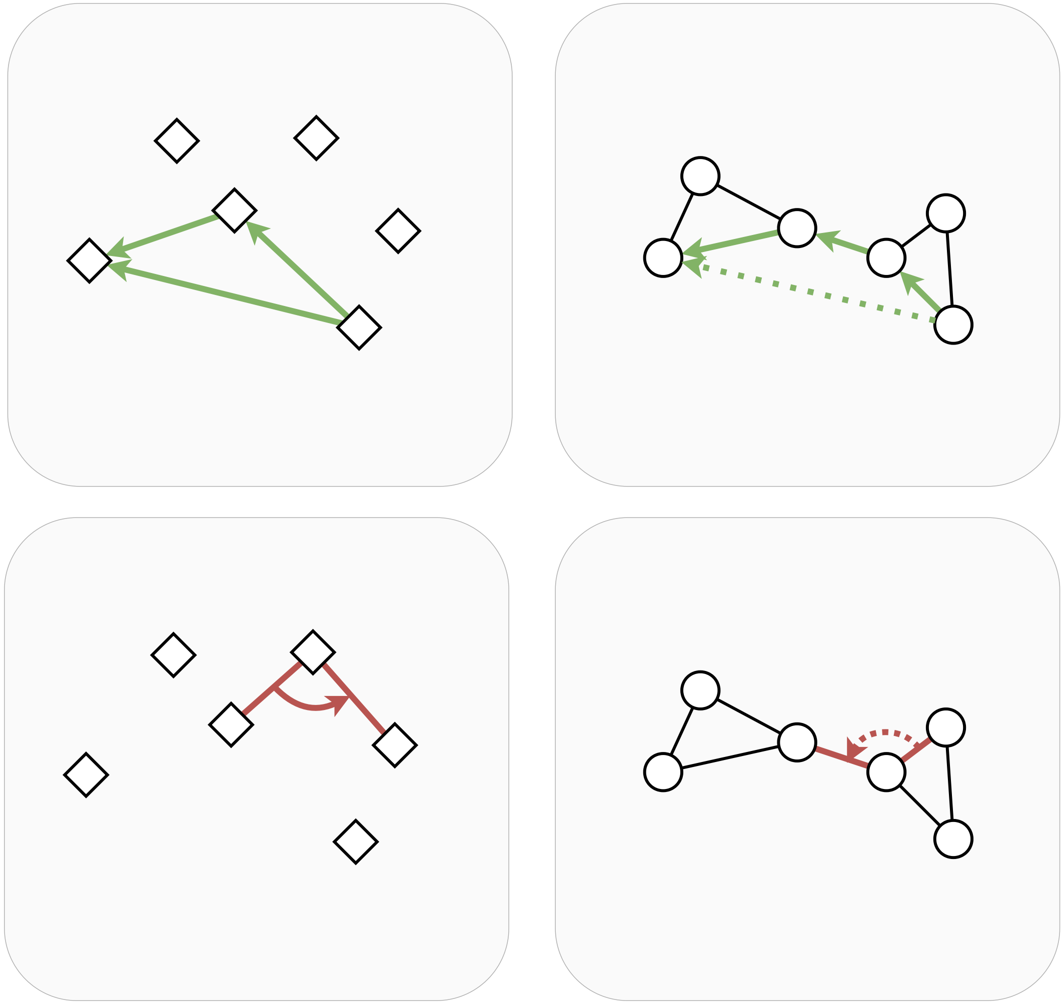




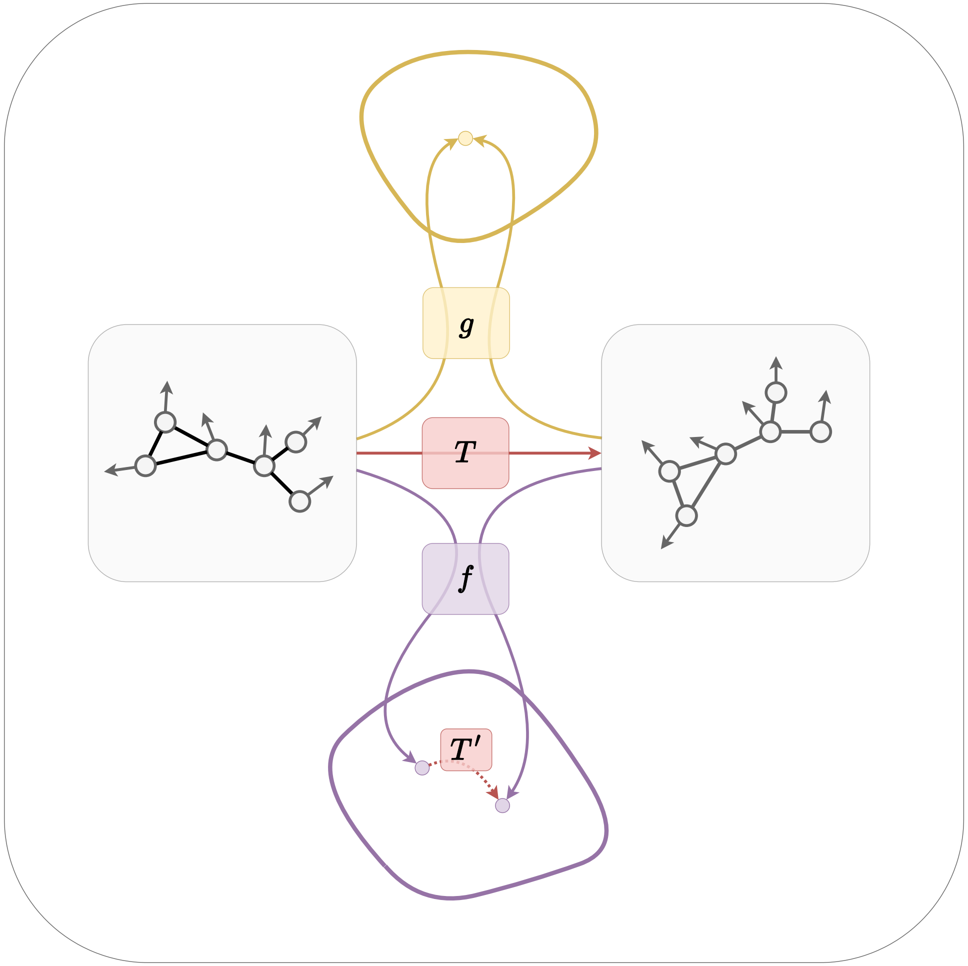


GEOMETRIC INFORMATION

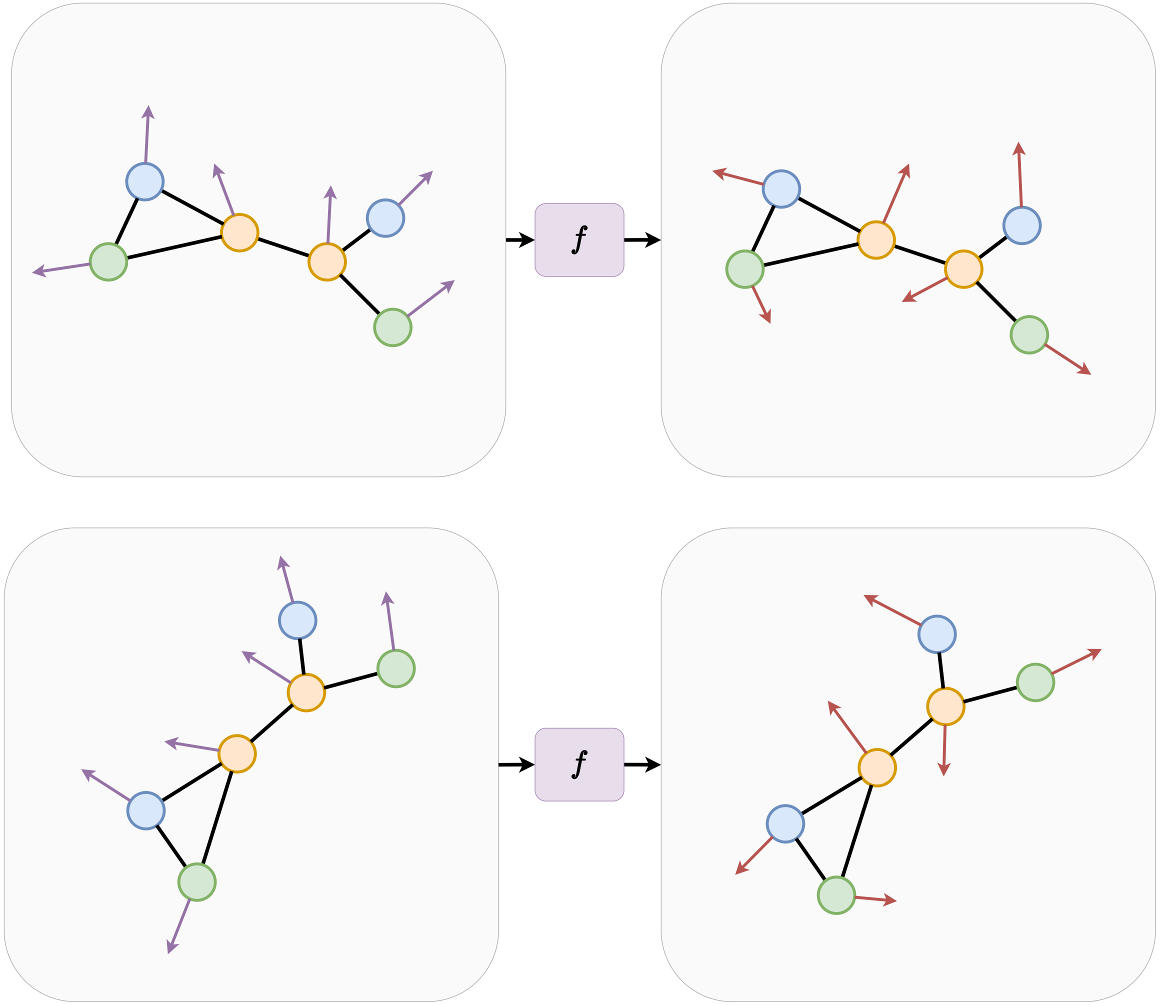
GEOMETRIC INFORMATION



ROTATION INVARIANCE AND EQUIVARIANCE



ROTATION INVARIANCE AND EQUIVARIANCE



ROTATION INVARIANCE AND EQUIVARIANCE