Northeastern University

REGE: A Method for Incorporating Uncertainty in Graph Embeddings

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

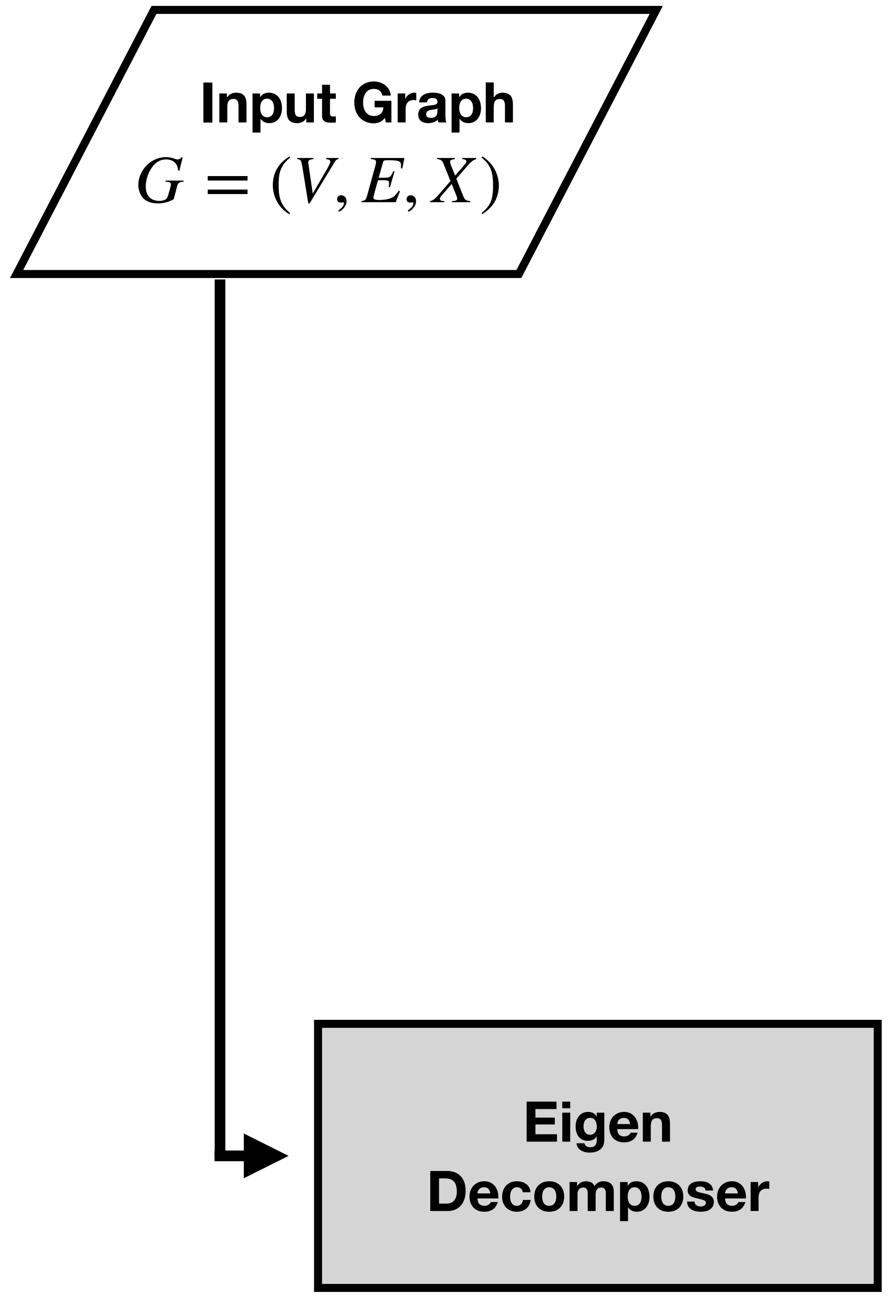
