

REGE: A Method for Incorporating Uncertainty in Graph Embeddings



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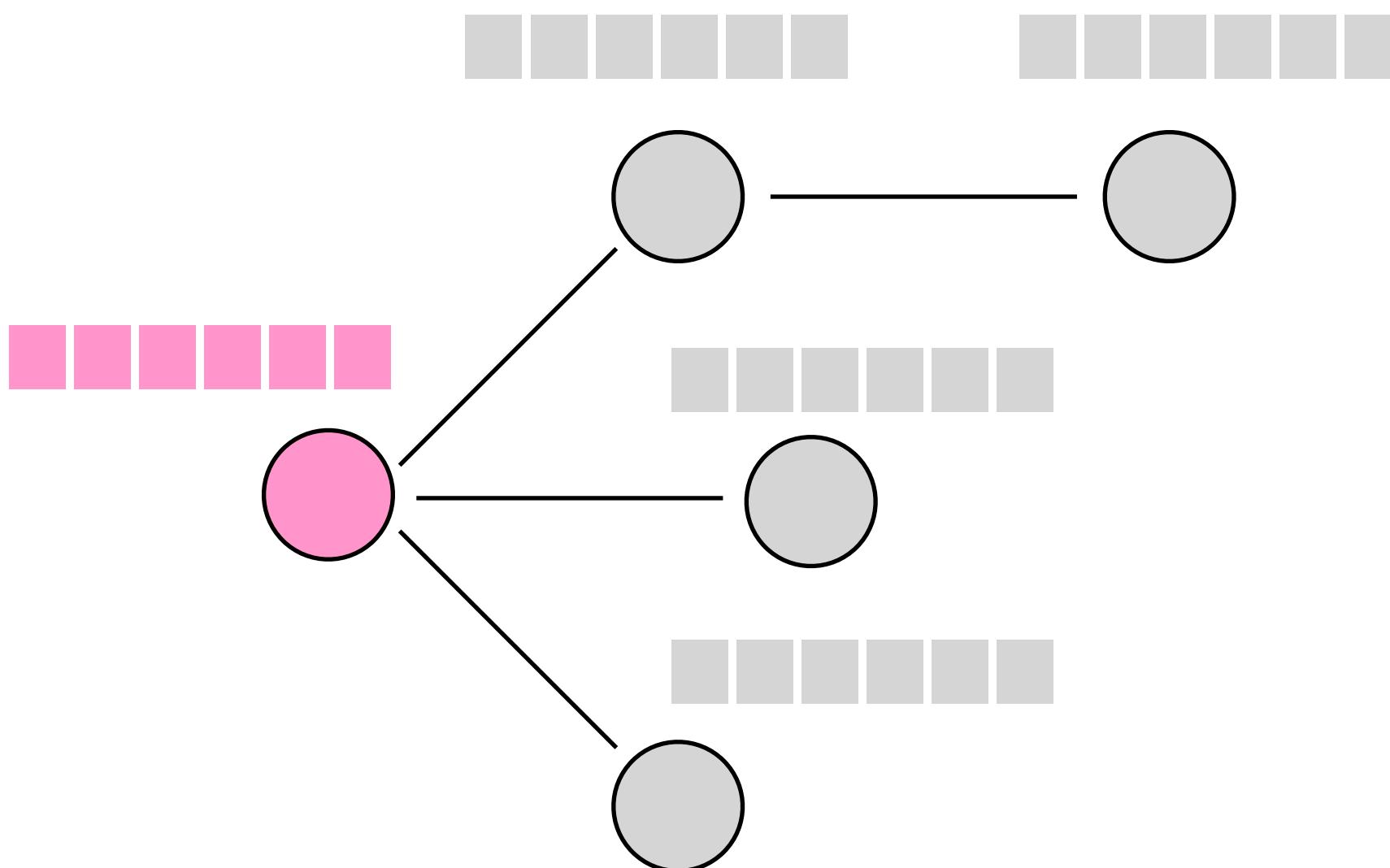
SDM 2025

Preliminaries

- Graph embedding
 - Let $G = (V, E, X)$ be a graph with $|V| = n$ nodes and $|E| = m$ edges.
 - $X \in \mathbb{R}^{n \times r}$ is a node feature matrix with r features per node.
 - $f(G(V, E, X)) = Z \in \mathbb{R}^{n \times d}$ is a graph embedding function. It maps each node onto a d -dimensional space.

