Cluster-wise Graph Transformer with Dual-granularity Kernelized Attention

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SHANGHAI JIAO TONG UNIVERSITY

NEURAL INFORMATION PROCESSING SYSTEMS

How to pool a graph step by step?

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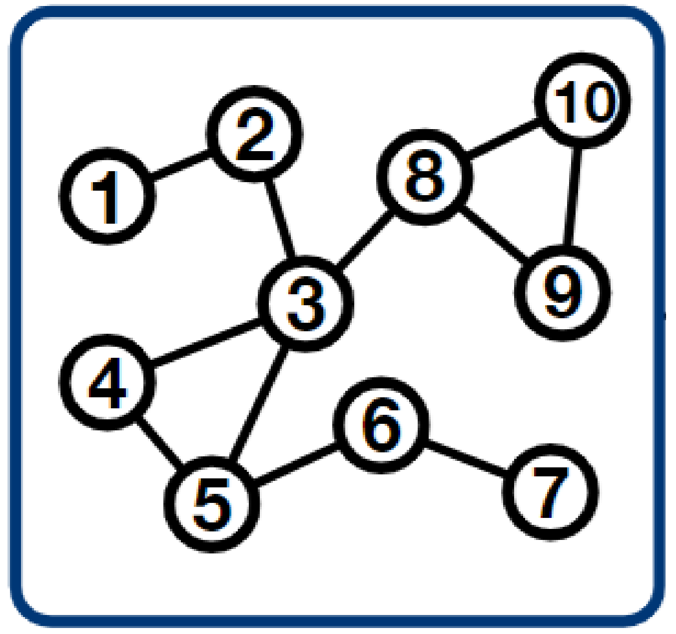
An illustrative example of **Node Clustering Pooling**



Input Graph
$\mathcal{G} = (\mathcal{V}, \mathcal{E})$

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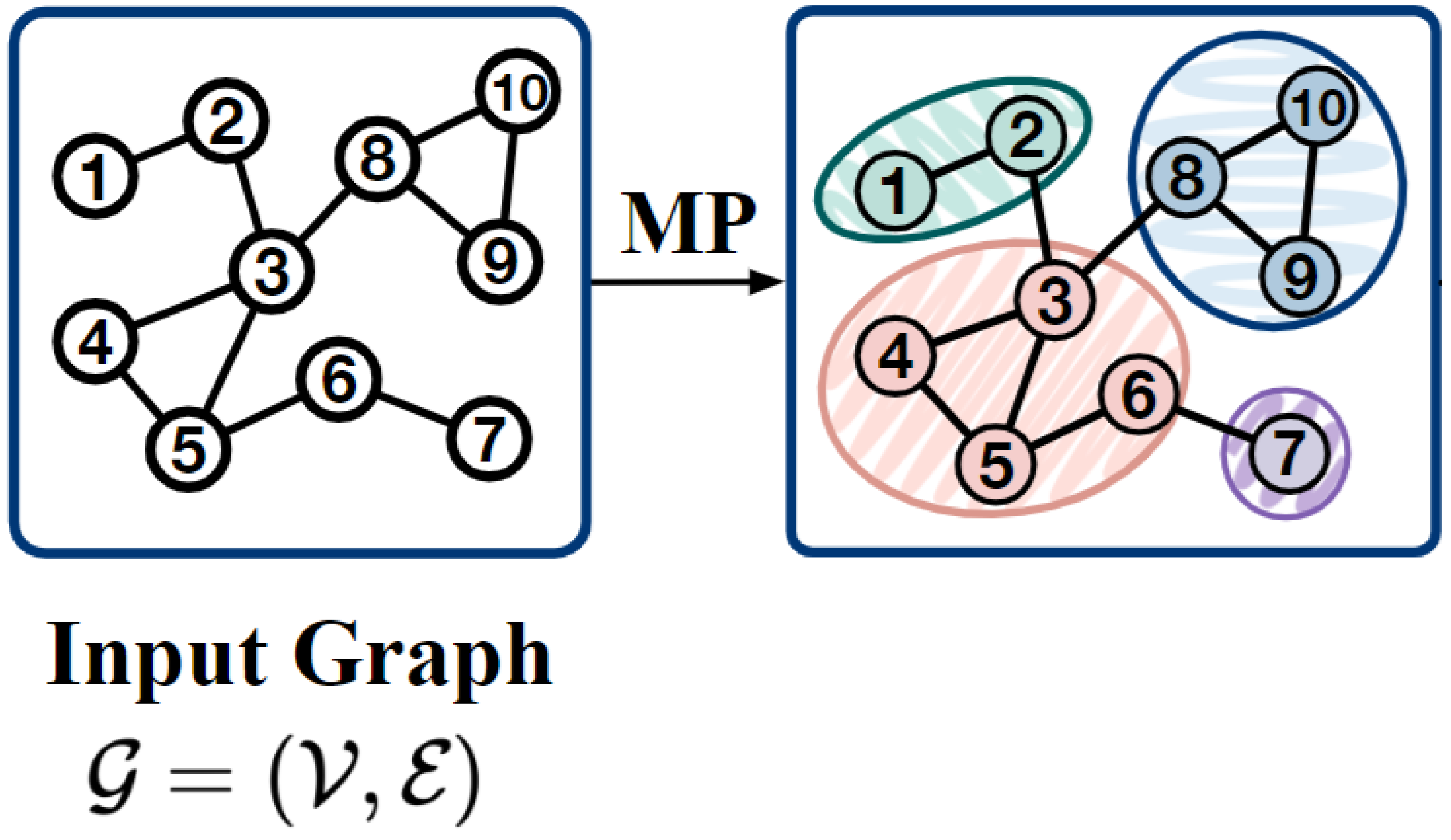

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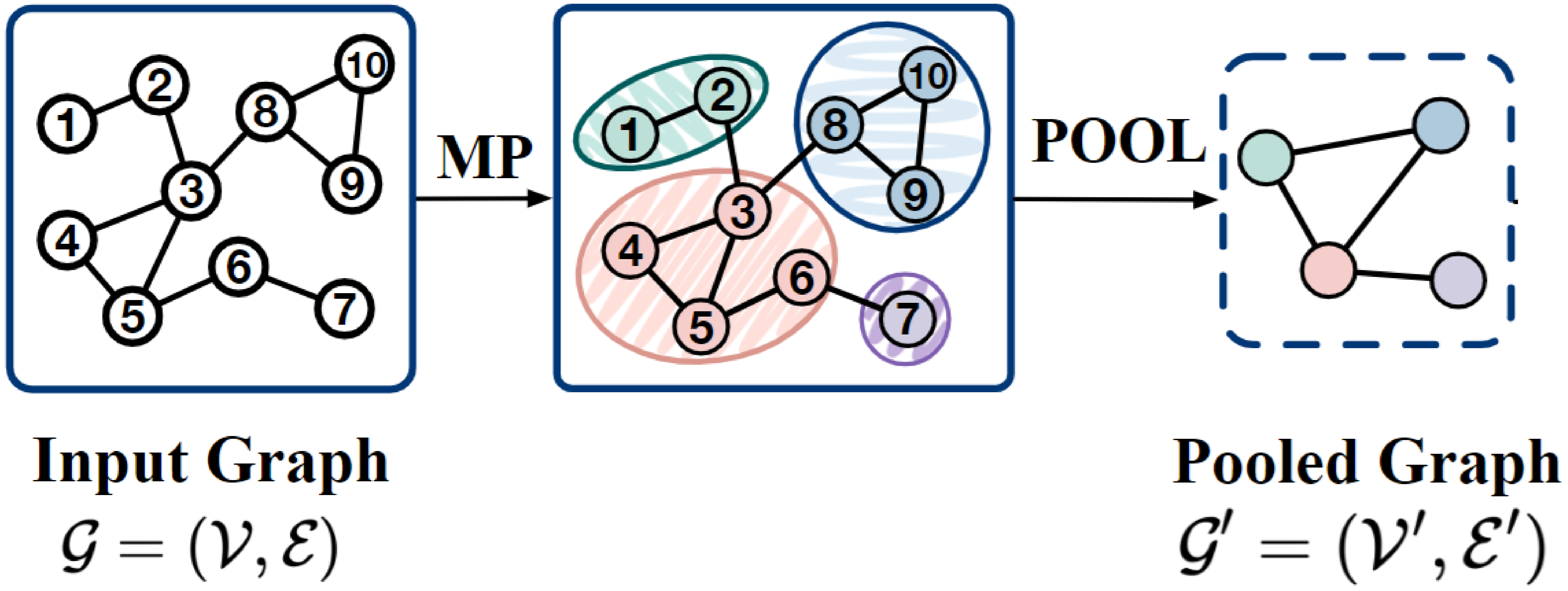

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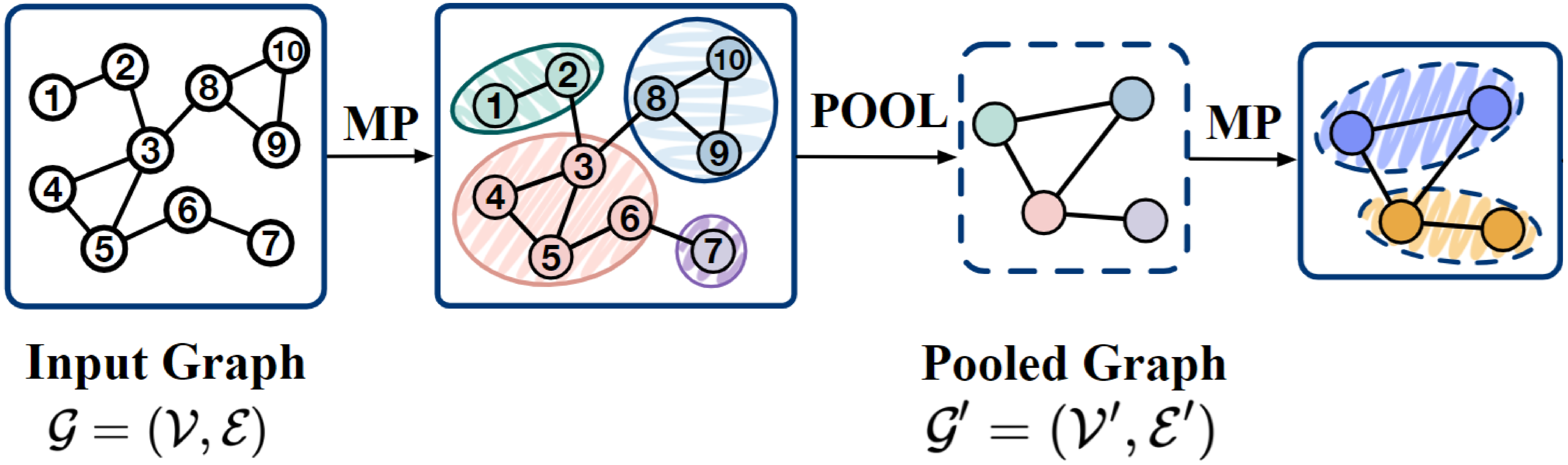

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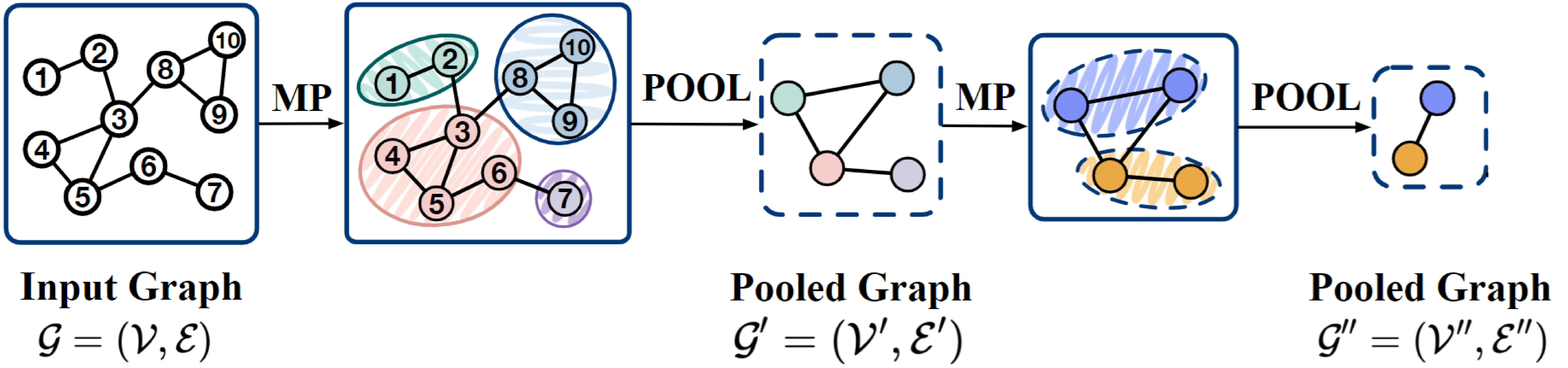