Motivation

- 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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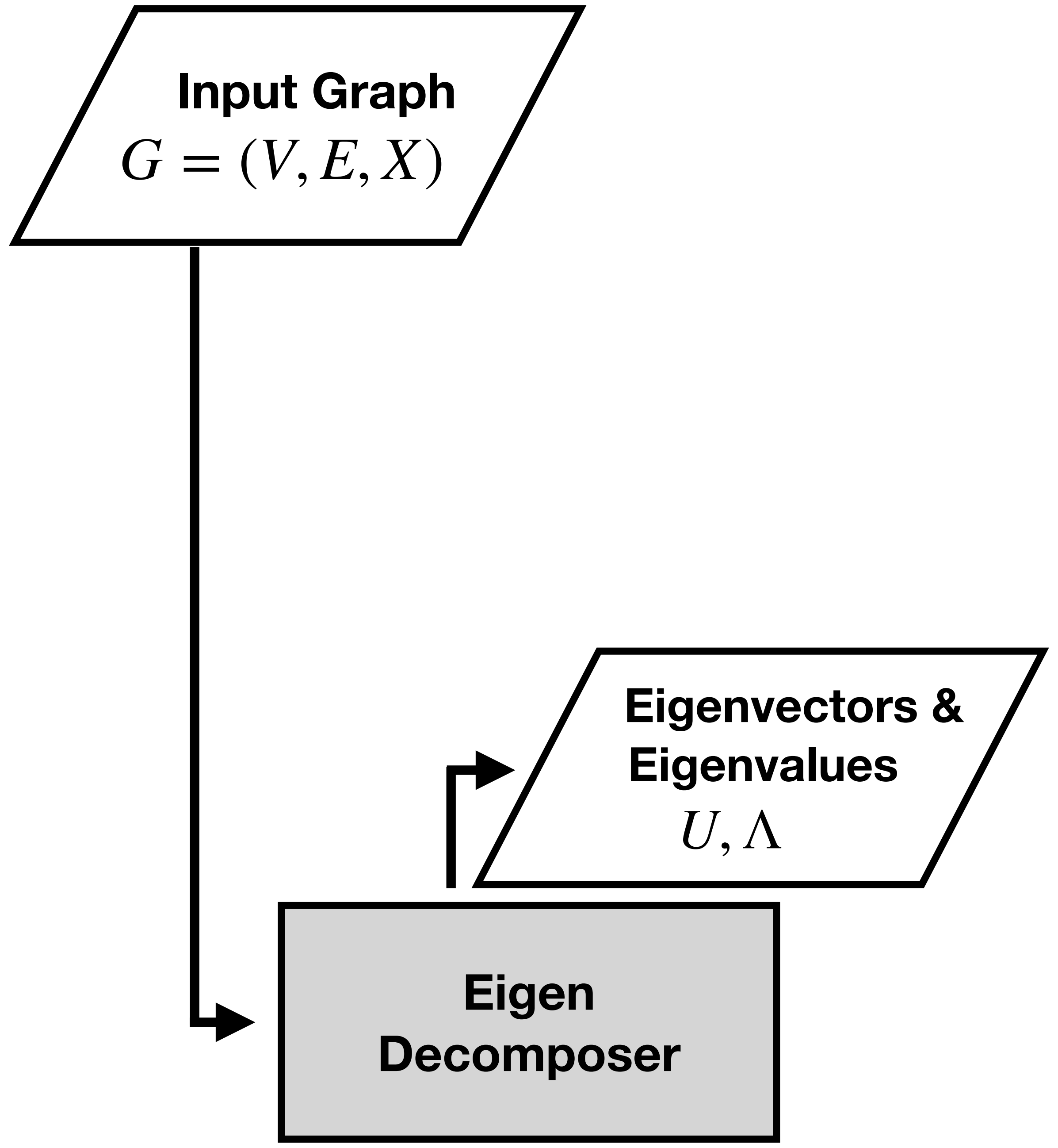