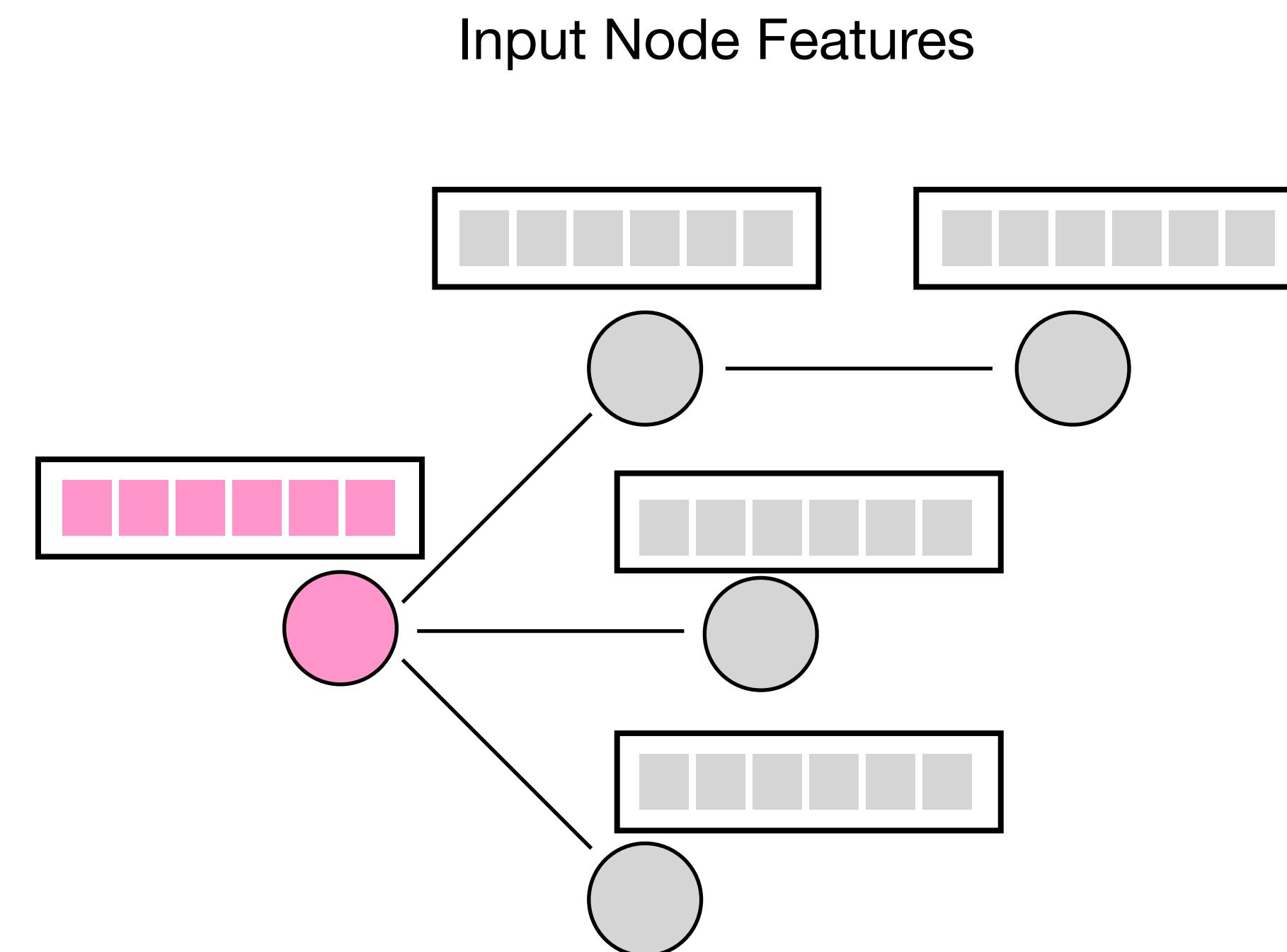
Preliminaries

- Graph embedding - message passing graph neural networks



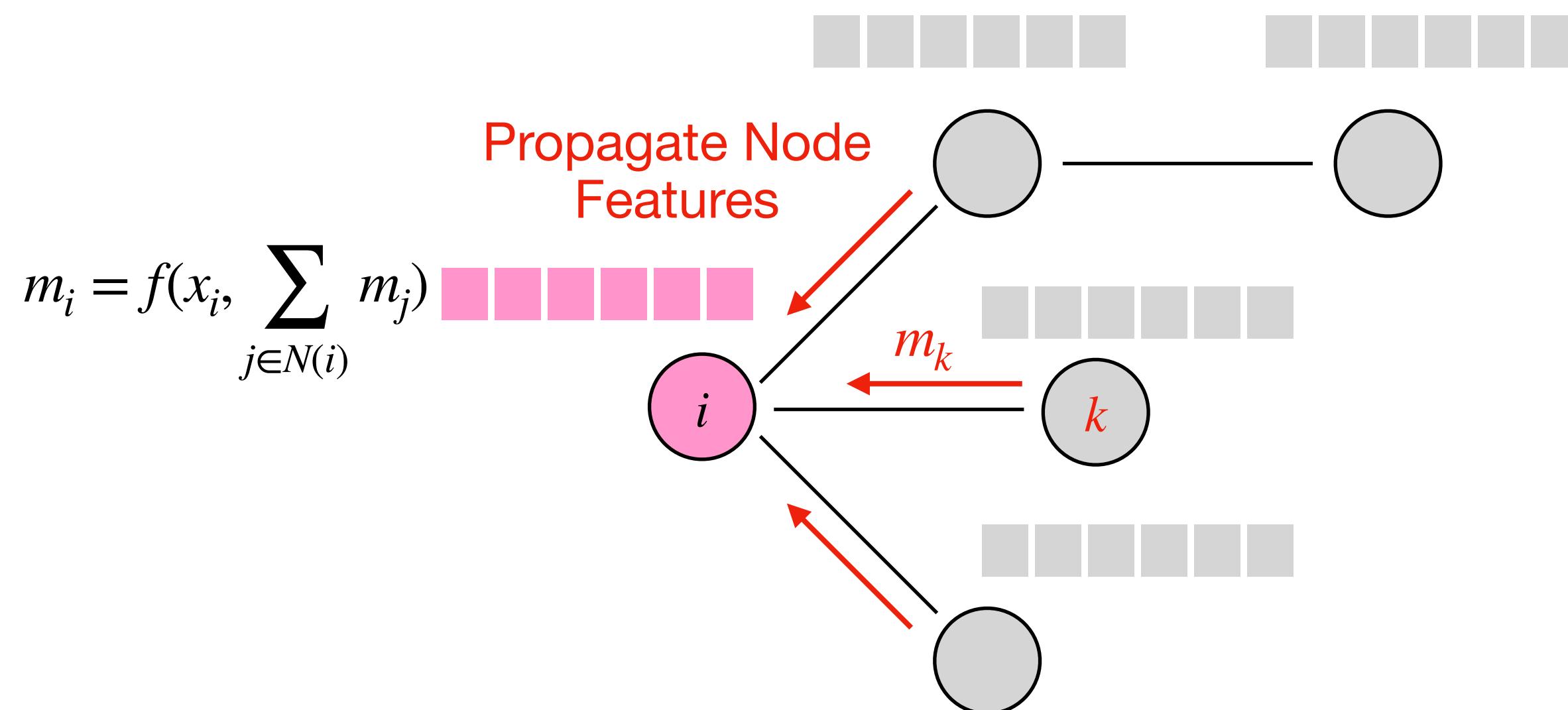
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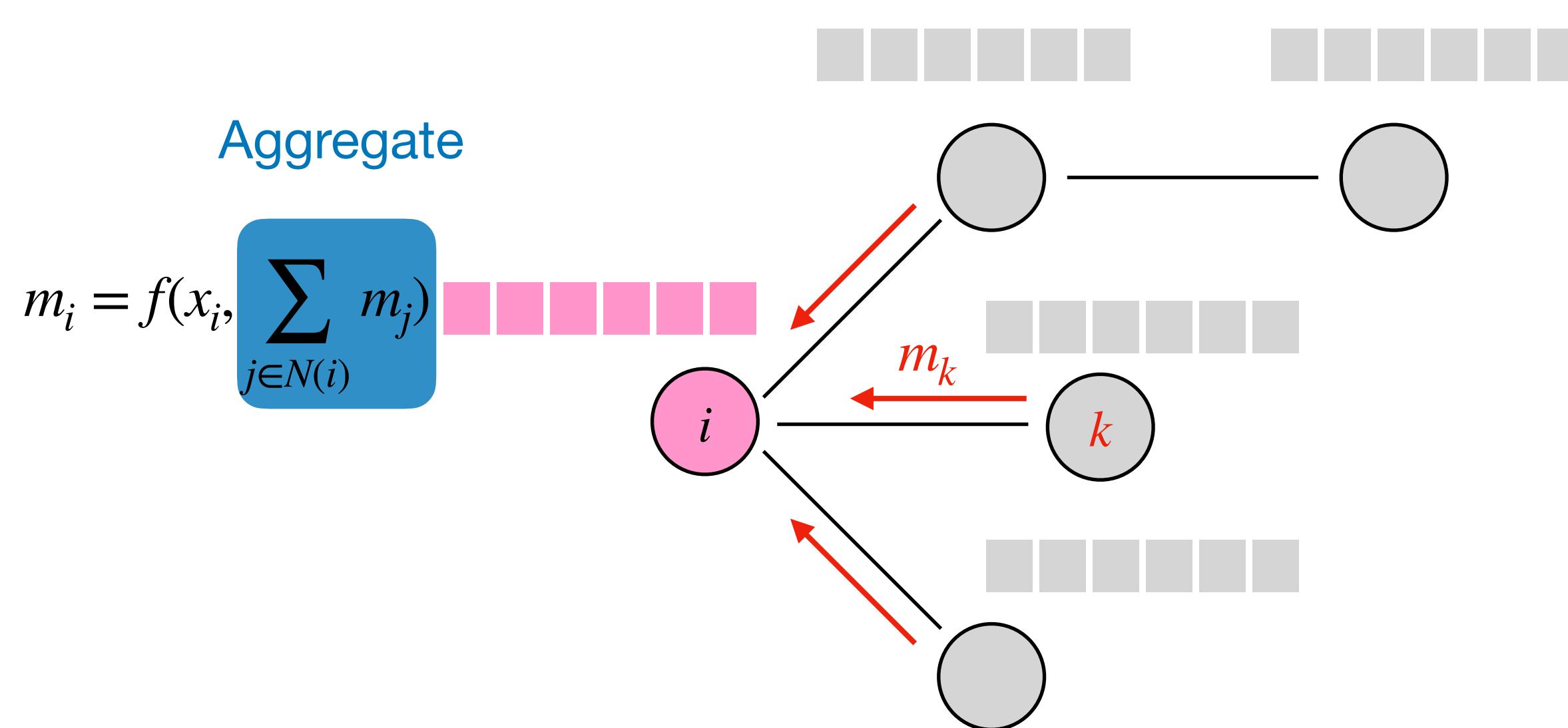
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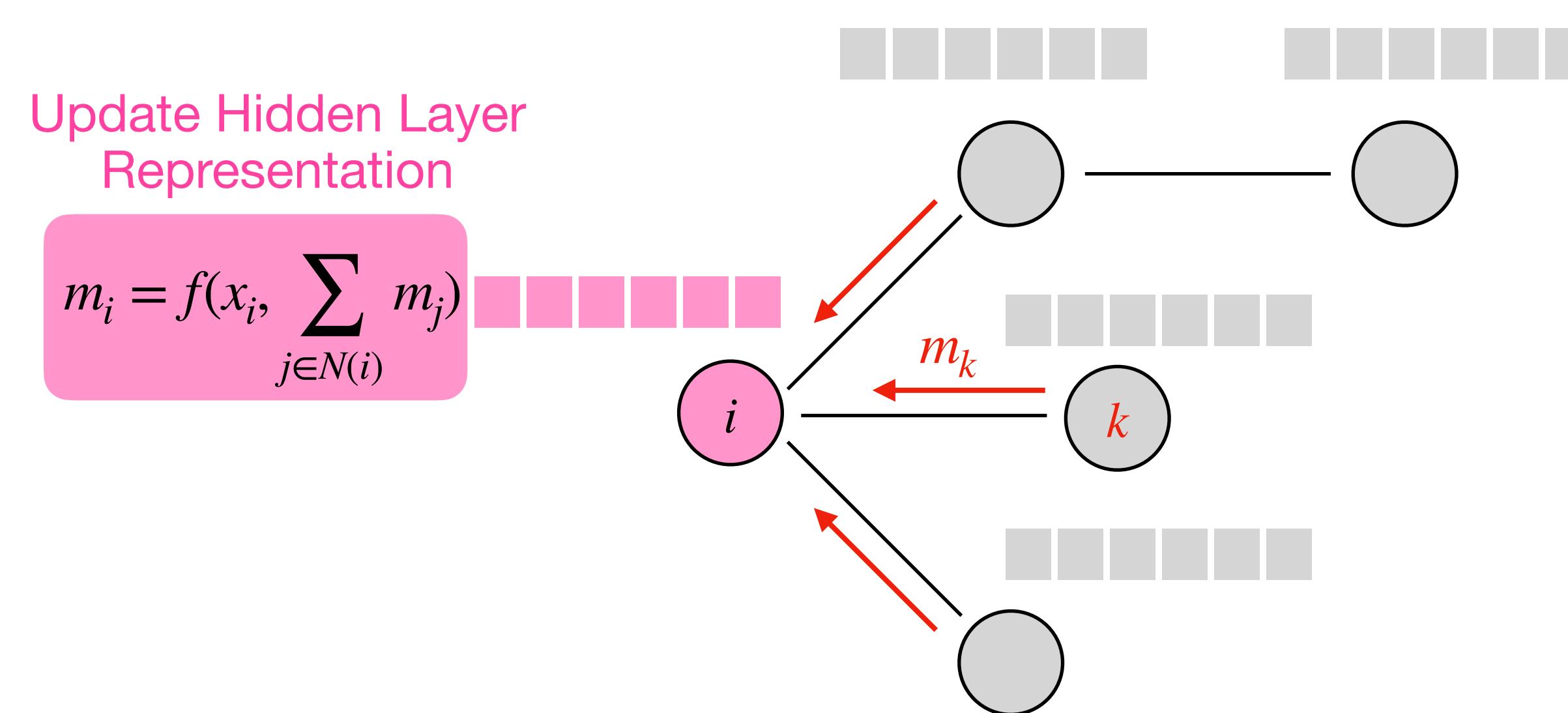
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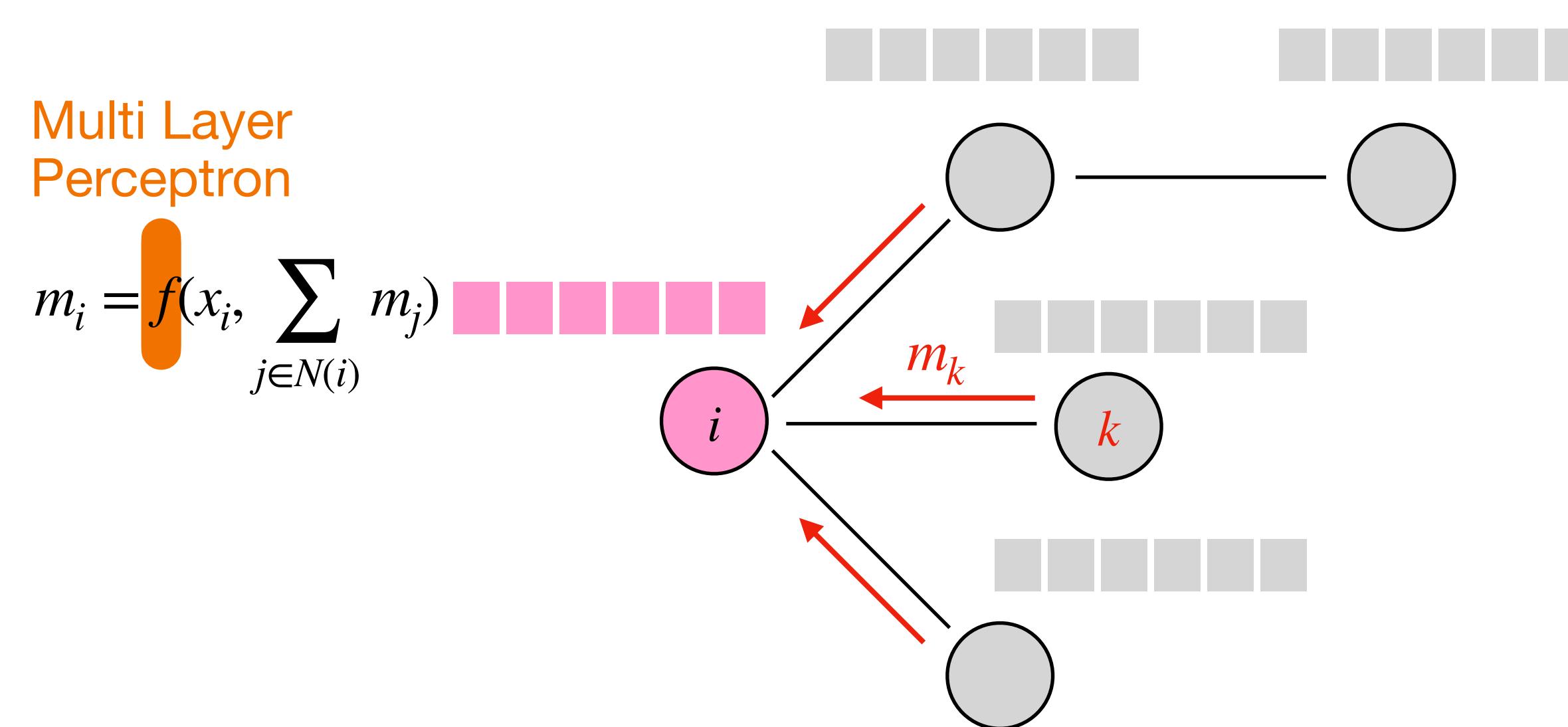
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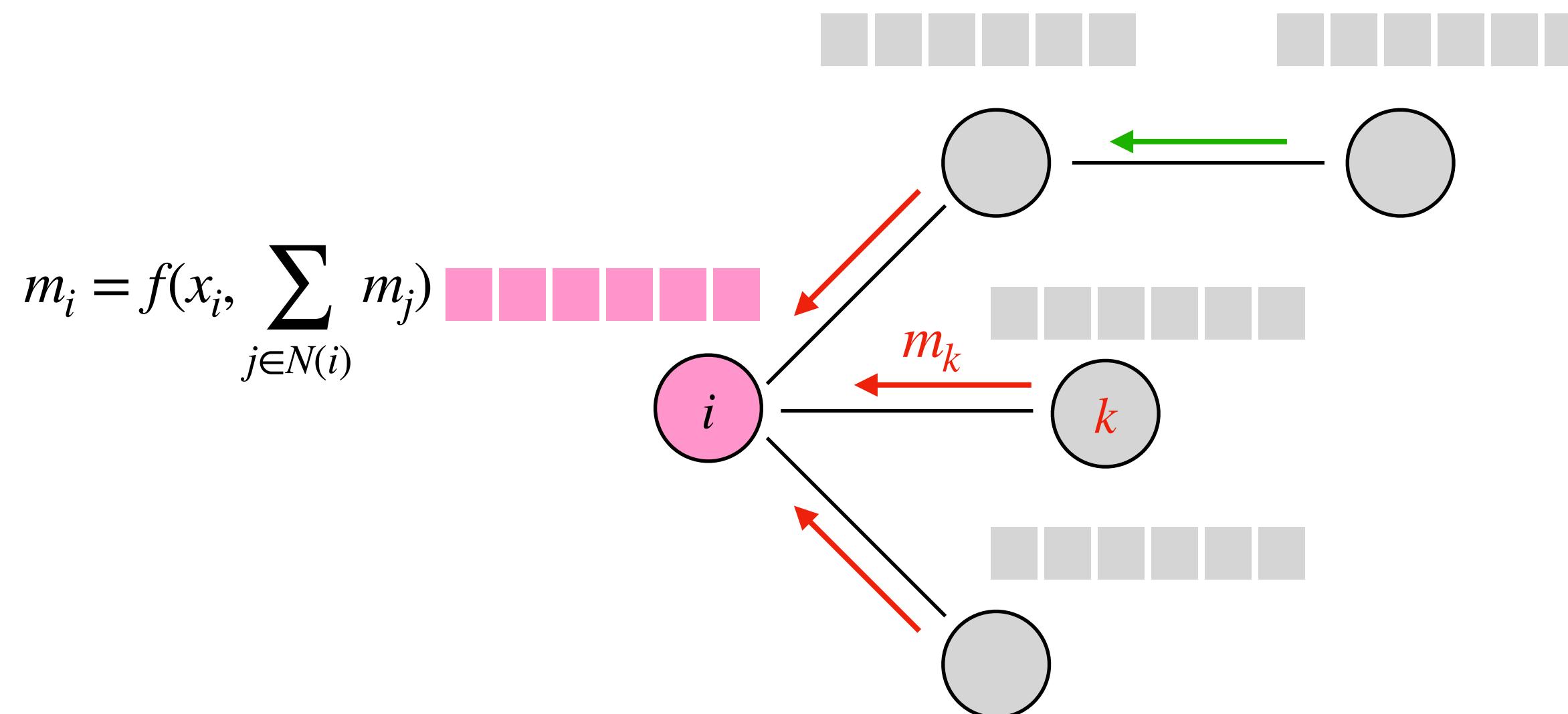
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Multiple message passing layers aggregates information from nodes further away



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- Uncertainty
 - Data: Uncertainty due to noisy or incomplete data
 - Model: Uncertainty due to parameters, optimization strategy, lack of training knowledge, etc.