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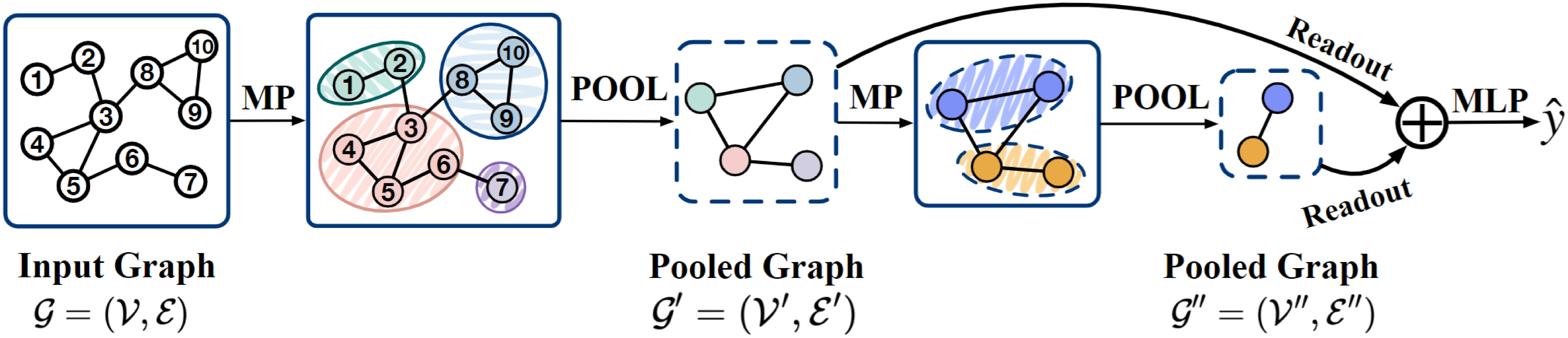

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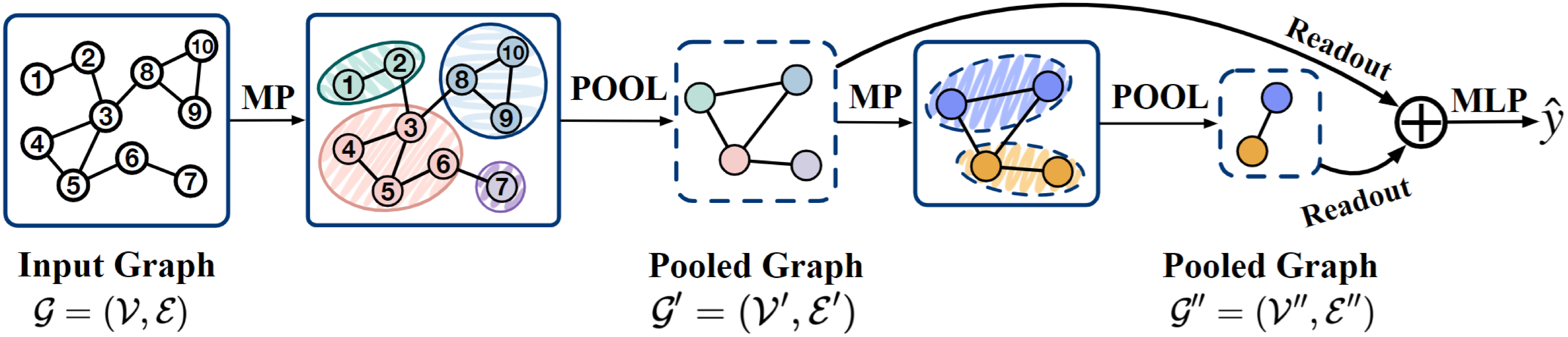

Cluster Assignment + Graph Coarsening

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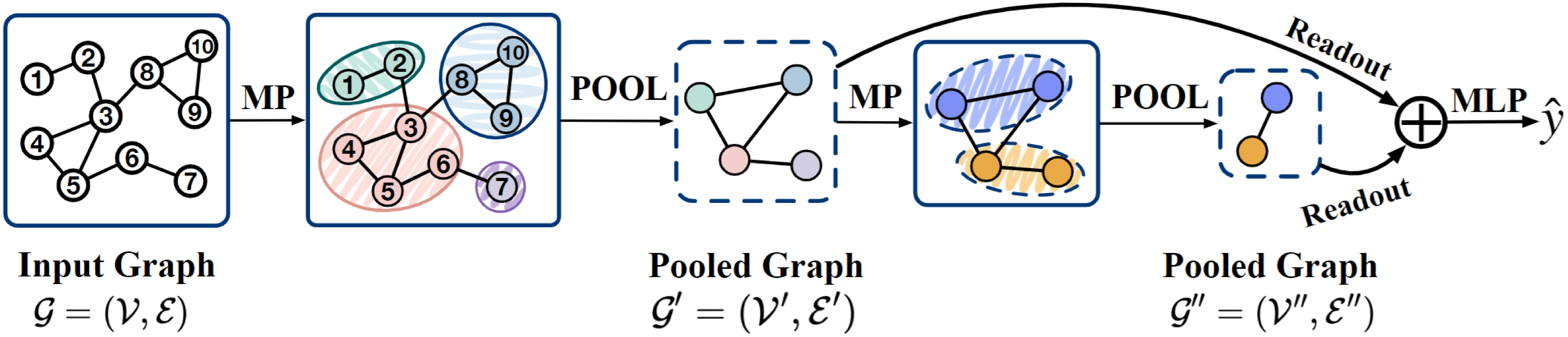

Cluster Assignment + Graph Coarsening

compressing each cluster into a single embedding

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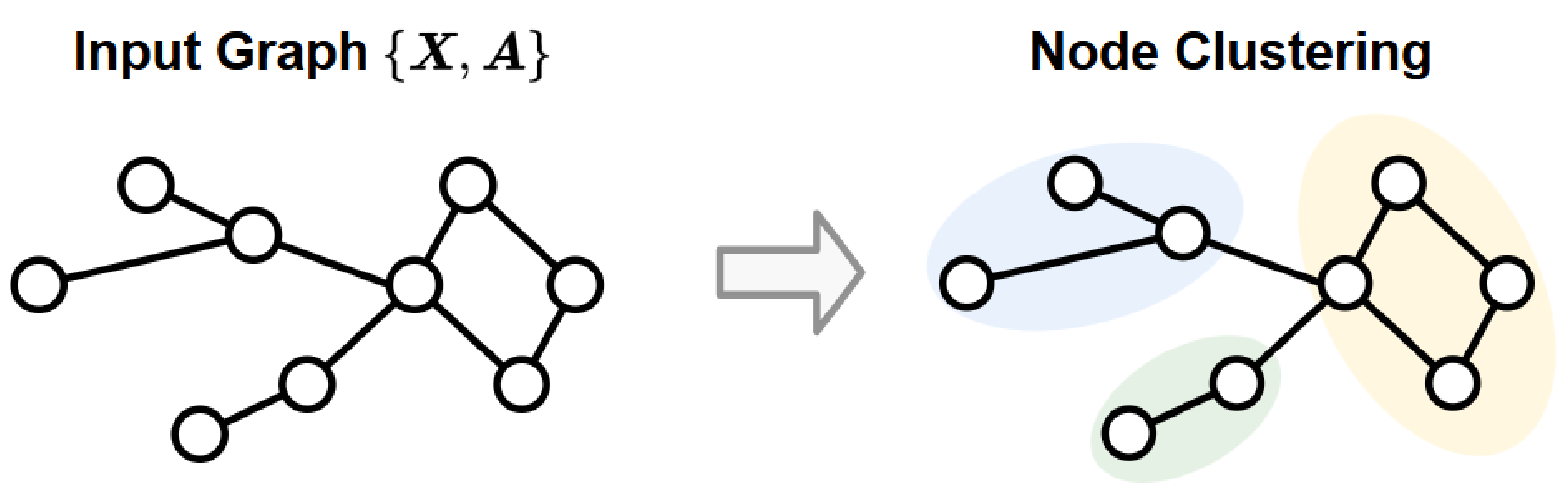
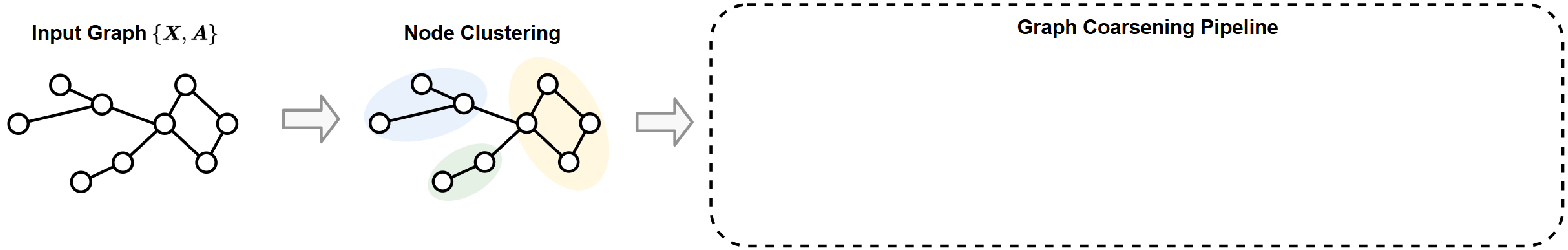
Graph Coarsening Pipeline leads to some problems when performing MP:

- overly homogeneous cluster representations
- loss of node-level information

➢ Can we avoid reducing each cluster to a single node?

➢ We can envision the graph as a network of interconnected node sets.