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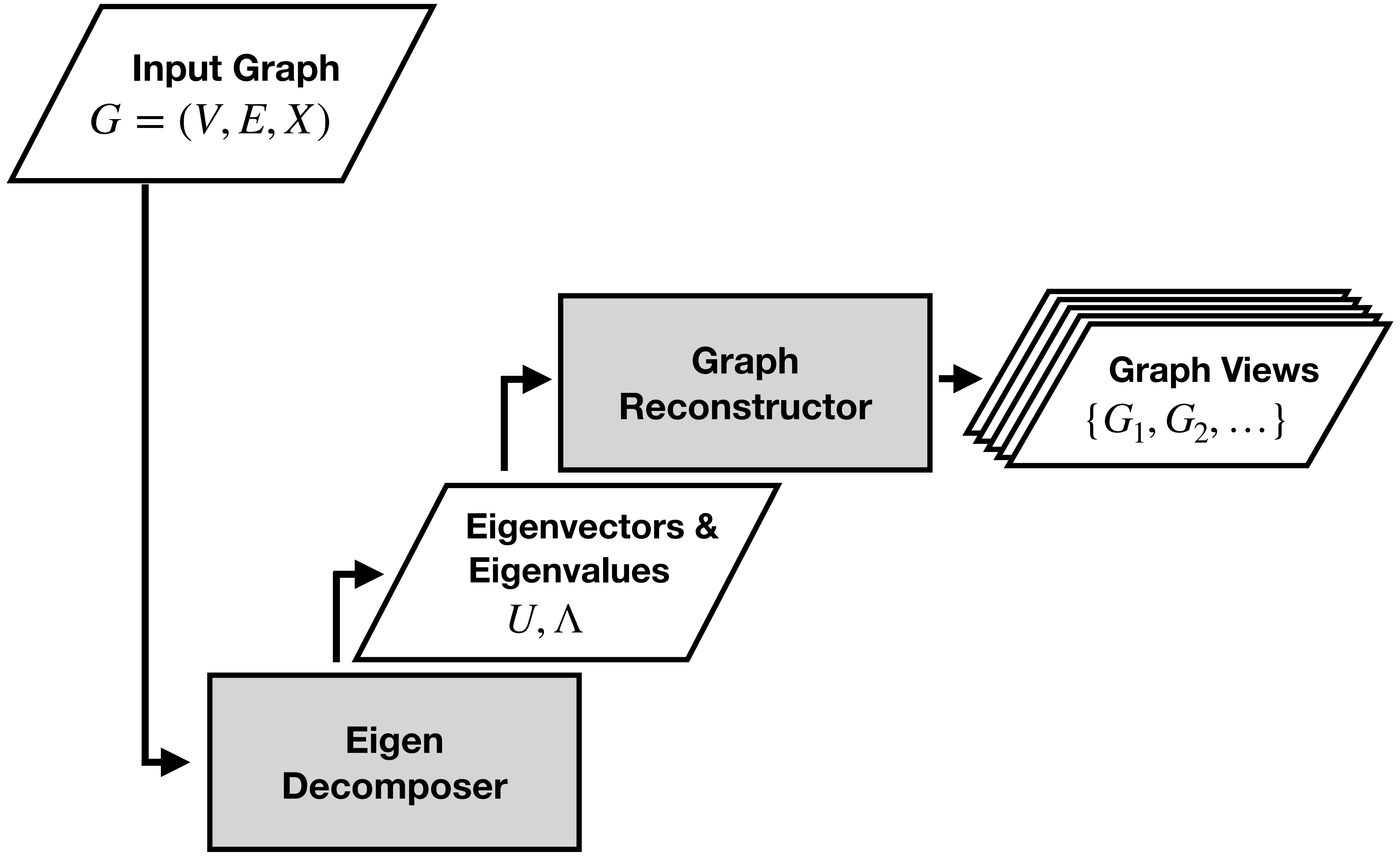

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