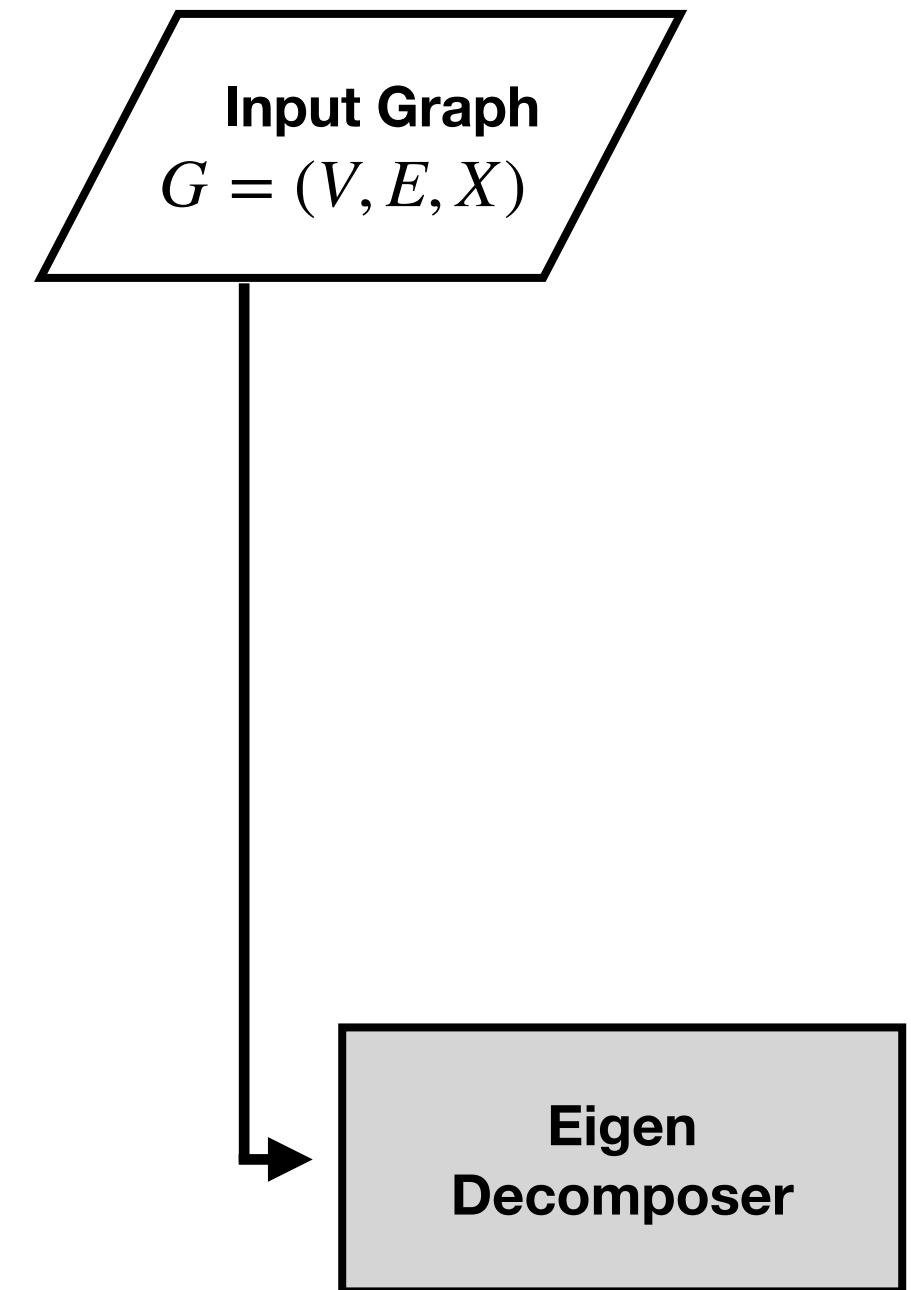
Motivation

- Why should we expect a node to embed in an exact spot in a d -dimensional space?
- Can we create a notion of a “radius” around each node where the node may embed?
- Could this “radius” help make node embeddings more robust to adversarial attacks?

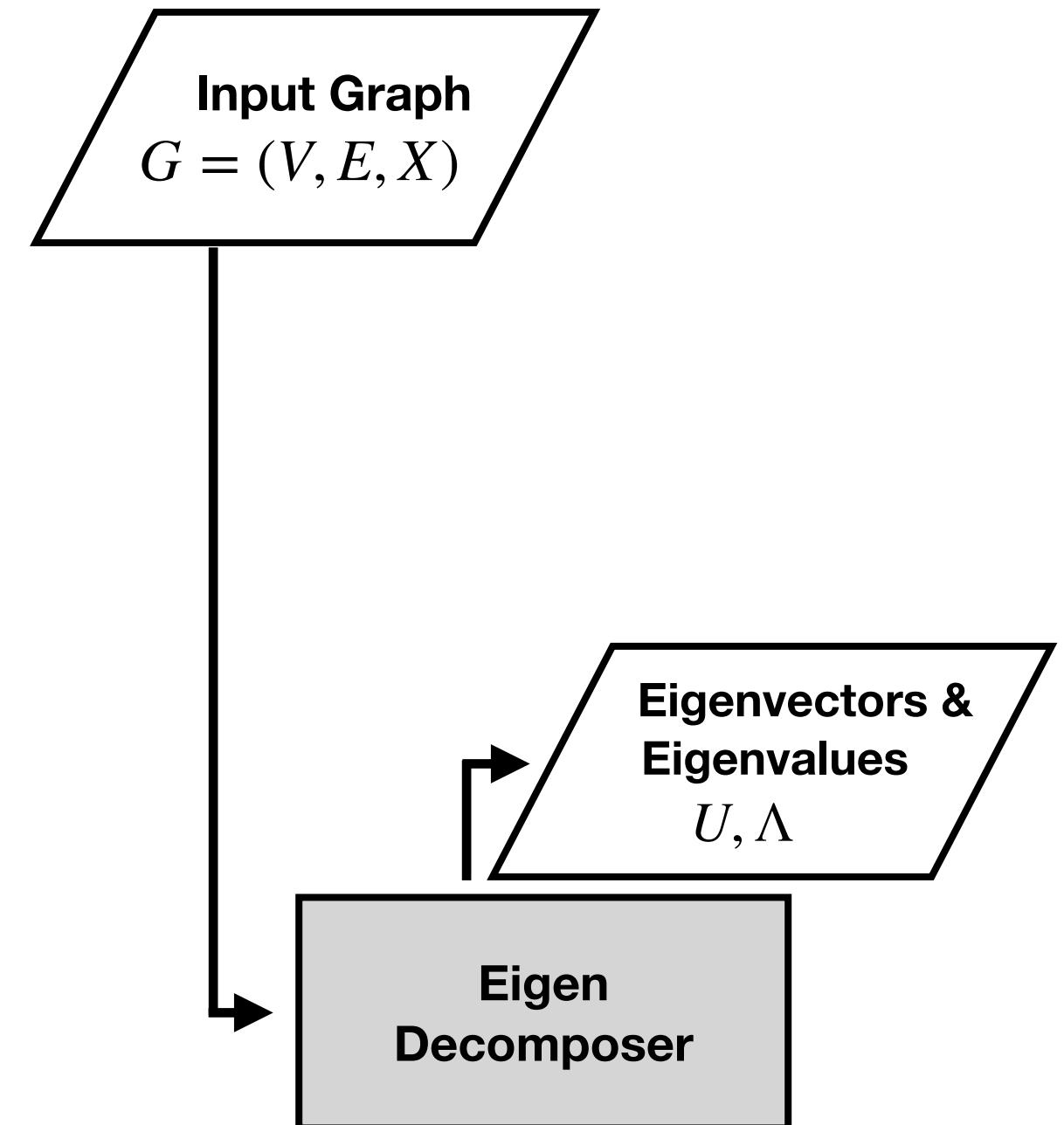
REGE: Radius Enhanced Graph Embeddings

- What does REGE do?
- How does it measure uncertainty in data?
- How does it measure uncertainty in the model?
- How does it incorporate uncertainty?
- How effective is it?

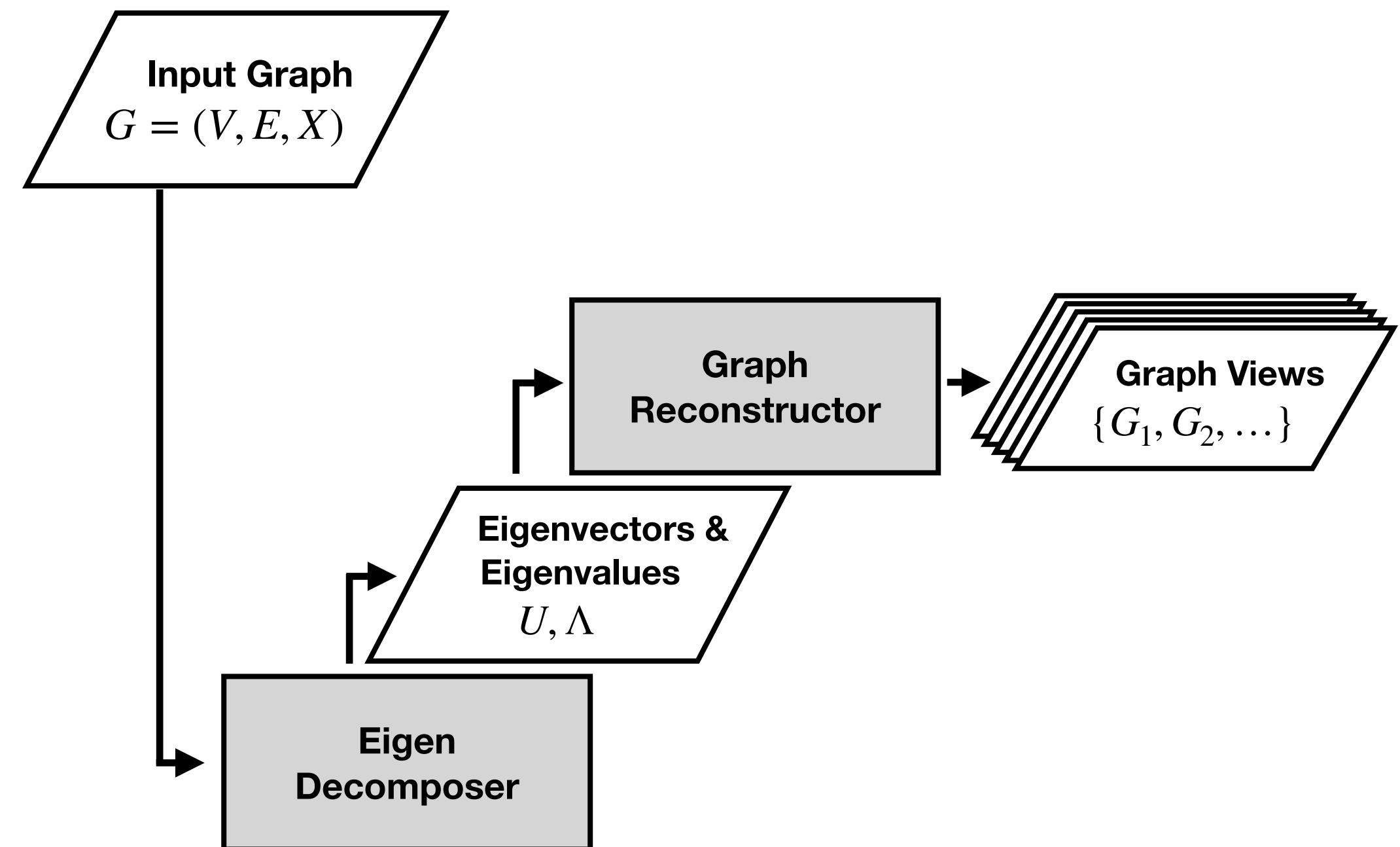
How does REGE measure uncertainty in data?