Input Graph $\{X, A\}$
Node Clustering


Input Graph $\{\boldsymbol{X}, \boldsymbol{A}\}$
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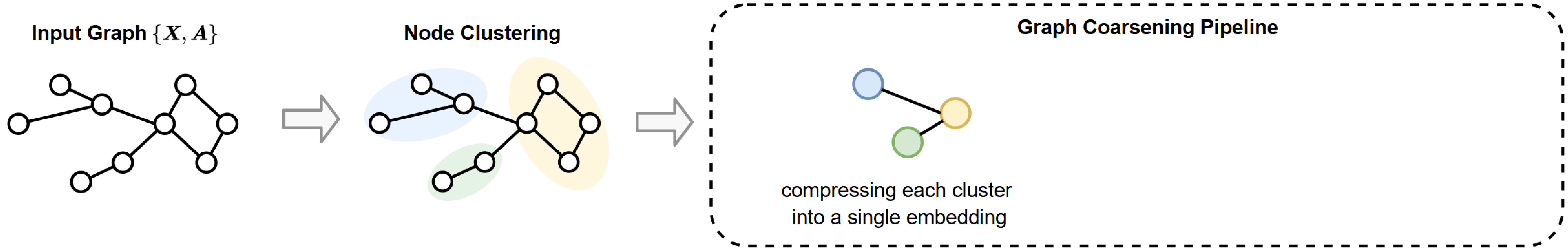
Graph Coarsening Pipeline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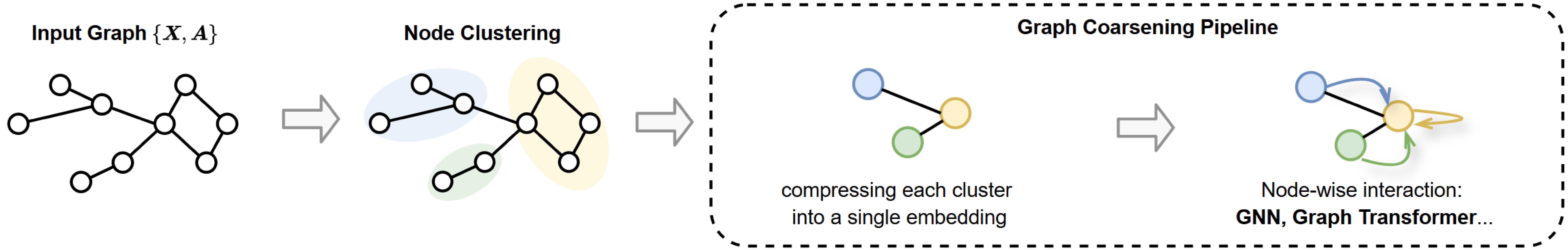
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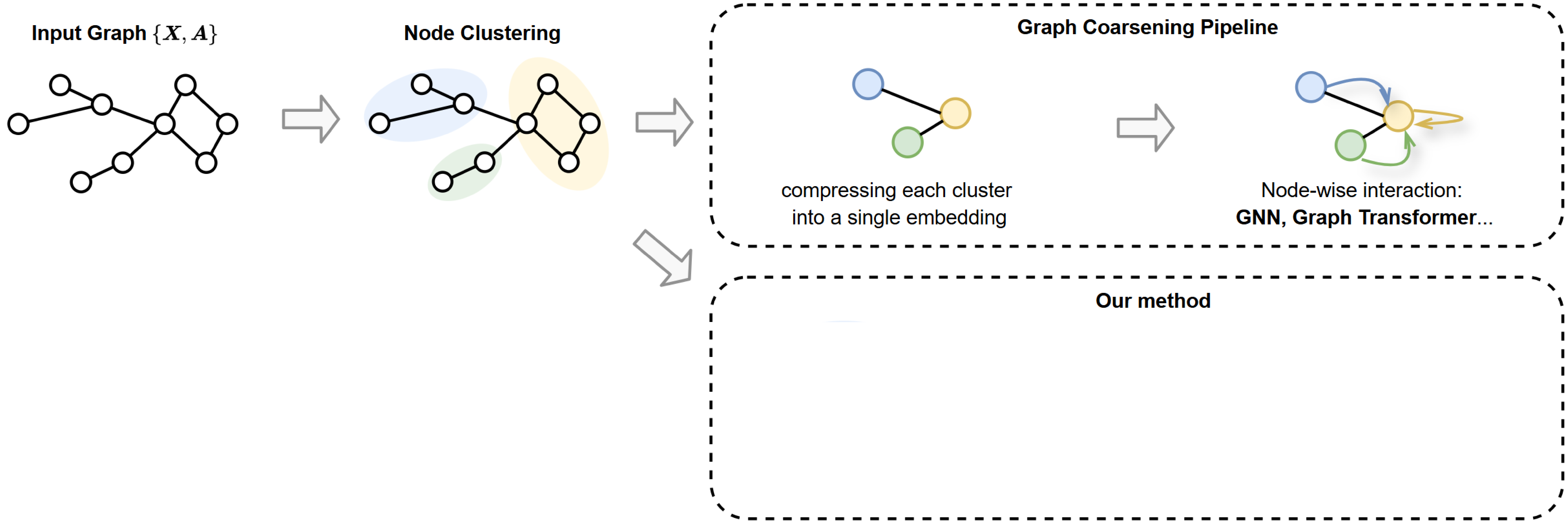
Node-wise interaction:
GNN, Graph Transformer...



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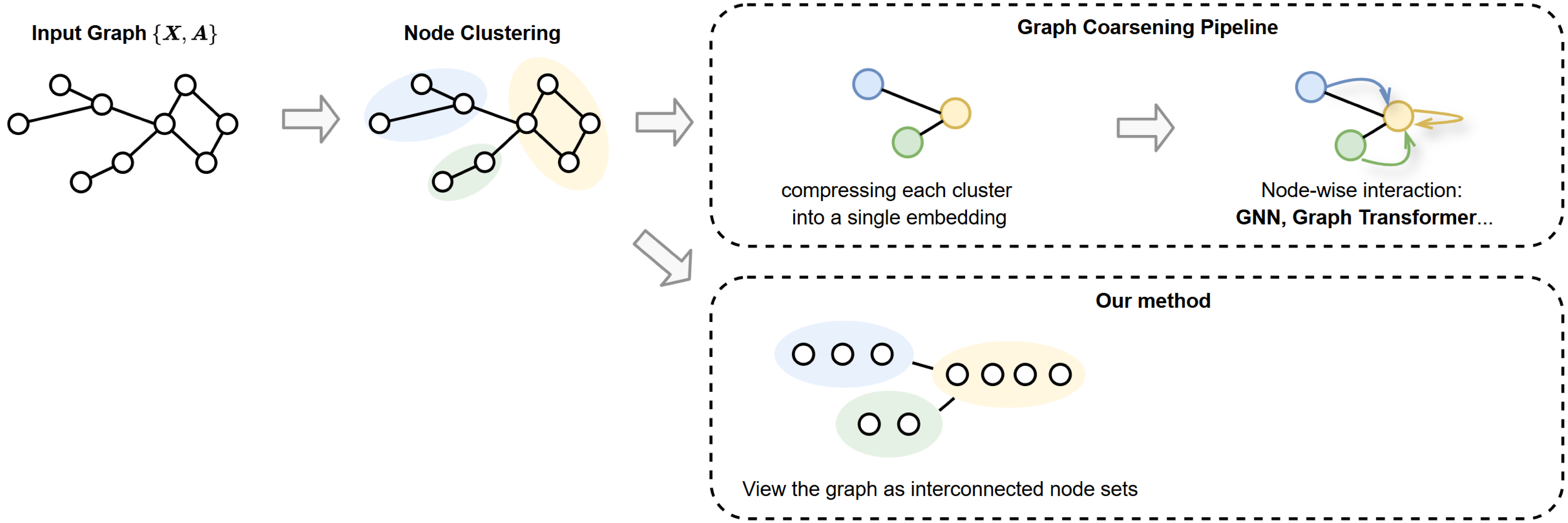

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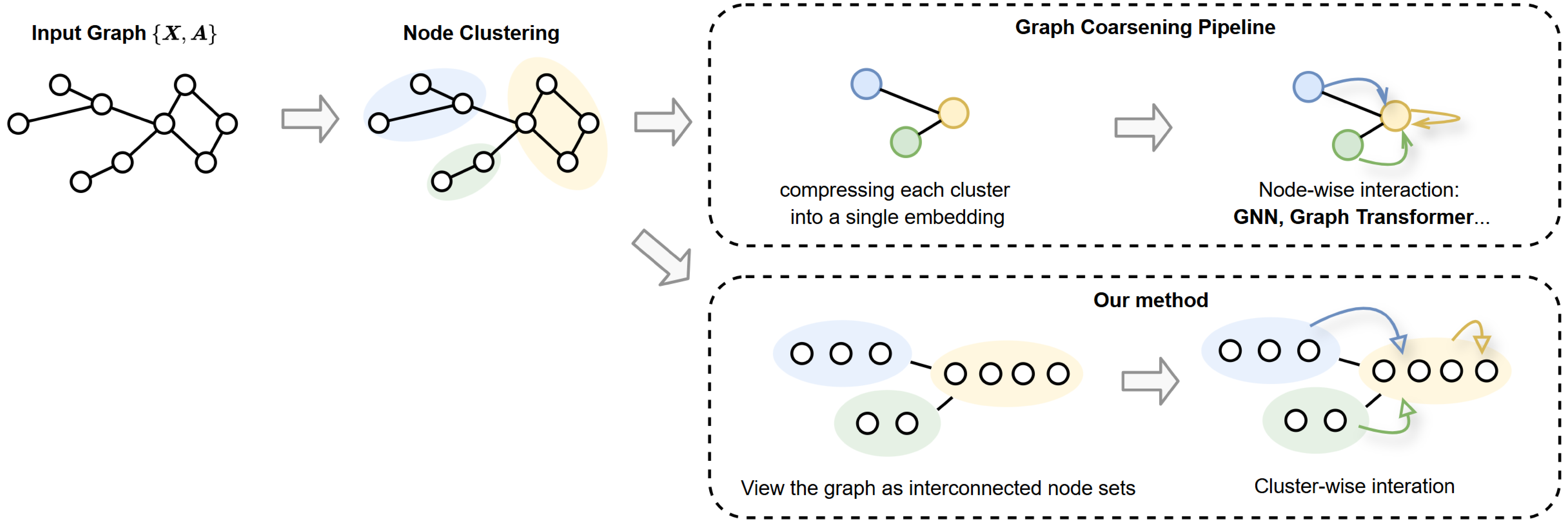
View the graph as interconnected node sets



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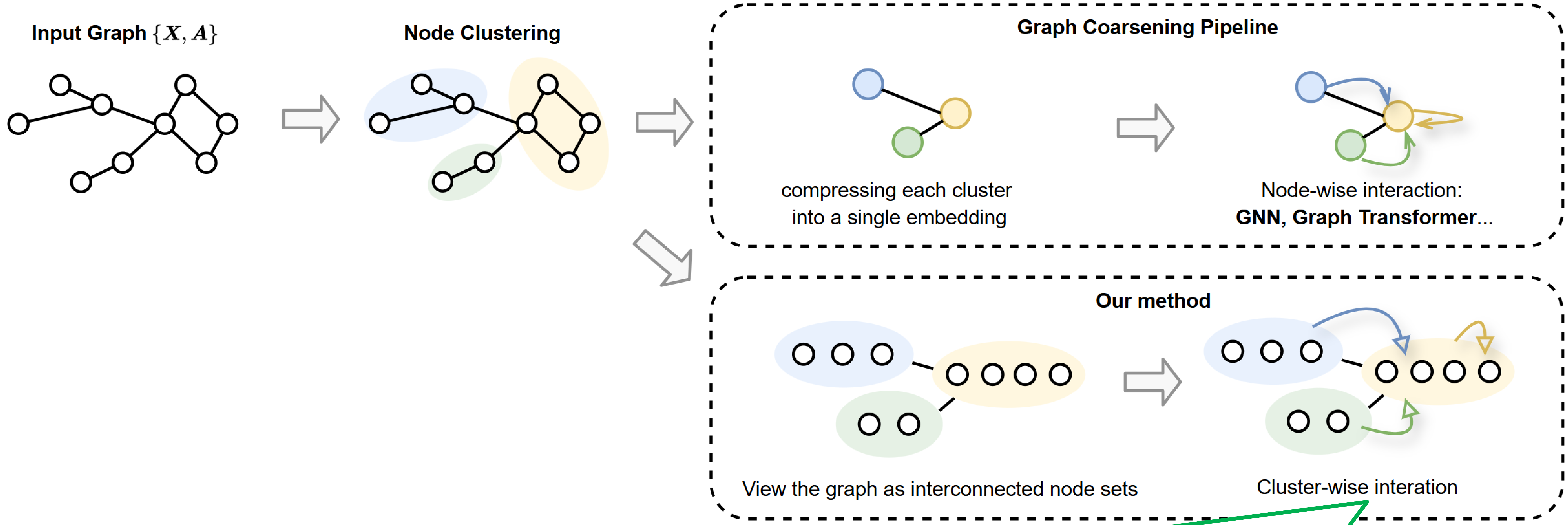
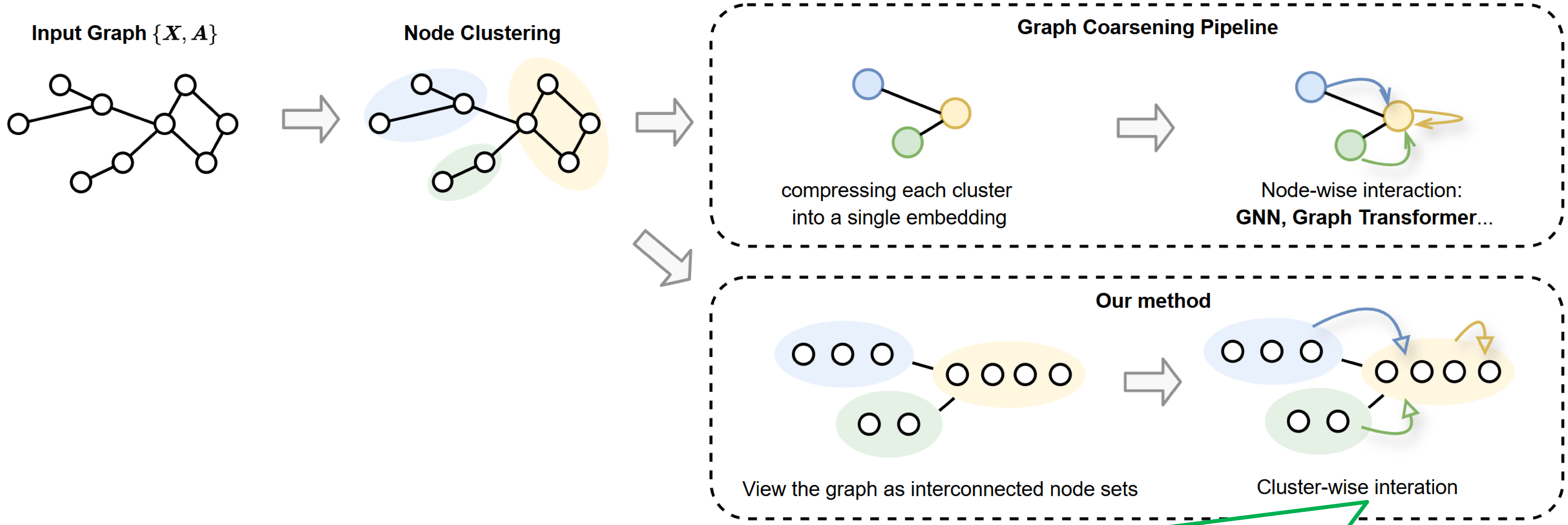
Cluster-wise interation



We need a method that captures information at both the node and cluster levels.