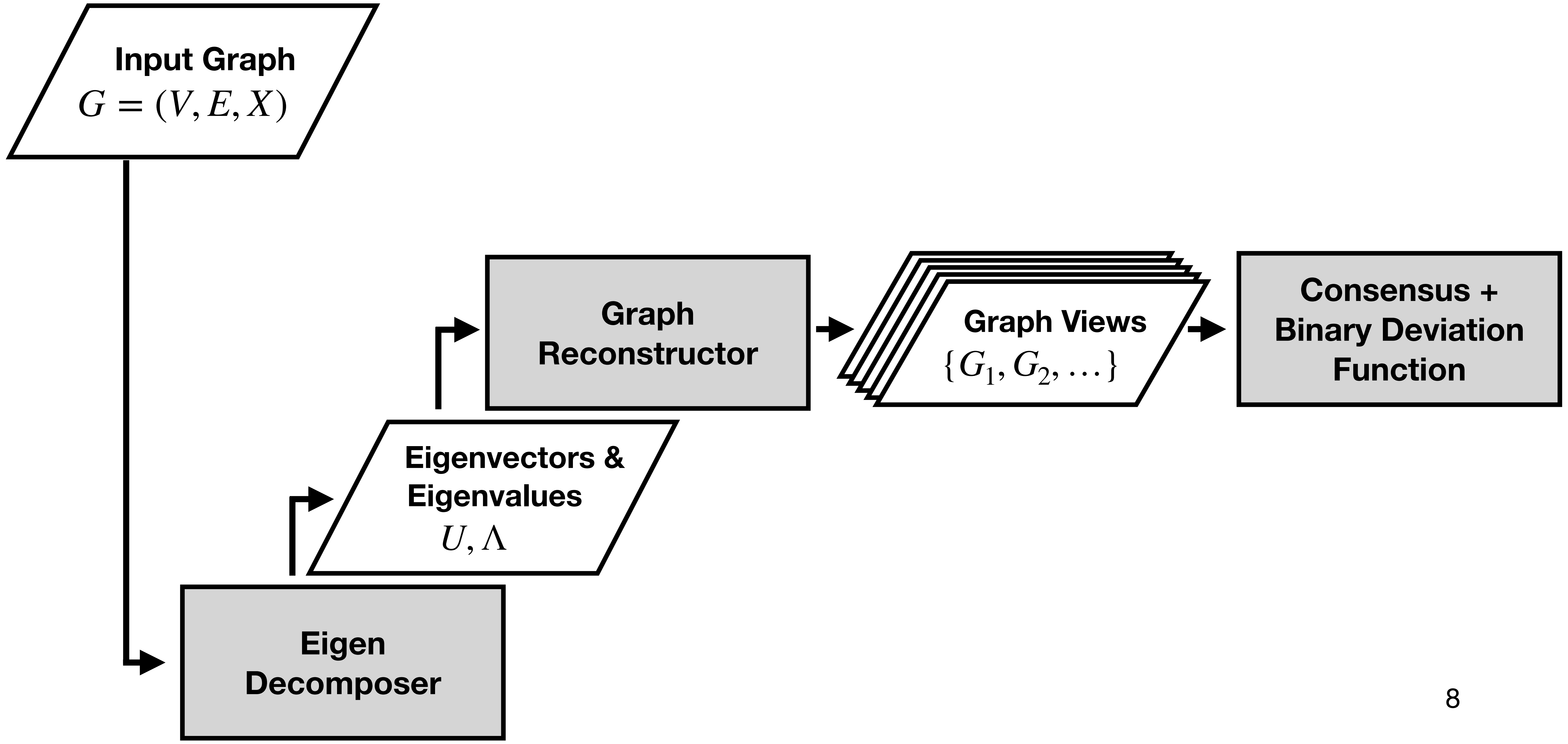

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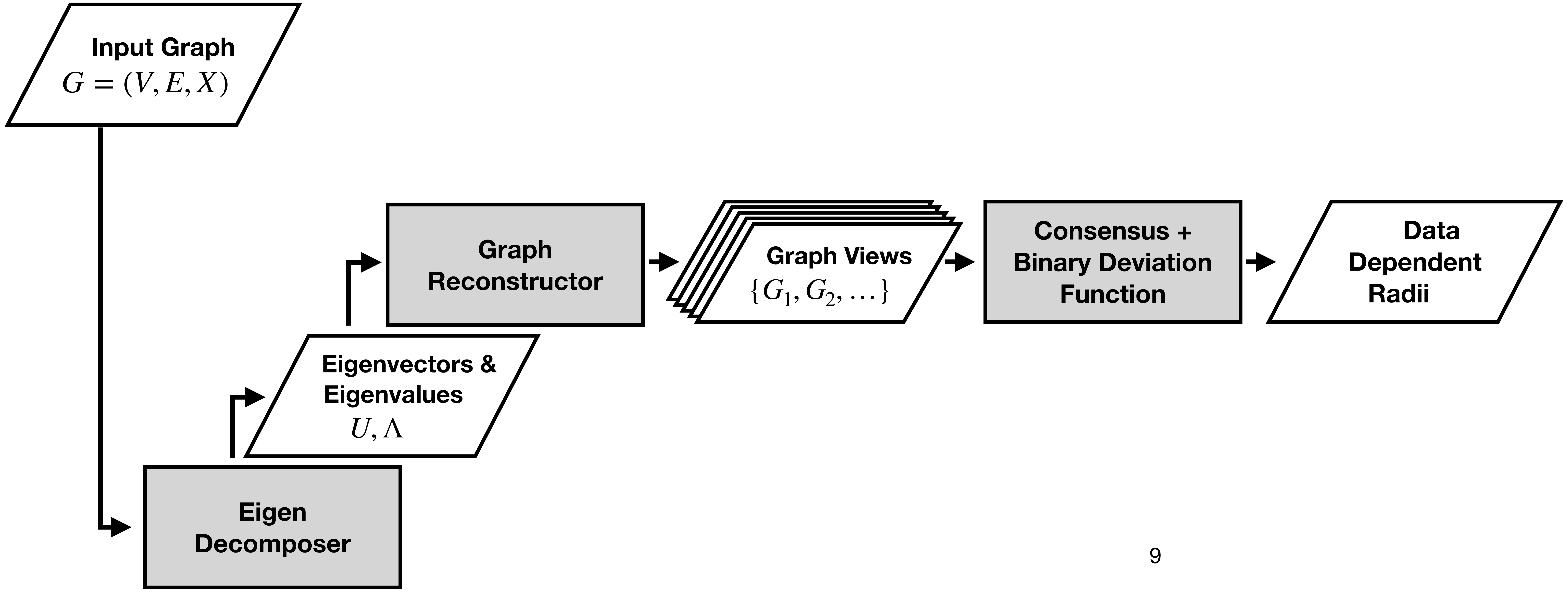
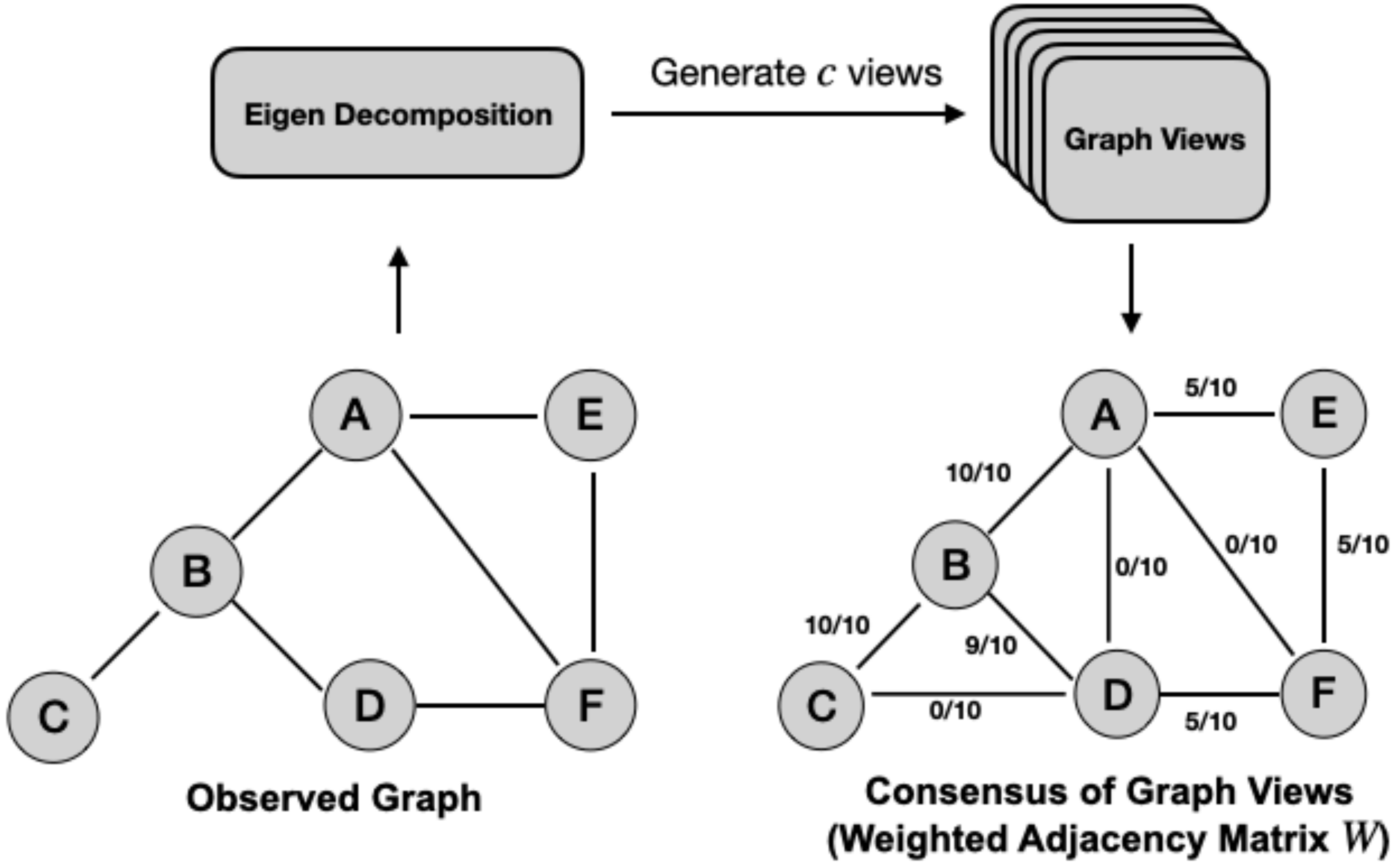