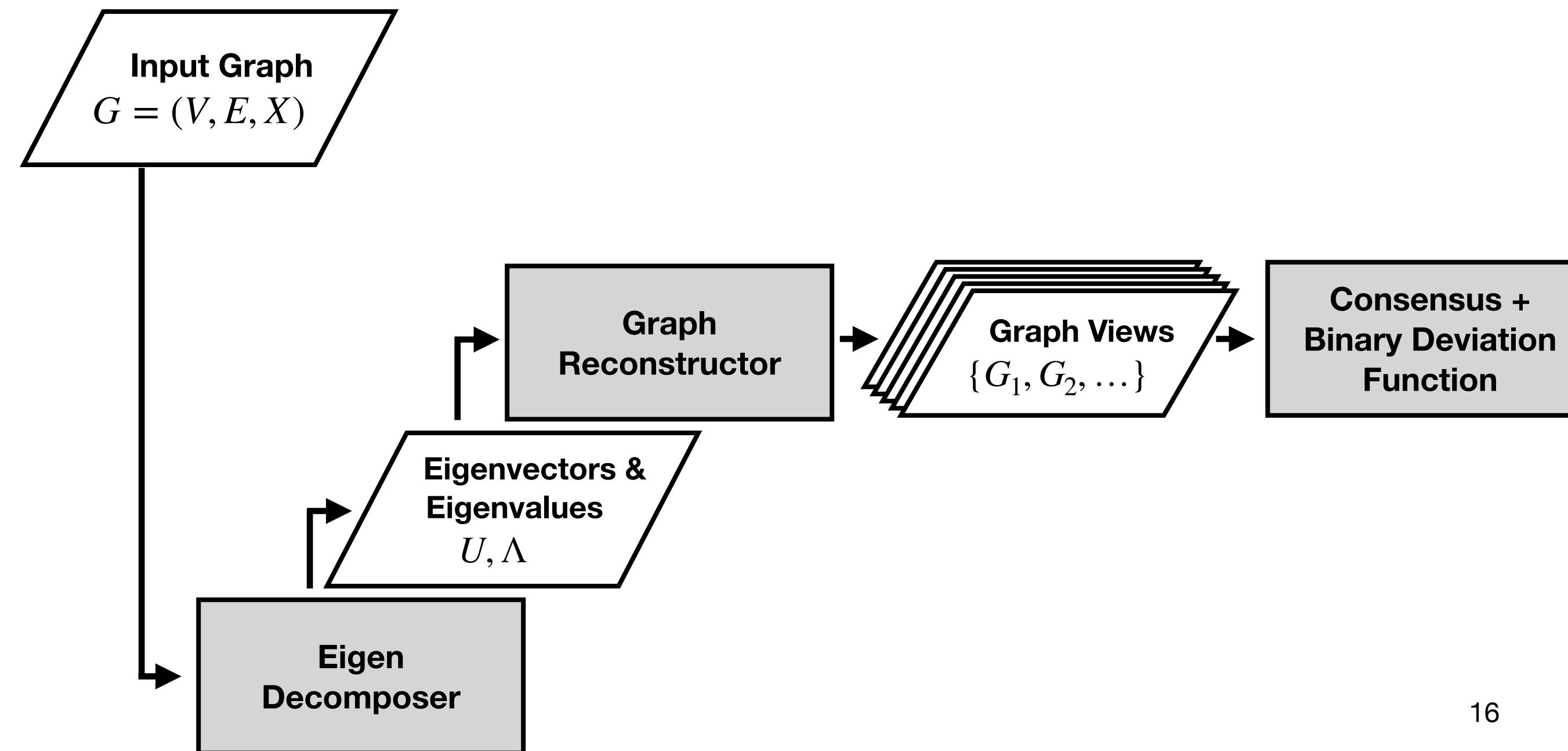
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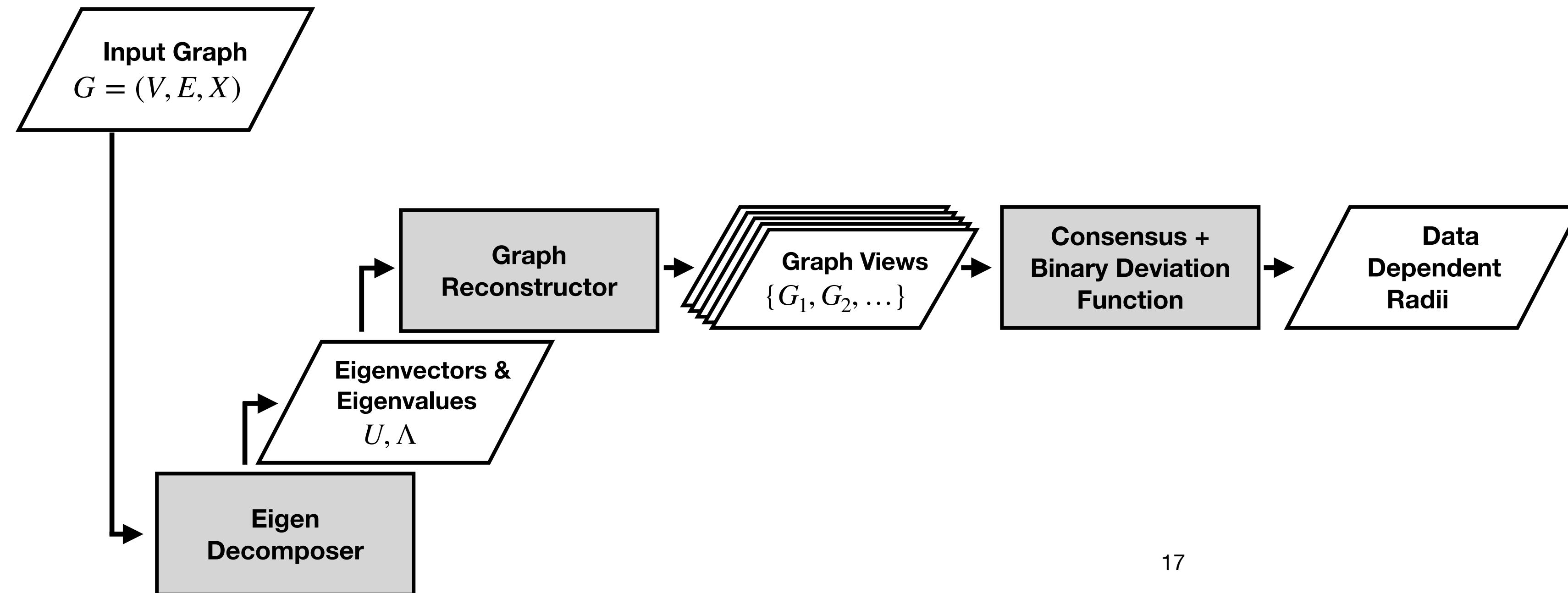
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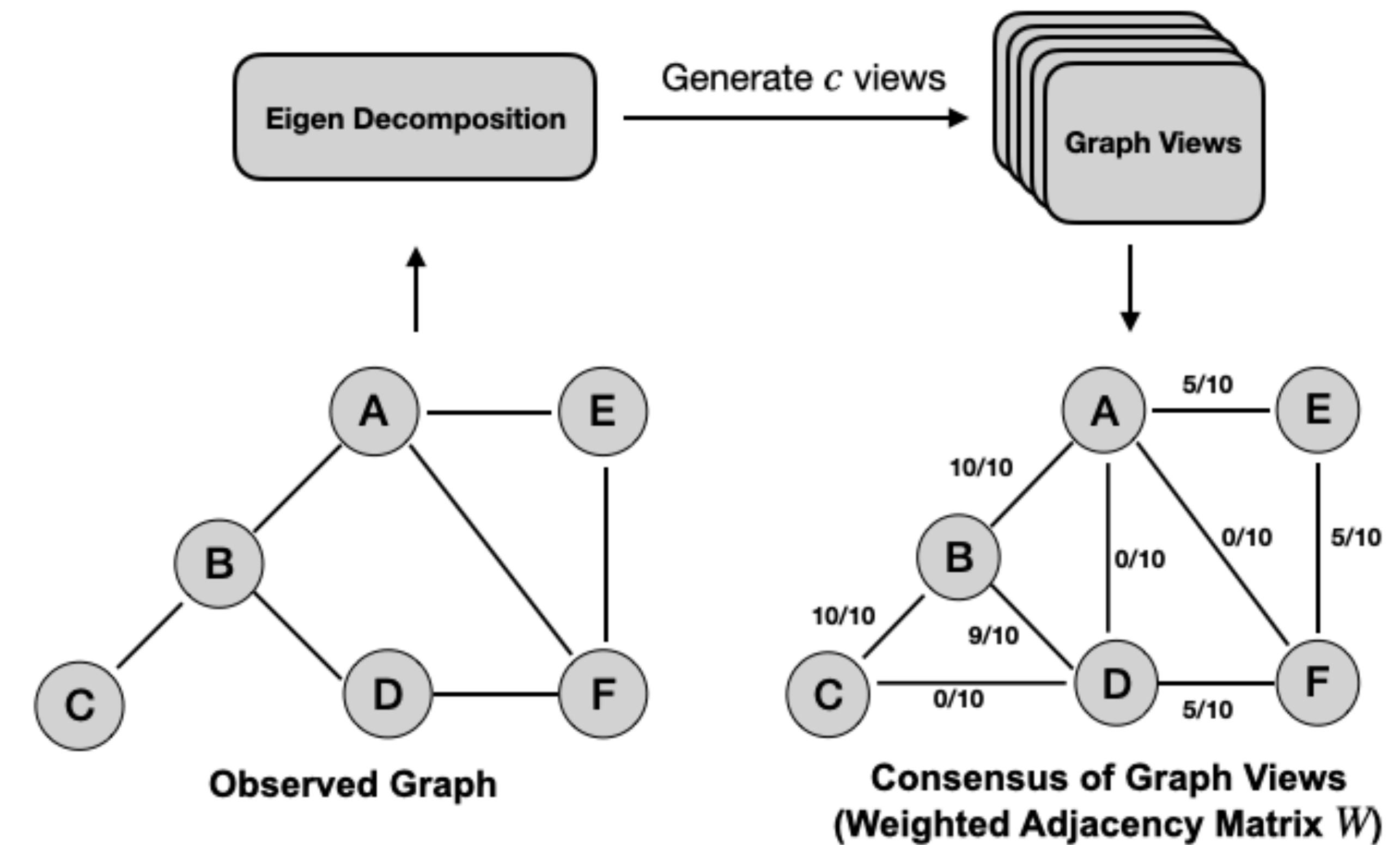