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Node-to-Cluster Attention Mechanism

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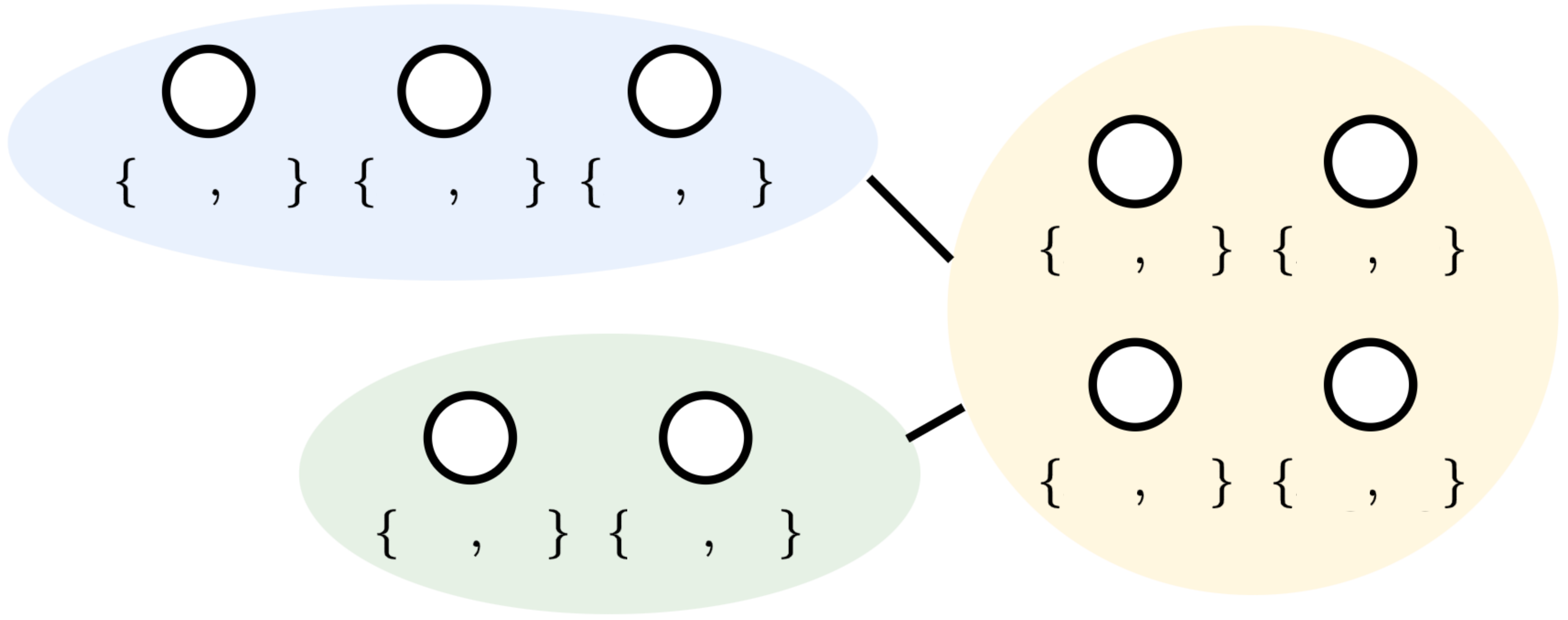
Queries of clusters		
Keys of nodes		



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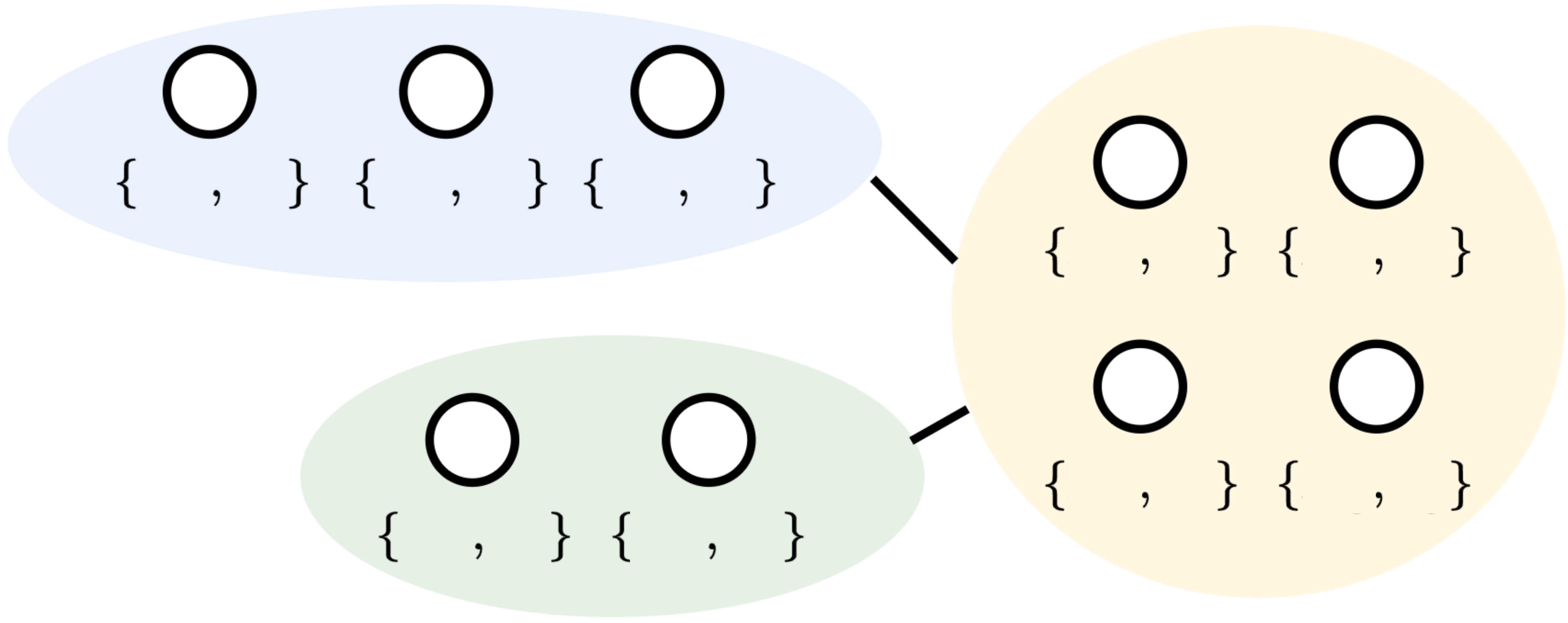

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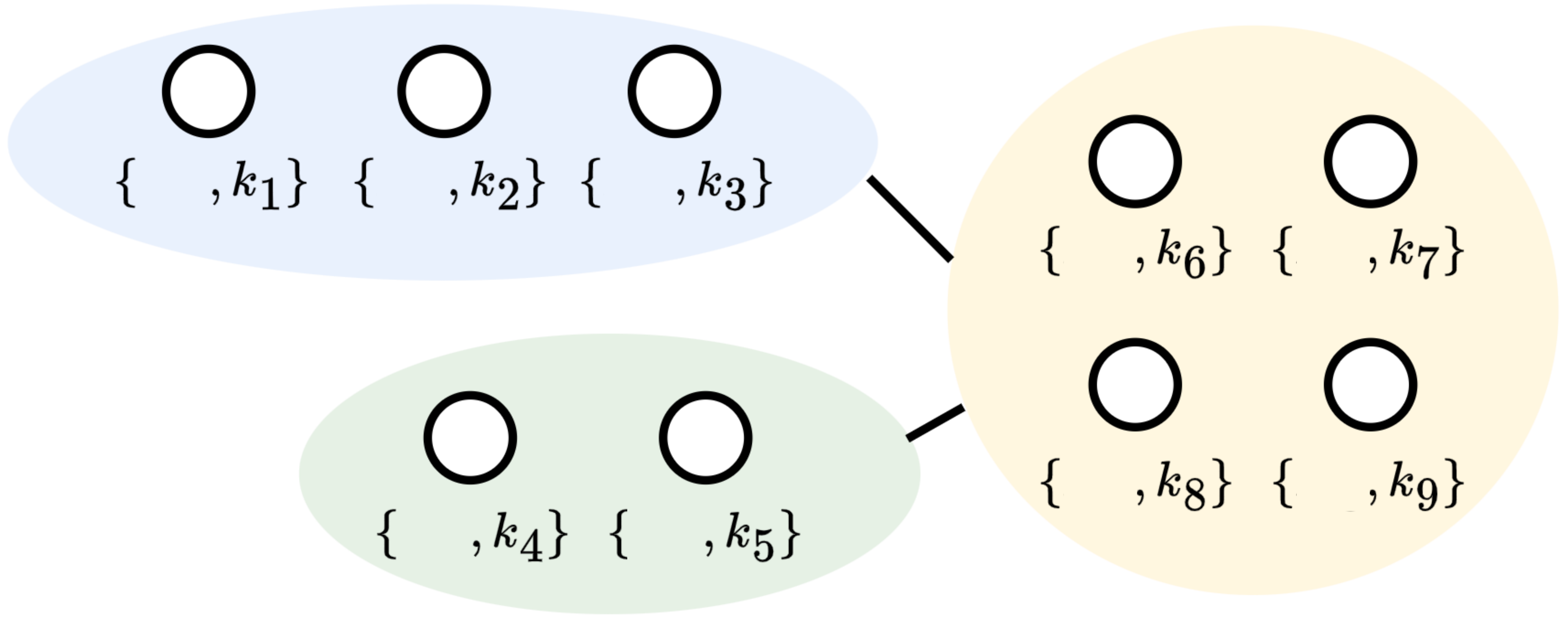

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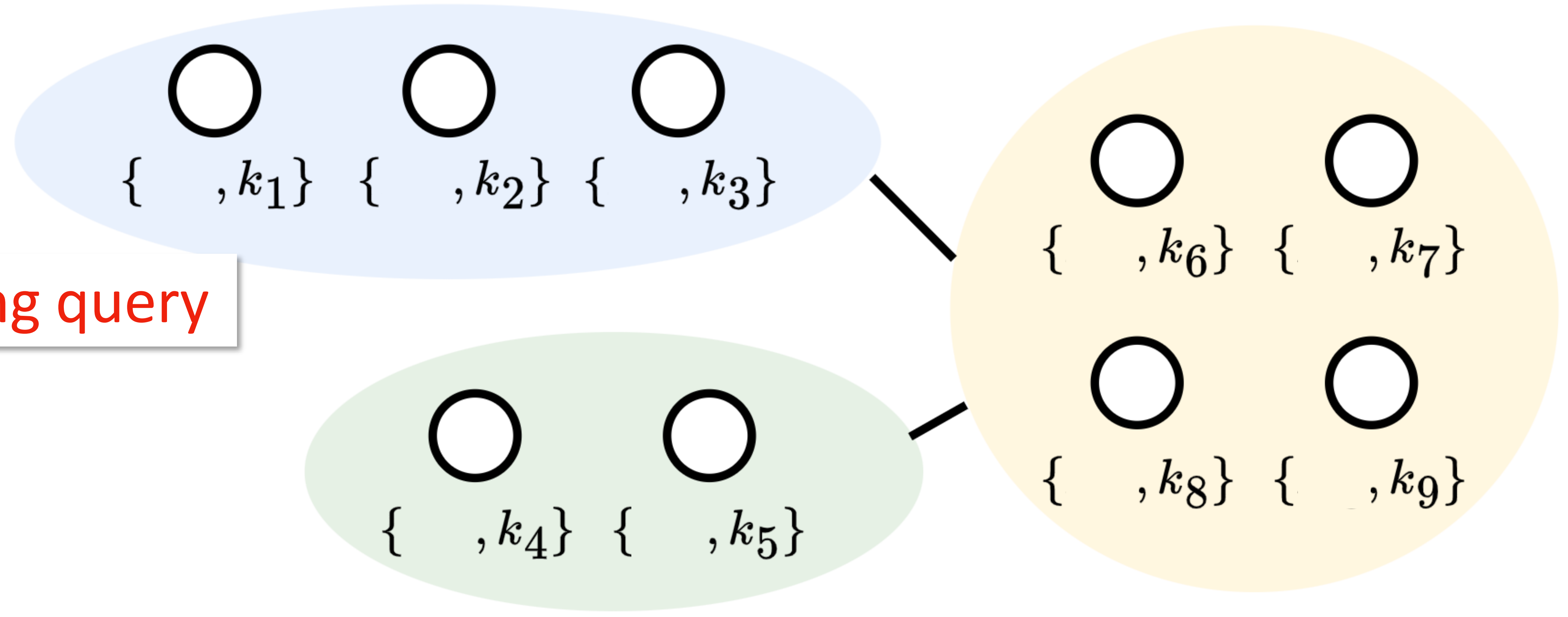
corresponding query



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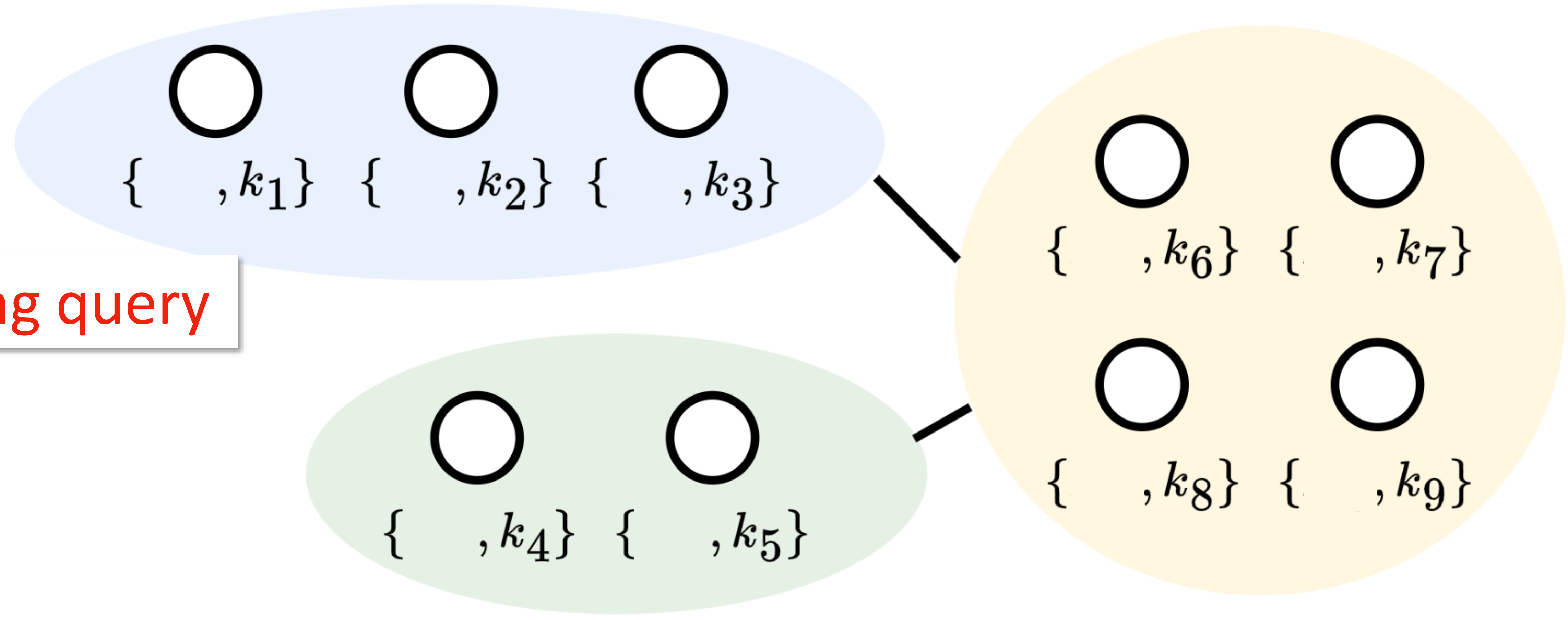

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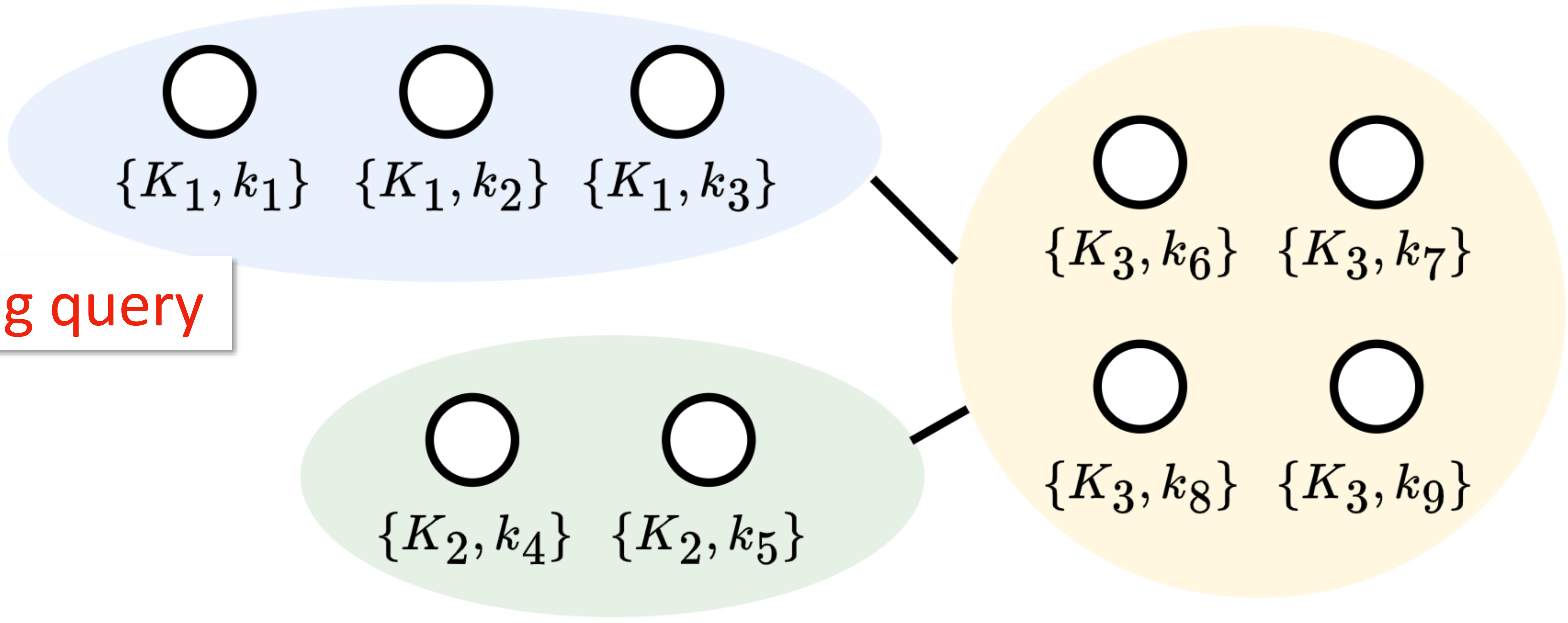

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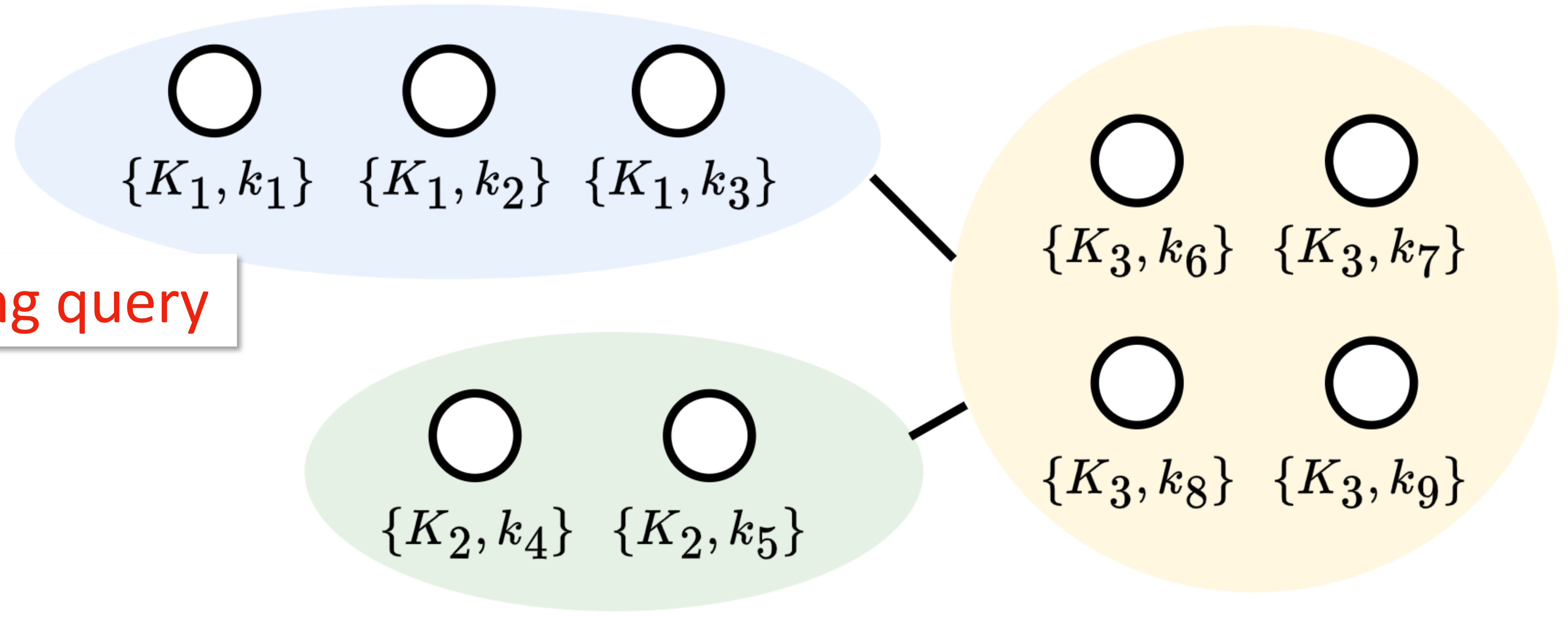