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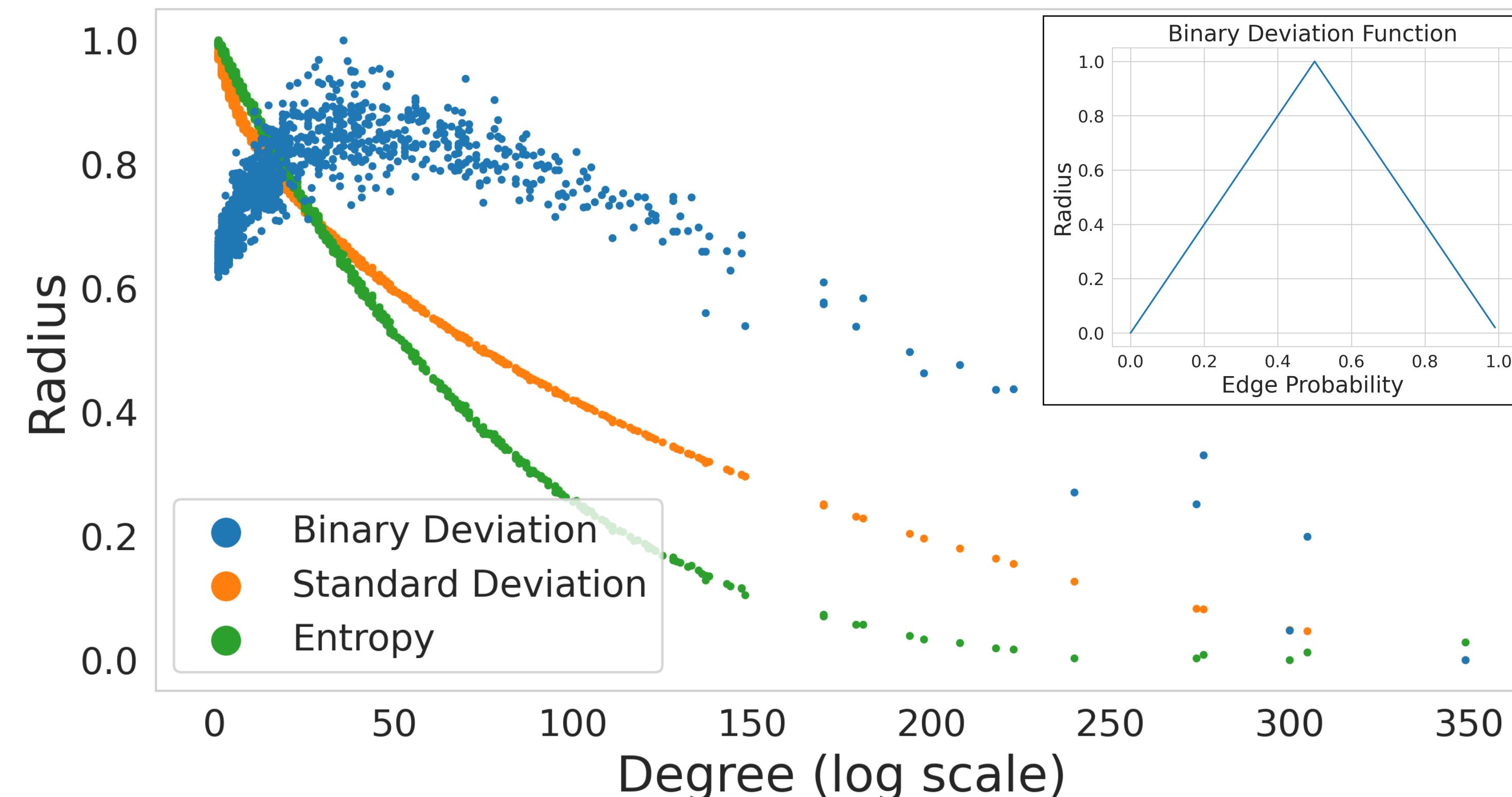
Data-dependent Radii (1/2)

- Given a graph G , compute its eigen-decomposition
- Reconstruct views of the graph (G_1, G_2, G_3, \dots)
- Compute weighted adjacency matrix W , by averaging the adjacency matrices of each reconstructed graph

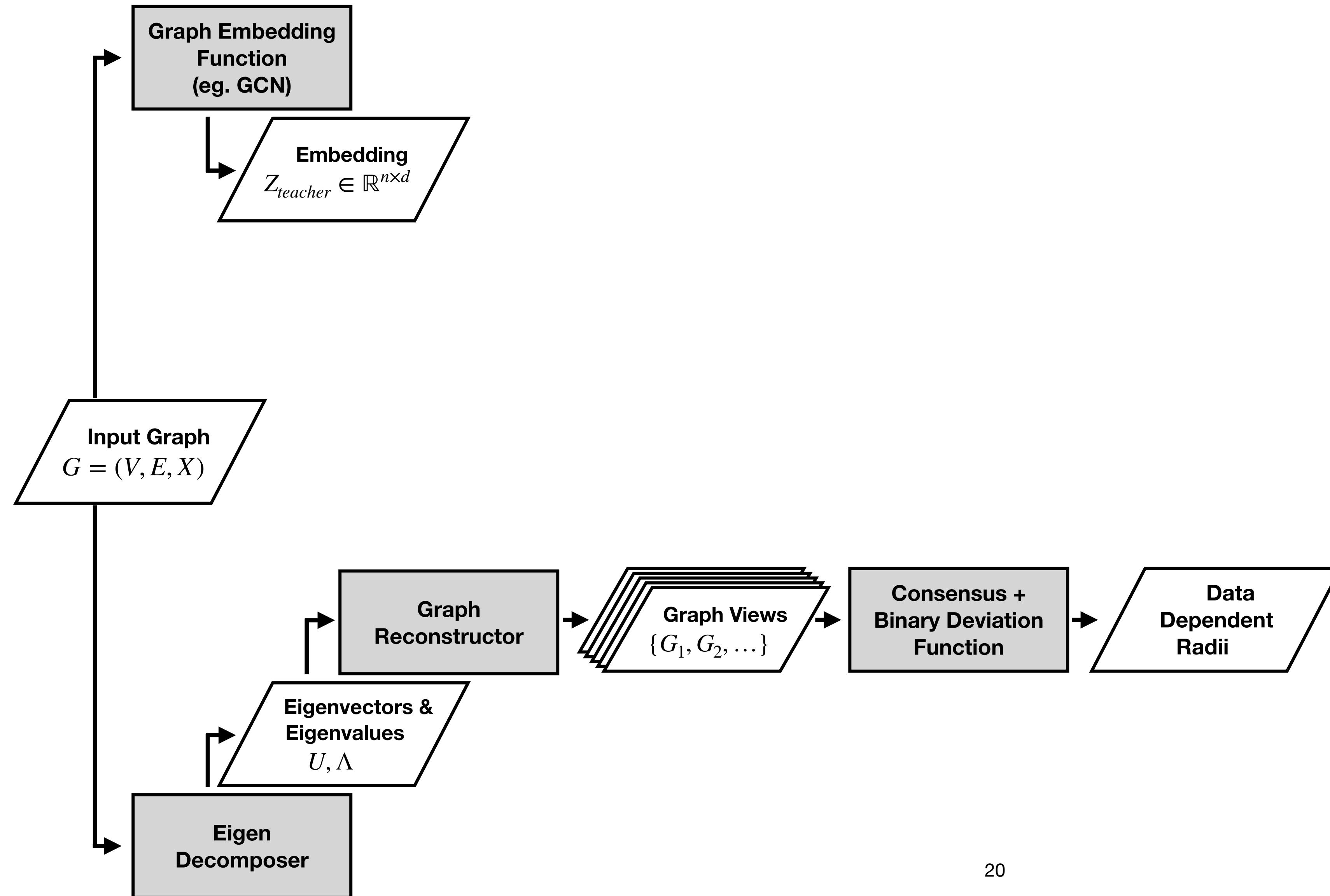


Data-dependent Radii (2/2)

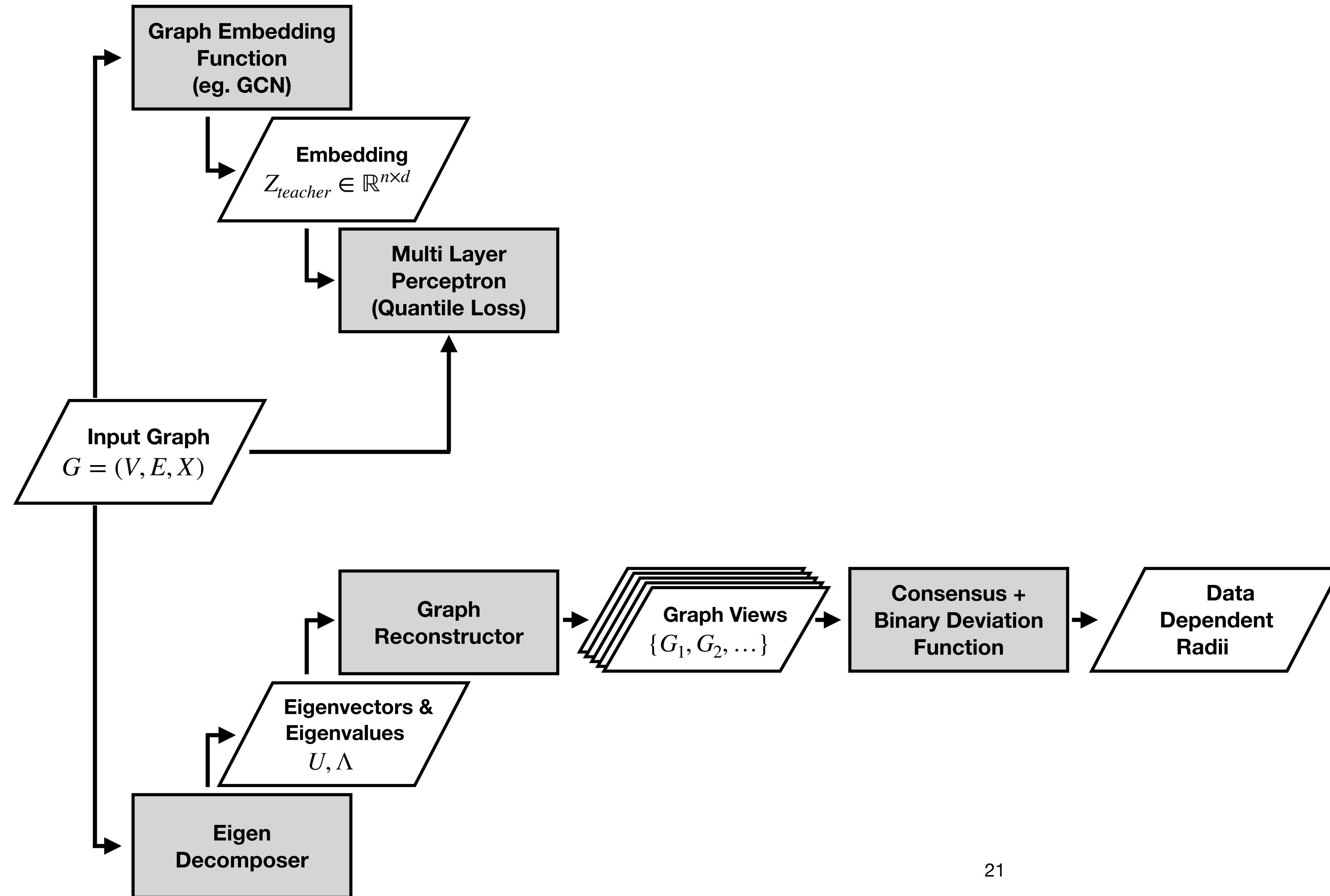
Given W , compute uncertainty for each edge e between nodes i, j using the binary deviation function: $u_e = 1 - |W_{ij} - (1 - W_{ij})|$