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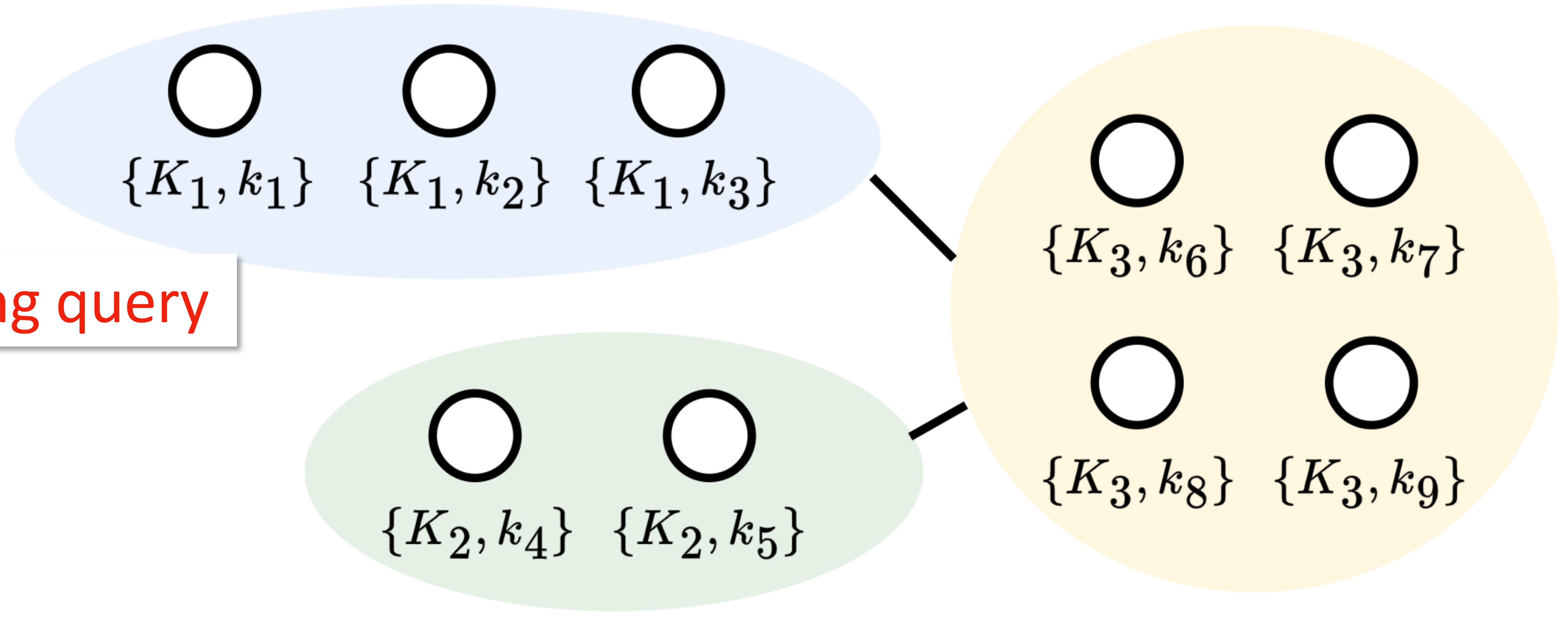

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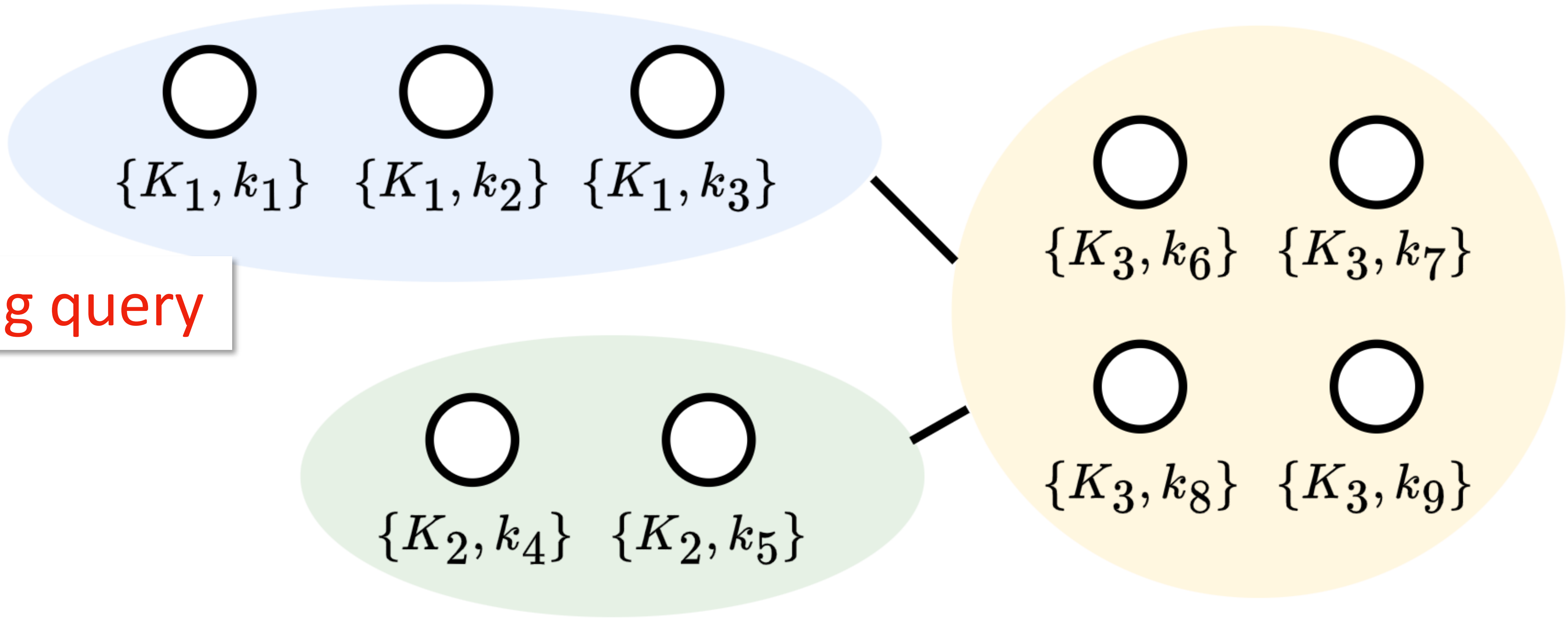

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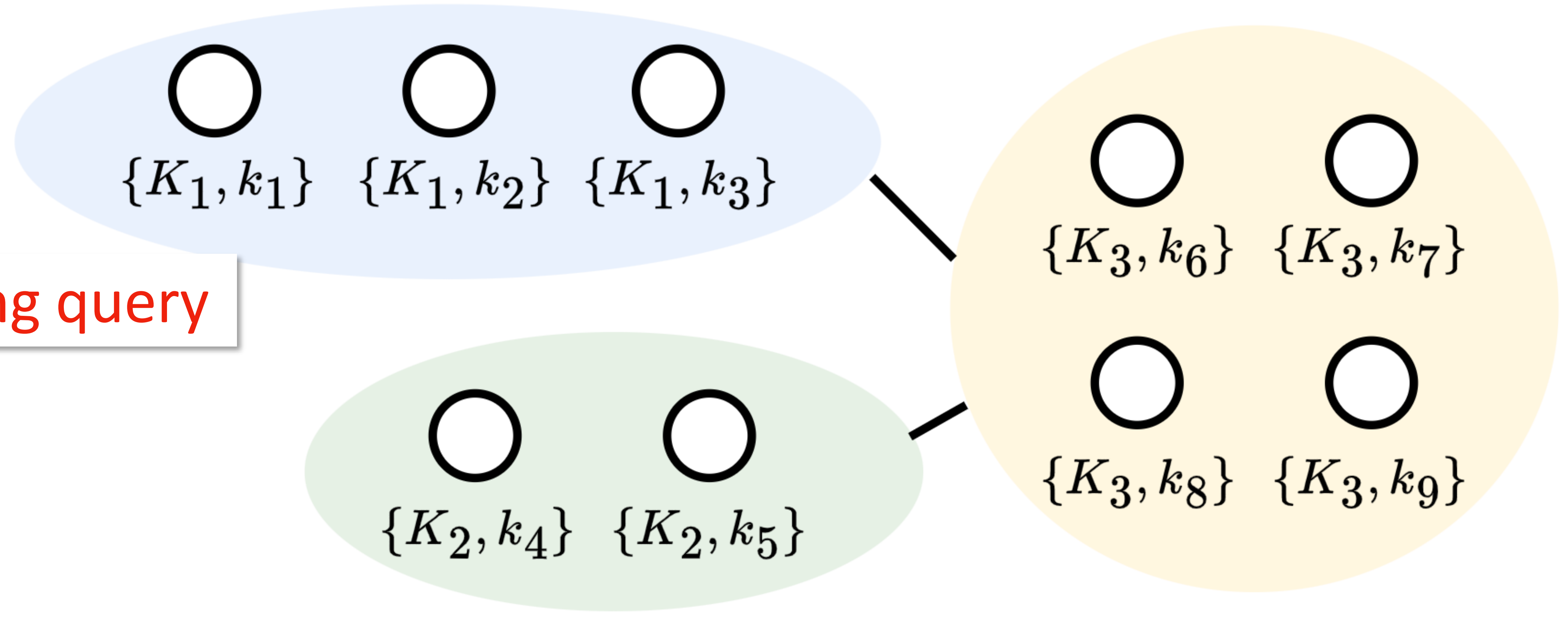

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$$\{Q_i, q_i\} \in \mathcal{X}_C \times \mathcal{X}_N$$

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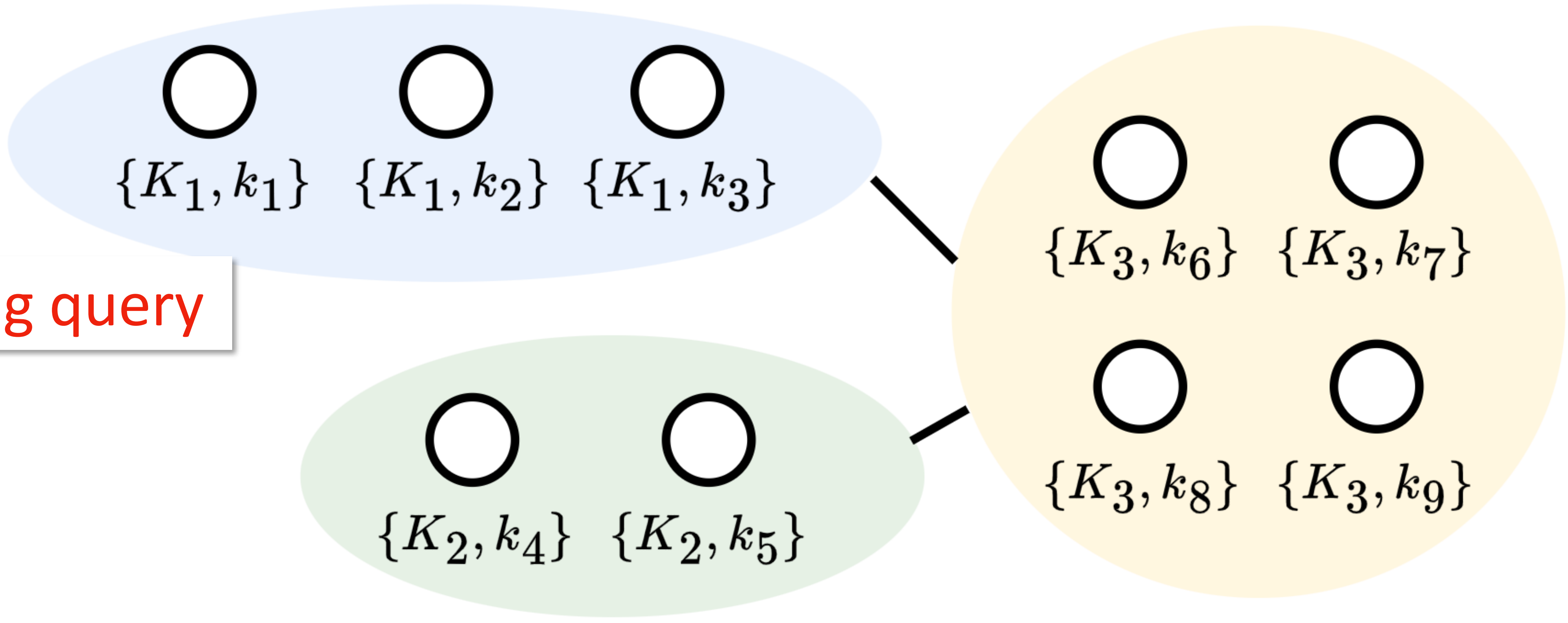

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We should construct a kernel on the tensor product space $\mathcal{X}_C \times \mathcal{X}_N$