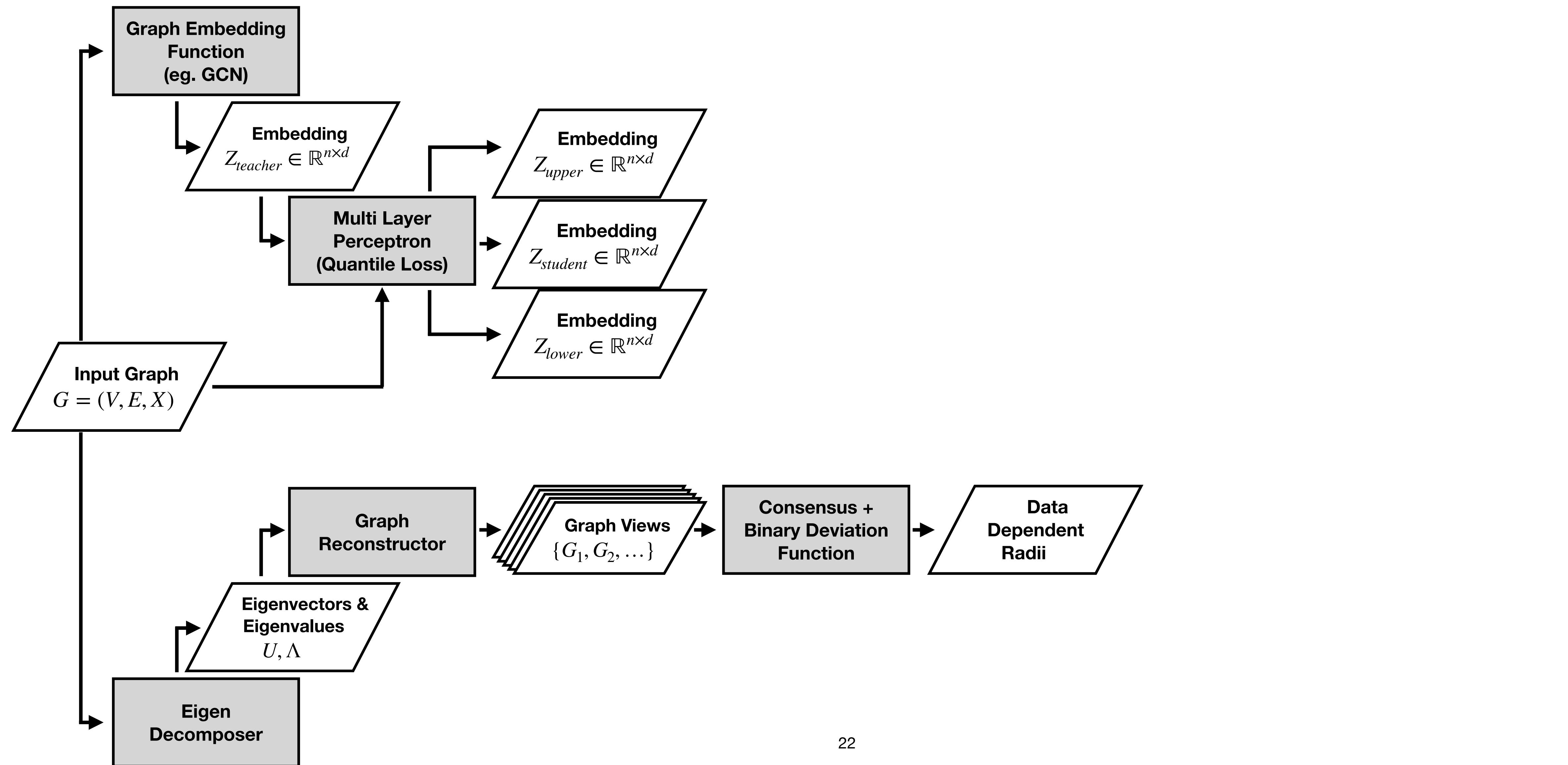
How does REGE measure uncertainty in the model?



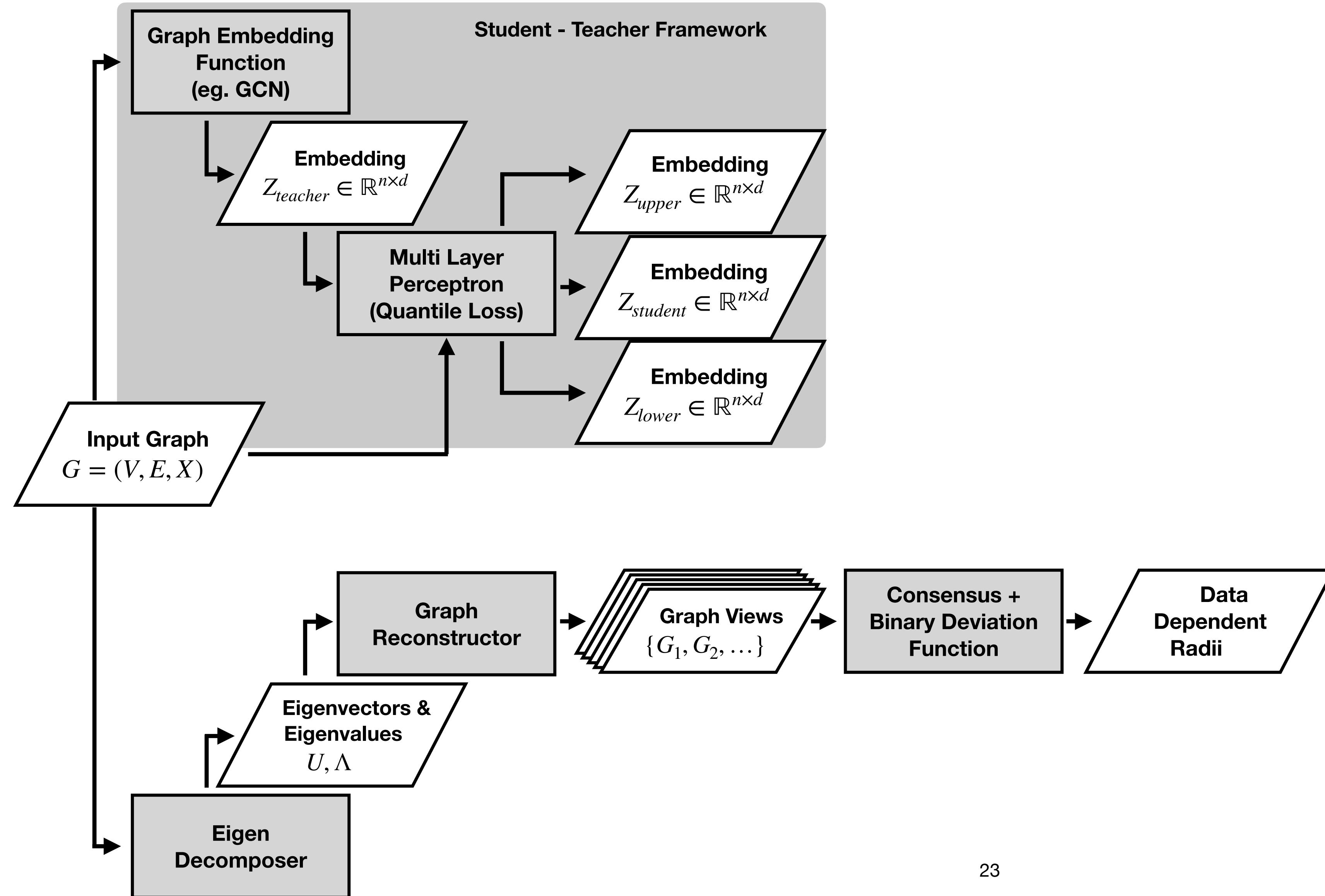
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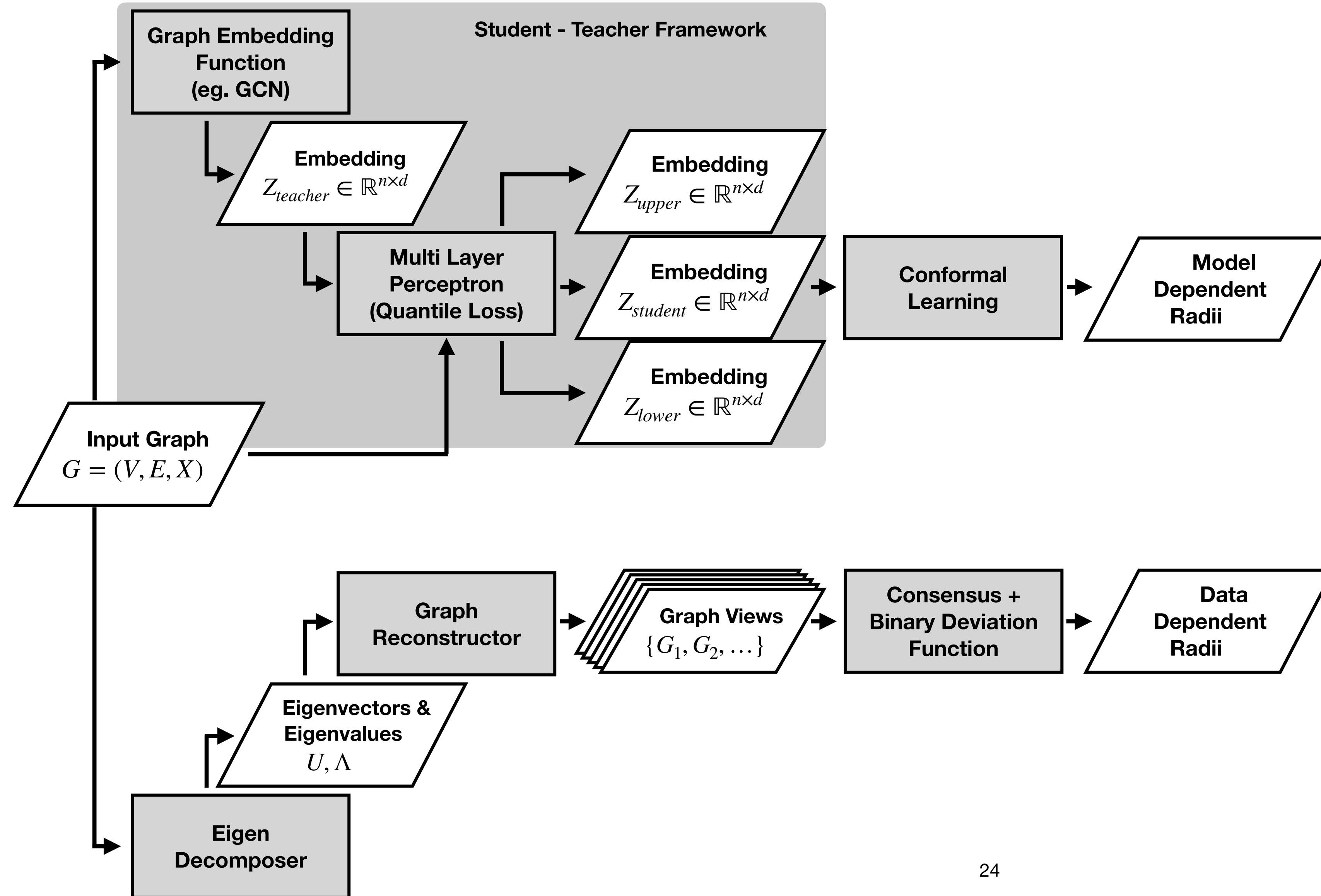
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How does REGE measure uncertainty in the model?

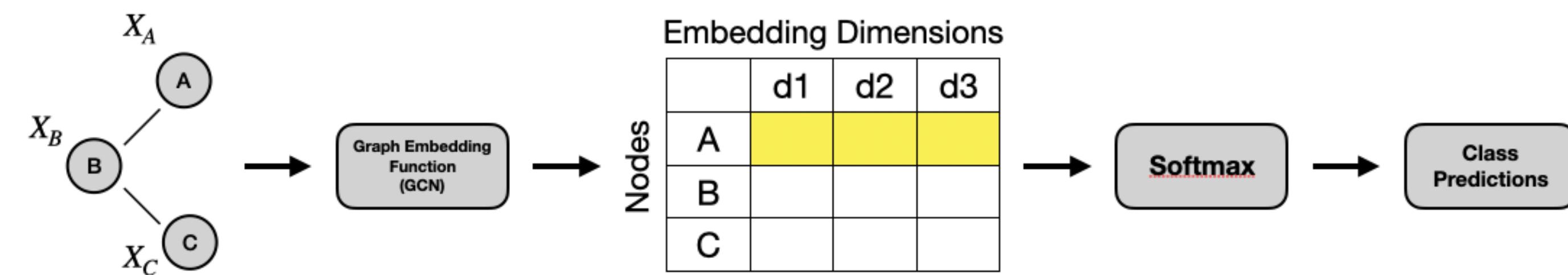


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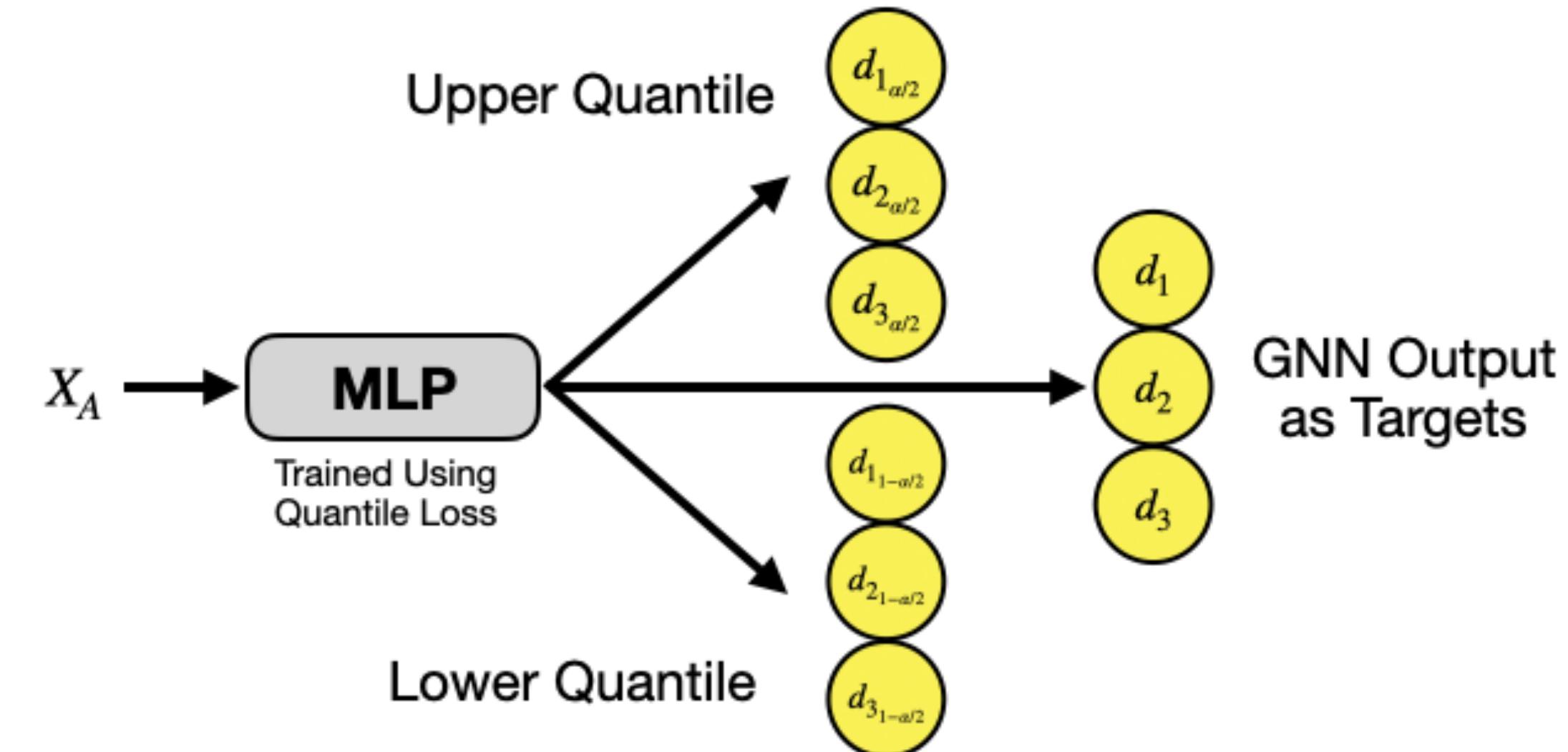


Model-dependent Radii

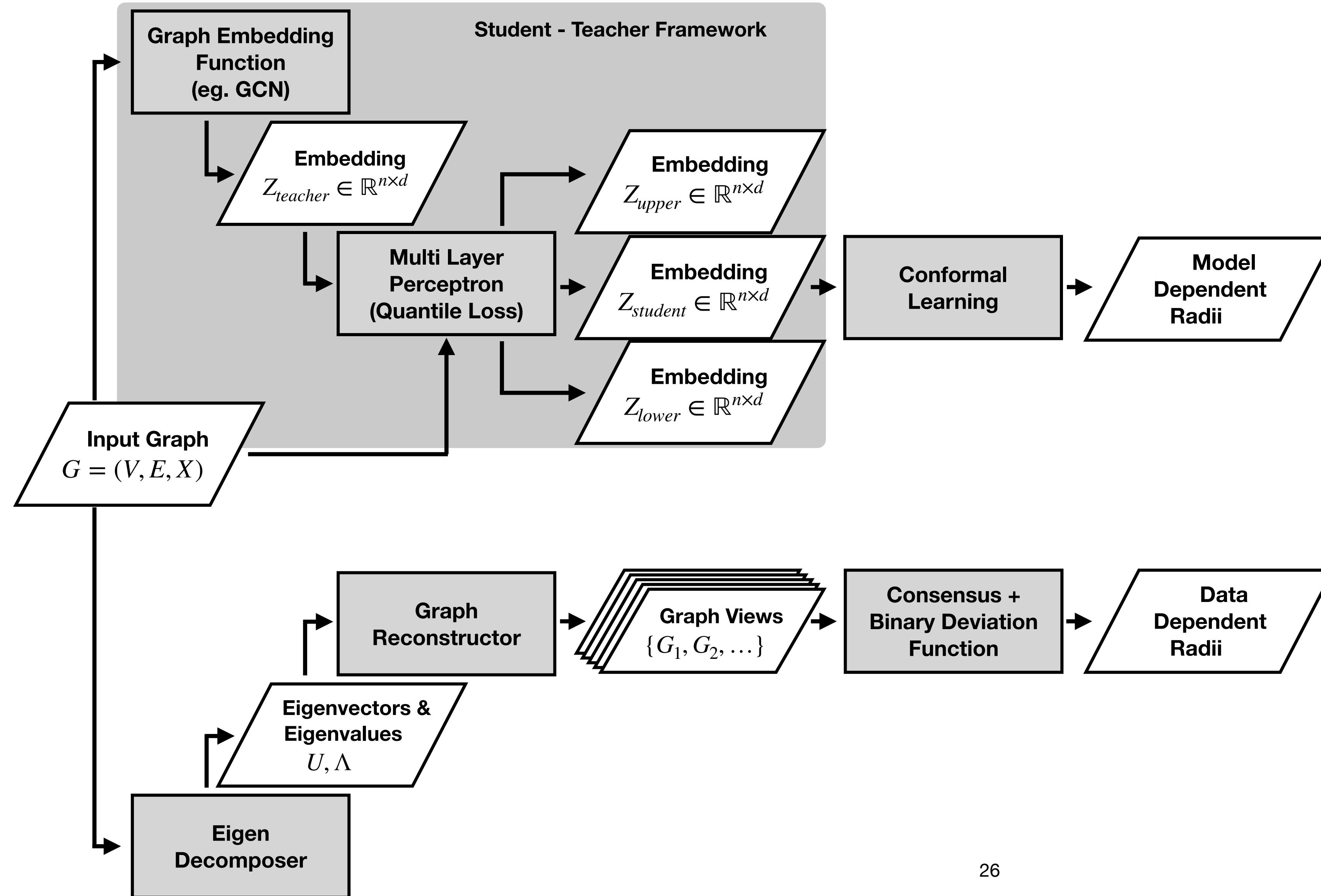
- Capture uncertainty around each embedding dimension
- Student-Teacher Framework
 - Learn an MLP to predict dimensions of a pre-trained GCN using quantile regression
 - This MLP predicts upper and lower quantiles
 - Conformal learning used to refine distance between quantiles
 - Distance between upper and lower quantile is considered as the uncertainty for that dimension



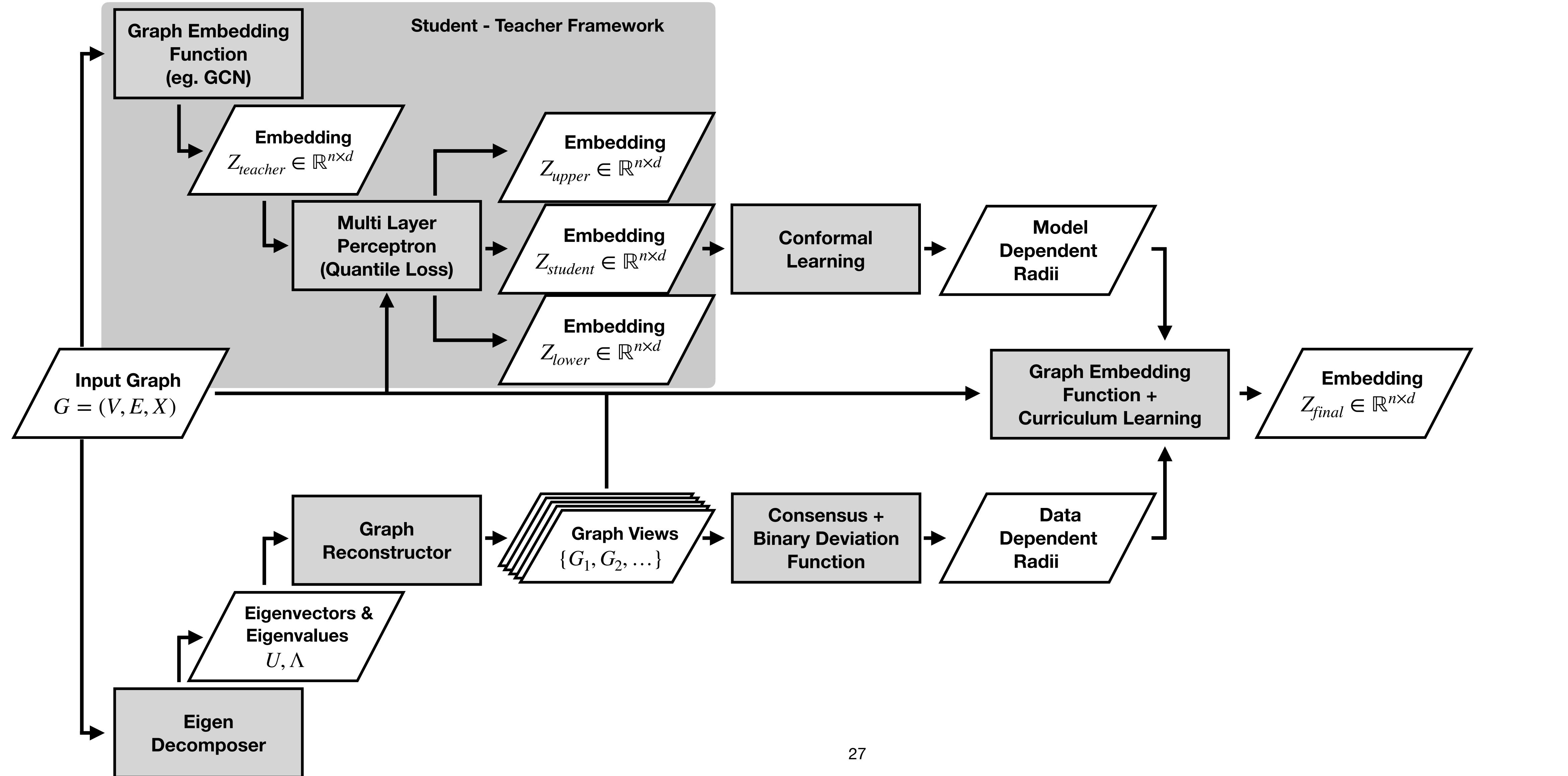
Student Model - Multi-layer Perceptron



How does REGE incorporate uncertainty?



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How does REGE incorporate uncertainty?