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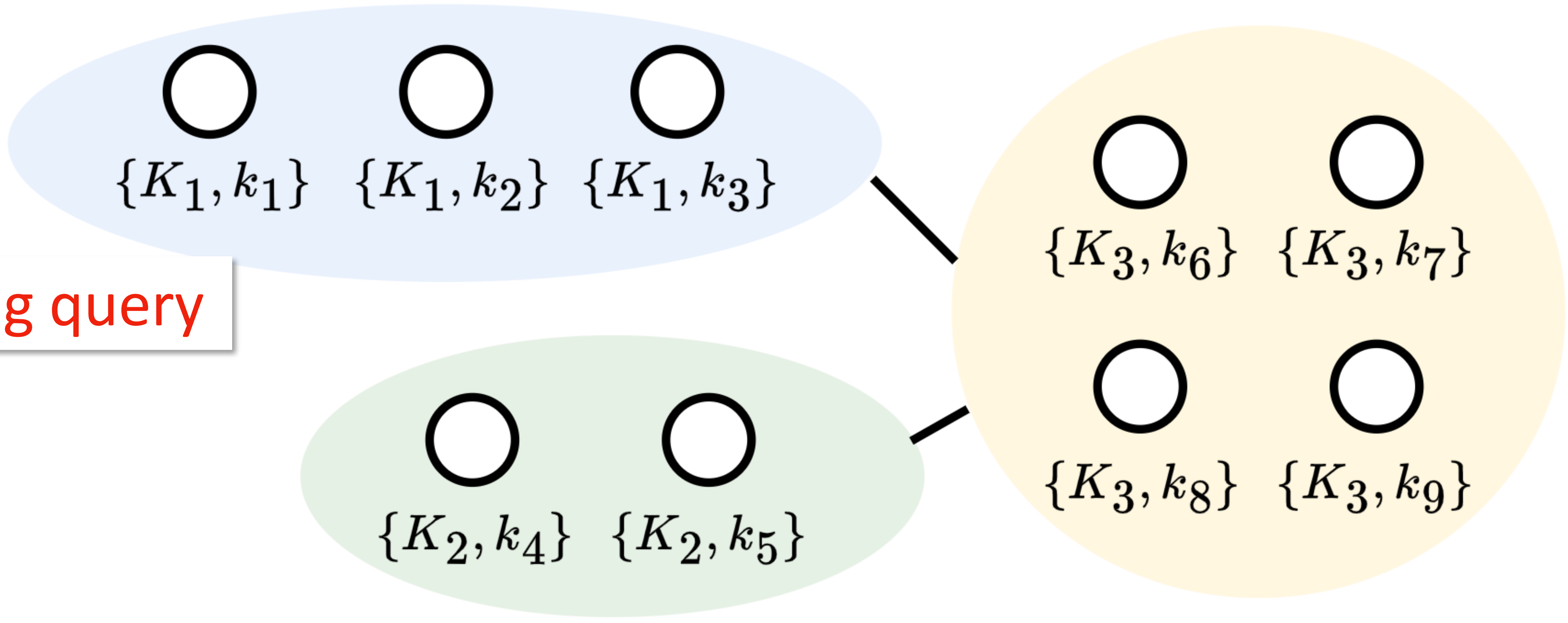

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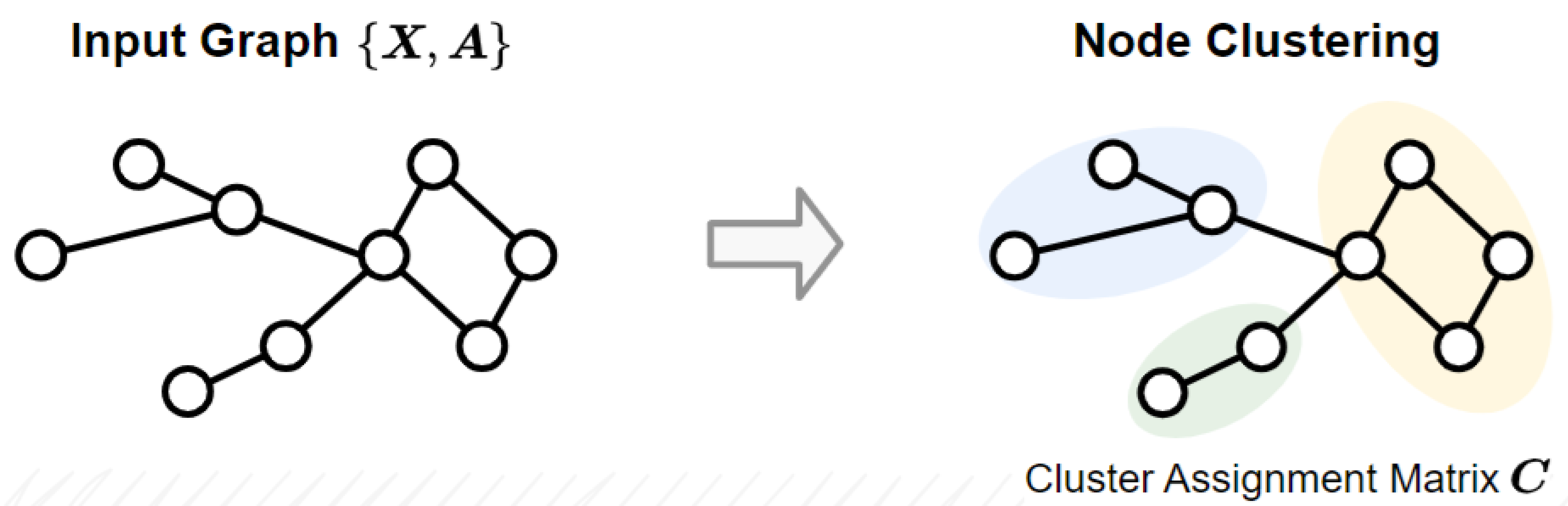
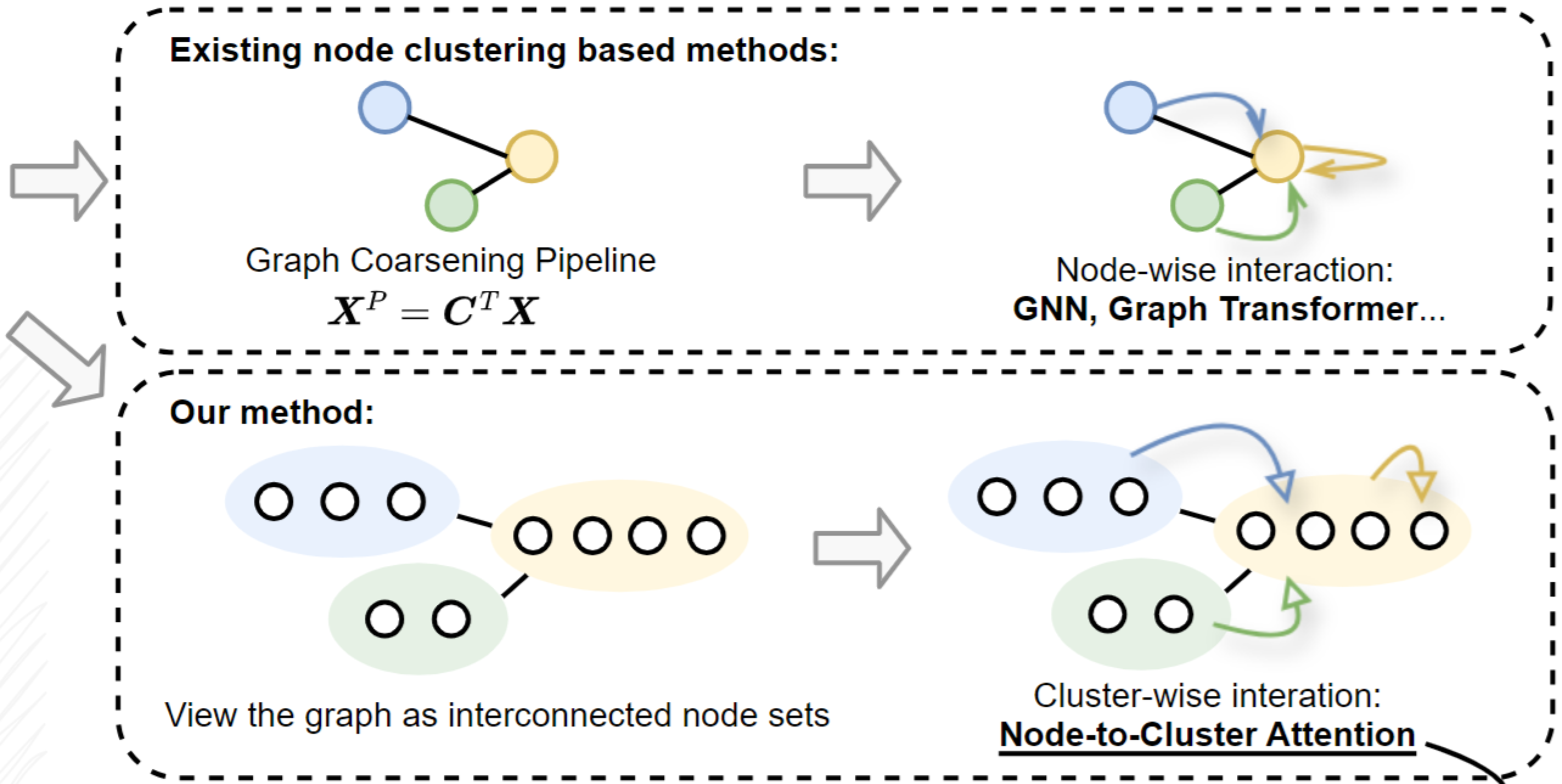
Refer to the paper for more details.

Our proposed Node-to-Cluster Attention





Graph Coarsening Pipeline:

1. Approximately homogenous cluster representations
2. Loss of fine-grained node-level information

Our Method:

1. Adaptive fusion of cluster-level and node-level information (subsection 3.3)
2. Maintain linear computational complexity (subsection 3.2)

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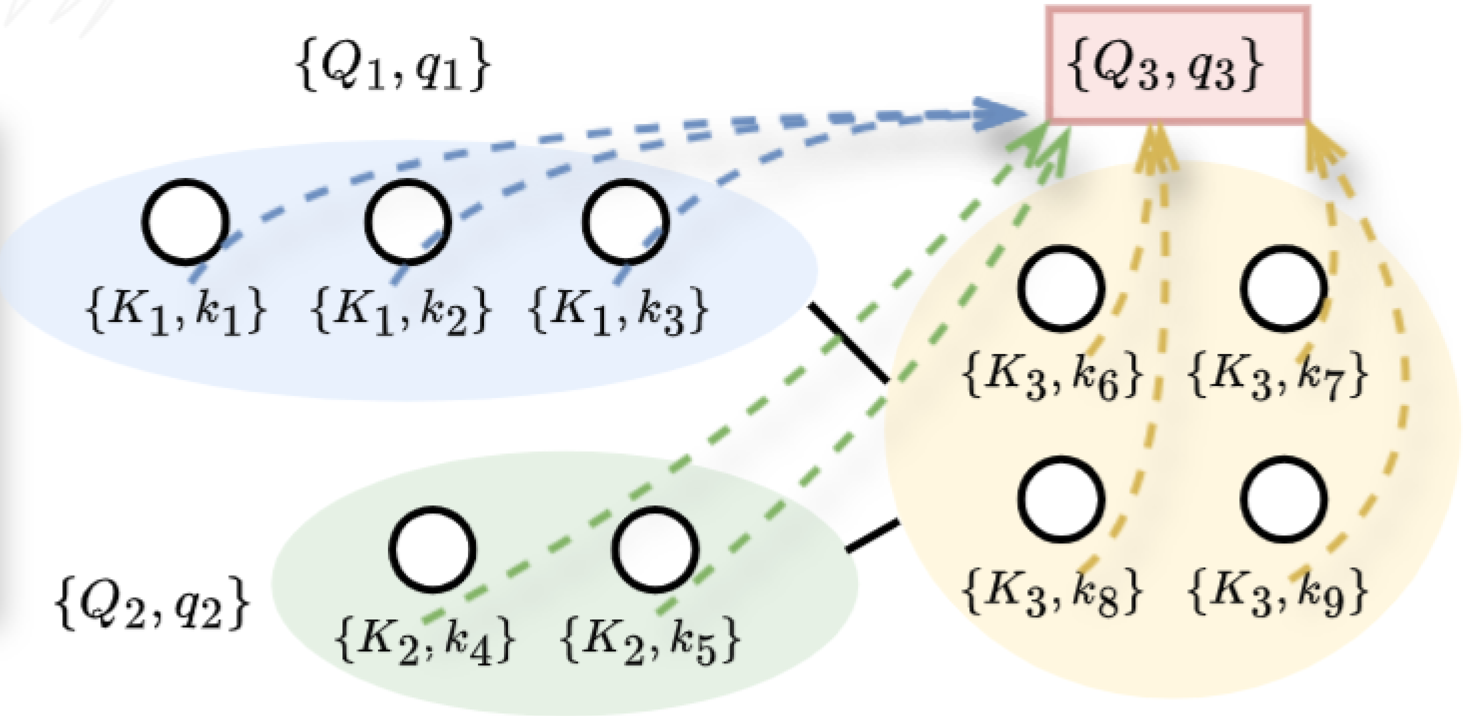

$$\text{N2C-Attn}(X)_i = \frac{\sum_j A^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_{\text{B}}(\{Q_i, q_i\}, \{K_j, k_t\}) v_t}{\sum_j A^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_{\text{B}}(\{Q_i, q_i\}, \{K_j, k_t\})}$$

where κ_{B} is a bi-level kernel on $\mathcal{X}_C \times \mathcal{X}_N$

Make it more Efficient

- Using the kernelized softmax trick

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- Using the kernelized softmax trick, but with a combined kernel!