Noise

- REGE adds noise to hidden layer representations of each node.
- This noise is proportional to the radius value of each node.
 - Nodes with low radius values have relatively stable embeddings.
 - Nodes with large radii have relatively unstable embeddings.
- This controlled instability makes the model learn robust representations for the nodes.

$$x_i^l \leftarrow x_i^l + \mathcal{N}(0, r_i)$$

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Curriculum Learning

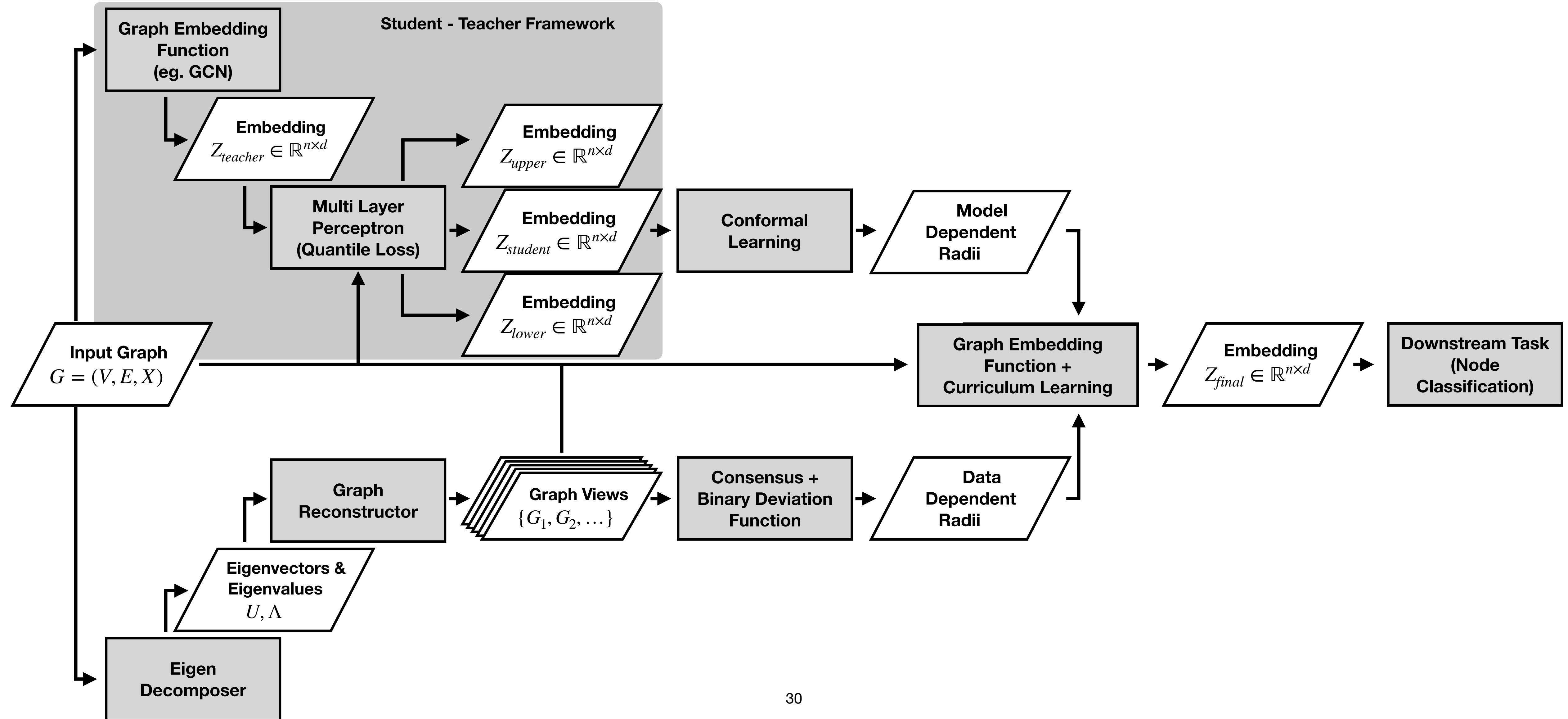
- Recall that we reconstruct multiple views of a graph.
- Graph G_1 is reconstructed by using the fewest components is the simplest graph with edges with high certainty
- As more components are added, so is more detail and smaller communities [1][2][3].
- We train the model starting on the simplest graph G_1 followed by G_2 and so on.

[1] S. Sawlani, L. Zhao, and L. Akoglu, “Fast attributed graph embedding via density of states,” in *ICDM* (2021)

[2] M. Cucuringu and M. W. Mahoney, “Localization on low-order eigenvectors of data matrices,” *arXiv preprint arXiv:1109.1355* (2011)

[3] M. Mitrović and B. Tadić, “Spectral and dynamical properties in classes of sparse networks with mesoscopic inhomogeneities,” *Physical Review E: Statistical, Nonlinear, and Soft Matter Physics* (2009)

All together



REGE: Radius Enhanced Graph Embeddings

- What does REGE do?
- How does it measure uncertainty in data?
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- How effective is it?

- REGE (D): Data-dependent Radii
- REGE (M): Model-dependent Radii

Evaluation on PolBlogs

(See paper for more results.)

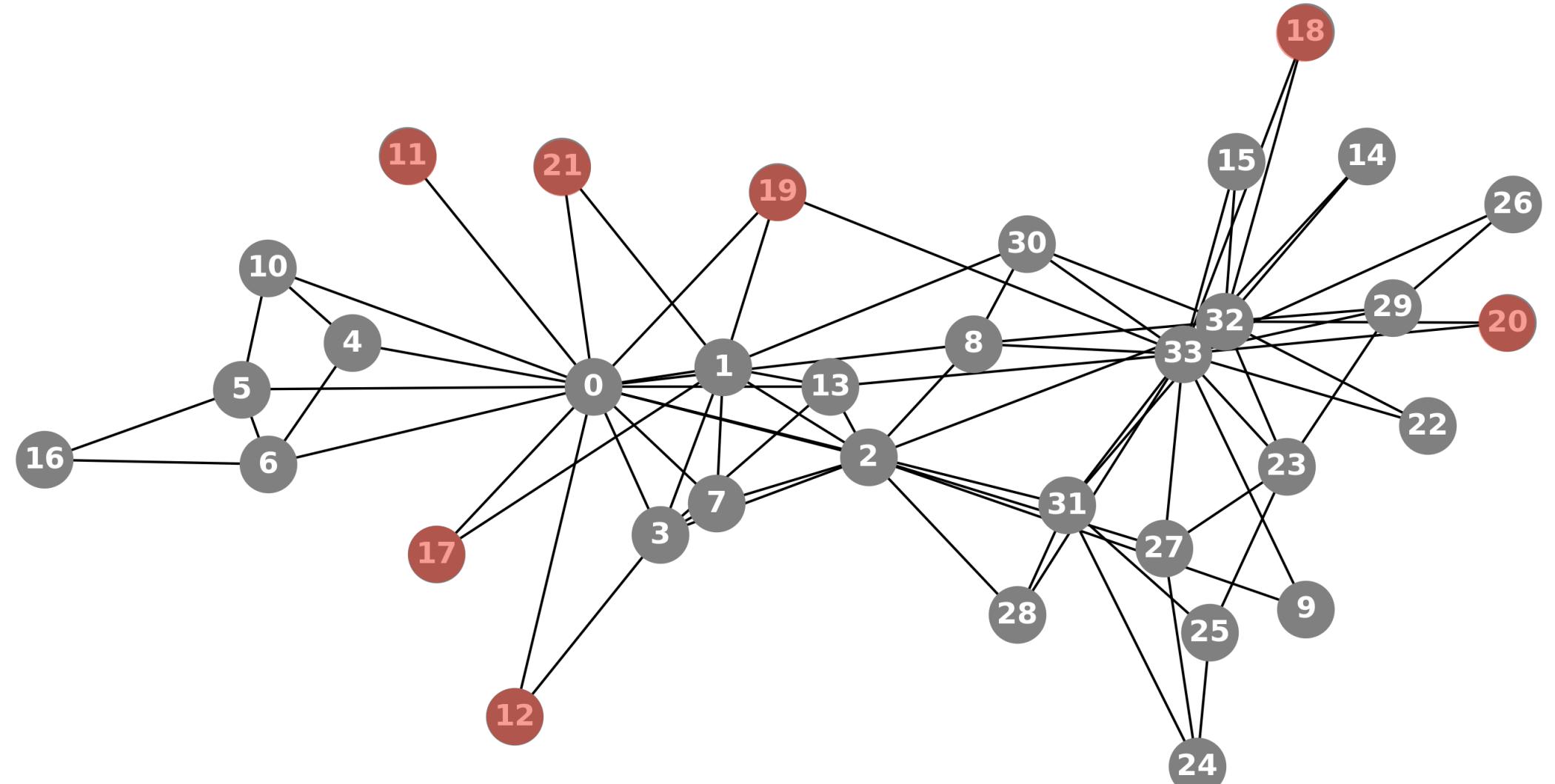
- Methods in the **red box** are some of the well-established defense methods
- Highlighted in **blue** are recent methods
- Best results are shown in **bold**, with second best underlined.

Method	MinMax (1%)	MinMax(10%)	Meta (1%)	Meta(10%)	GraD (1%)	GraD (10%)
GCN	.944 ± .001	.871 ± .002	.859 ± .002	.726 ± .004	.876 ± .005	.795 ± .002
RGCN	.936 ± .002	.854 ± .002	.850 ± .002	.699 ± .007	.866 ± .003	.811 ± .003
GCN-SVD	.939 ± .005	<u>.885 ± .002</u>	.926 ± .002	.894 ± .007	.883 ± .004	.865 ± .003
GNNGuard	.950 ± .004	.861 ± .001	.854 ± .002	.707 ± .014	.855 ± .005	.812 ± .002
ProGNN	.935 ± .017	.869 ± .029	<u>.936 ± .023</u>	.823 ± .055	.829 ± .029	.859 ± .005
GADC	.512 ± .008	.512 ± .008	.512 ± .008	.512 ± .008	.498 ± .009	.497 ± .014
GraphReshape	.935 ± .007	.847 ± .002	.850 ± .006	.694 ± .002	.851 ± .003	.803 ± .004
Ricci-GNN	.941 ± .004	.874 ± .004	.932 ± .003	.928 ± .010	.875 ± .011	.865 ± .008
REGE (D)	<u>.946 ± .004</u>	.890 ± .004	.946 ± .007	.950 ± .005	<u>.887 ± .002</u>	.865 ± .003
REGE (M)	.929 ± .009	.880 ± .006	.931 ± .017	<u>.942 ± .017</u>	.889 ± .002	.861 ± .004

REGE on Karate Club Network

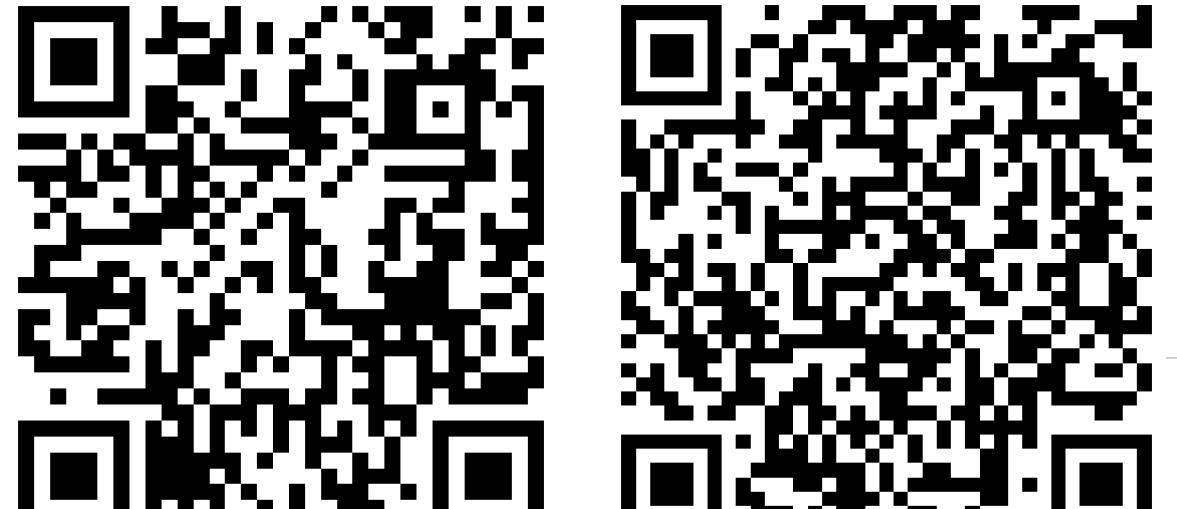
Data vs. Model Dependent Radii

- DDR - Data-dependent radii
- MDR - Model-dependent radii
- Low degree nodes (red) show low DDR - possibly due to consistent edge reconstruction
- The same nodes show high MDR - indicating that GNNs may not do as well for low degree nodes



Node	Degree	DDR	MDR
0	16	1.0	0.25
1	9	0.41	0.13
2	10	0.5	0.21
3	6	0.45	0.55
4	3	0.16	0.33
5	4	0.22	0.42
6	4	0.19	0.37
7	4	0.24	0.1
8	5	0.29	0.06
9	2	0.0	0.0
10	3	0.16	0.4
11	1	0.01	0.34
12	2	0.02	0.26
13	5	0.31	0.19
14	2	0.07	0.24
15	2	0.08	0.3
16	2	0.12	0.39
17	2	0.0	0.3
18	2	0.0	0.27
19	3	0.06	0.23
20	2	0.04	0.35
21	2	0.03	0.32
22	2	0.06	0.0
23	5	0.25	0.12
24	3	0.13	0.06
25	3	0.02	0.03
26	2	0.08	0.12
27	4	0.21	0.16
28	3	0.1	0.09
29	4	0.23	0.55
30	4	0.26	0.22
31	6	0.2	0.12
32	12	0.73	1.0
33	17	0.98	0.71

REGE: Takeaway points



- REGE improves the robustness of graph embeddings.
- How?
 - It incorporates data and model uncertainty during training.
- How effective is it?
 - It outperforms state of the art methods in terms of node classification accuracy on adversarially attacked datasets.