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- Take Node-to-Cluster Attention with Tensor Product of Kernels as an example:

$$\text{N2C-Attn-T}(X)_i = \frac{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C(Q_i, K_j)\, \kappa_N(q_i, k_t) v_t}{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C(Q_i, K_j)\, \kappa_N(q_i, k_t)}$$

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- Take Node-to-Cluster Attention with Tensor Product of Kernels as an example:

$$\text{N2C-Attn-T}(X)_i = \frac{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \kappa_N\left(q_i, k_t\right) v_t}{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \kappa_N\left(q_i, k_t\right)}$$

$$= \frac{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \left(\psi(q_i)^T \psi(k_t)\right) v_t}{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \left(\psi(q_i)^T \psi(k_t)\right)}$$

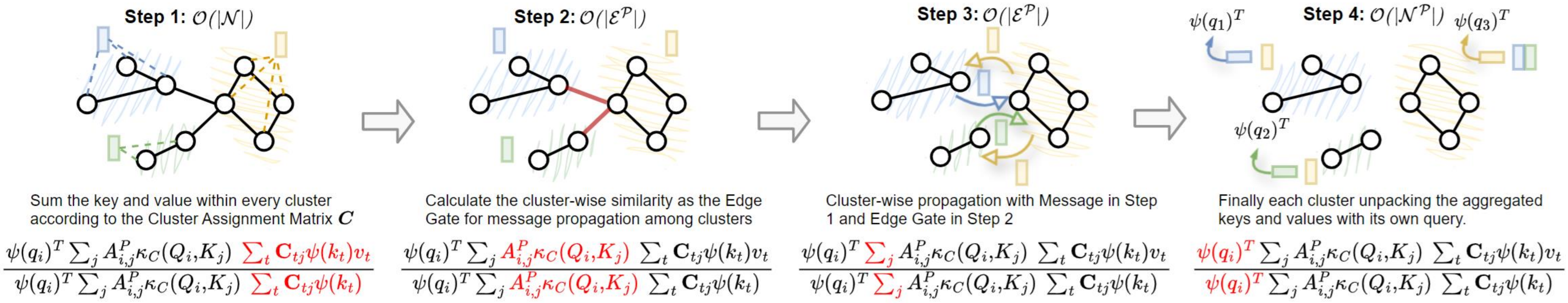
Make it more Efficient

- Using the kernelized softmax trick, but with a combined kernel!
- Take Node-to-Cluster Attention with Tensor Product of Kernels as an example:

$$
\begin{aligned}
\text{N2C-Attn-T}(X)_i &= \frac{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \kappa_N\left(q_i, k_t\right) v_t}{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \kappa_N\left(q_i, k_t\right)} \\
&= \frac{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \left(\psi(q_i)^T \psi(k_t)\right) v_t}{\sum_j \mathbf{A}^P_{i,j} \sum_t \mathbf{C}_{tj} \kappa_C\left(Q_i, K_j\right) \left(\psi(q_i)^T \psi(k_t)\right)} \\
&= \frac{\psi(q_i)^T \sum_j \mathbf{A}^P_{i,j} \kappa_C\left(Q_i, K_j\right) \sum_t \mathbf{C}_{tj} \psi(k_t) v_t}{\psi(q_i)^T \sum_j \mathbf{A}^P_{i,j} \kappa_C\left(Q_i, K_j\right) \sum_t \mathbf{C}_{tj} \psi(k_t)}
\end{aligned}
$$

Make it more Efficient

- Using the kernelized softmax trick, but with a combined kernel!
- Take Node-to-Cluster Attention with Tensor Product of Kernels as an example:



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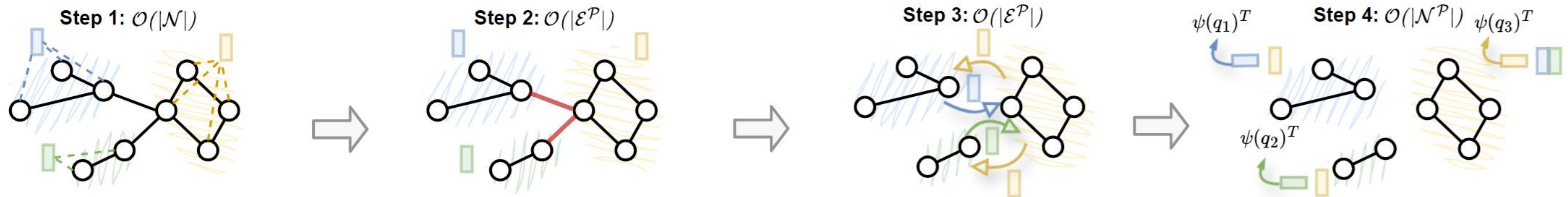

Sum the key and value within every cluster according to the Cluster Assignment Matrix $\boldsymbol{C}$

$$\frac{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)v_t}{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)}$$

Calculate the cluster-wise similarity as the Edge Gate for message propagation among clusters

$$\frac{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)v_t}{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)}$$

Cluster-wise propagation with Message in Step 1 and Edge Gate in Step 2

$$\frac{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)v_t}{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)}$$

Finally each cluster unpacking the aggregated keys and values with its own query.

$$\frac{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)v_t}{\psi(q_i)^T \sum_j A^P_{i,j}\kappa_C(Q_i,K_j) \ \sum_t \mathbf{C}_{tj}\psi(k_t)}$$

This process can be implemented as cluster-wise message propagation with PyG/DGL…

Refer to the paper for more details.

Some Experimental Results

- Visualization of weight of the cluster-level kernel during the training process

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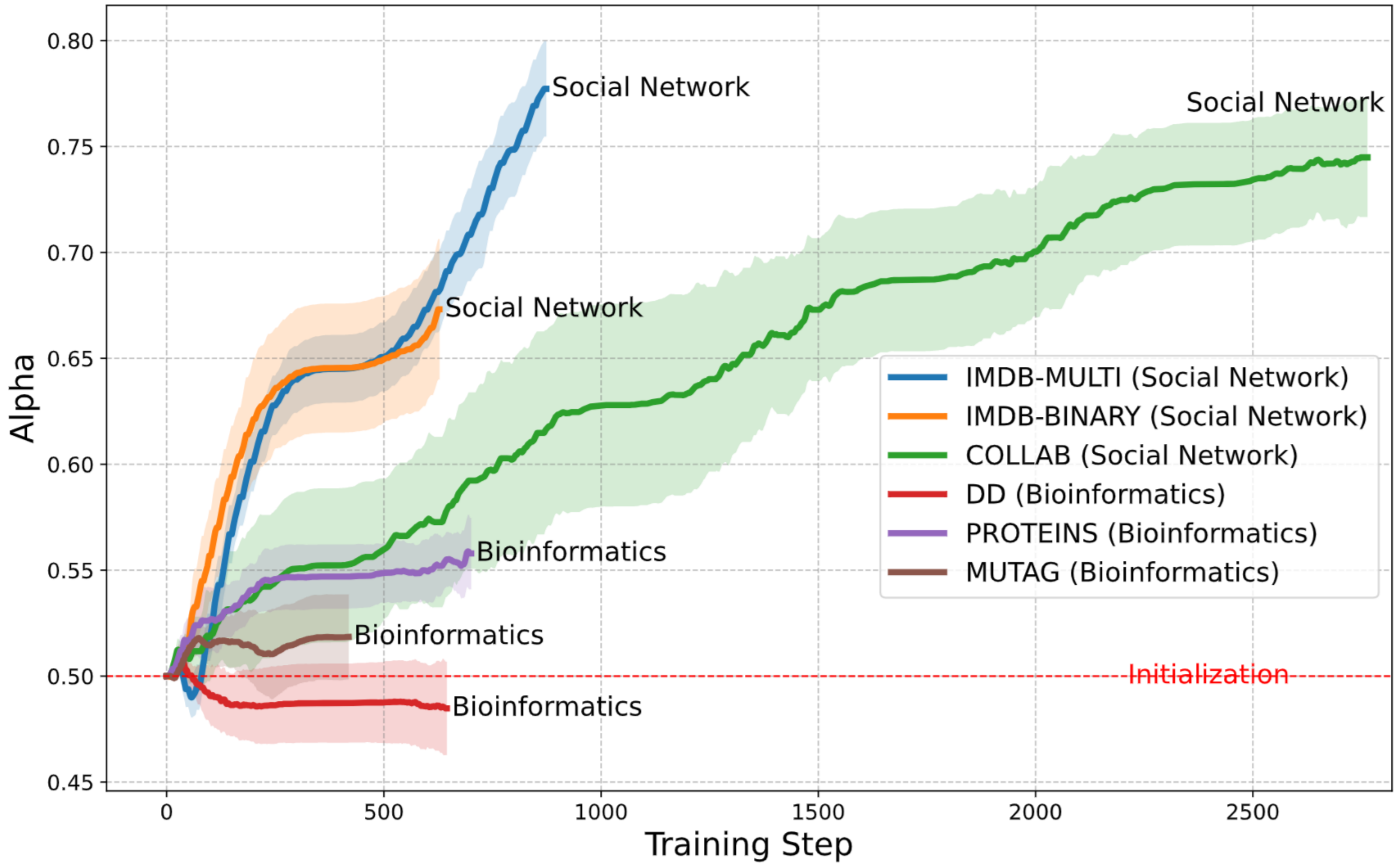
- Visualization of weight of the cluster-level kernel during the training process
  - For social network datasets, N2C-Attn prefers cluster-level information
  - For biology datasets, N2C-Attn balances its attention more equally between both granularities



Some Experimental Results

- Comparison of attention strategies with different granularities

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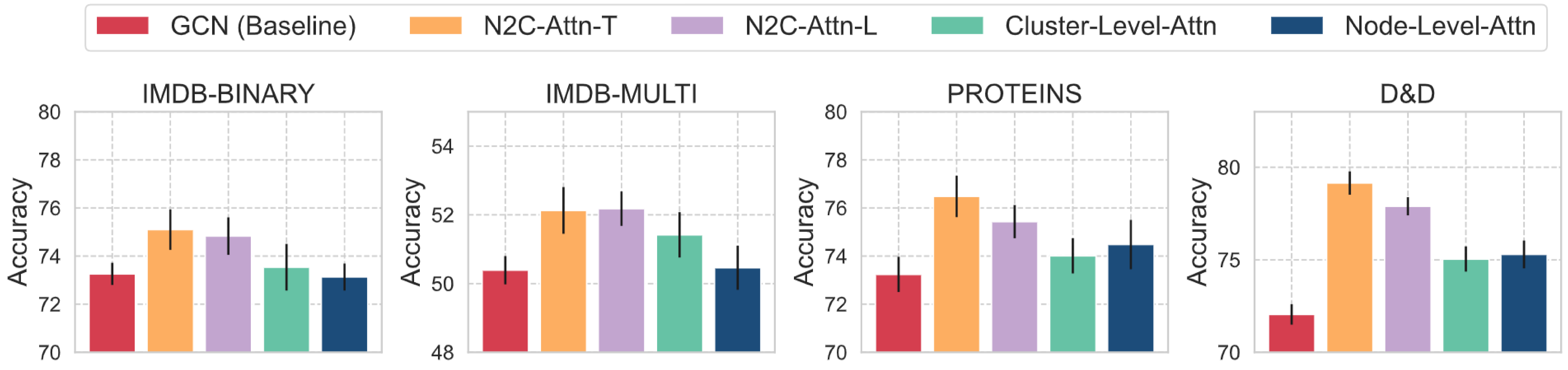
- Comparison of attention strategies with different granularities
  - We find that the variants that combine attention from both levels significantly surpass those that do not.



Thanks