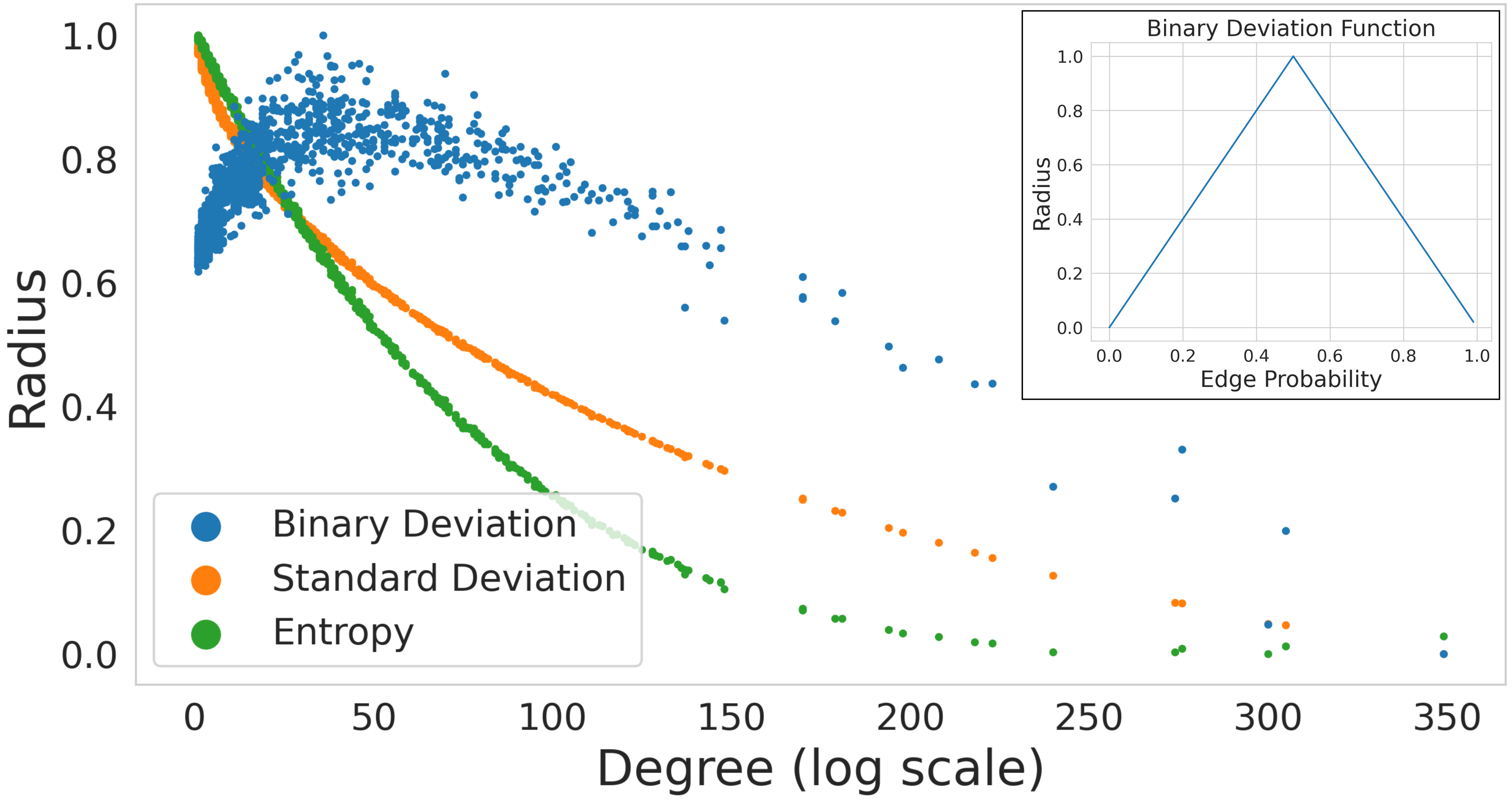
Data-dependent Radii (1/2)

- Given a graph G, compute its eigen-decomposition
- Reconstruct views of the graph $(G_1, G_2, G_3, \ldots)$
- 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: $u_e = 1 - |W_{ij} - (1 - W_{ij})|$



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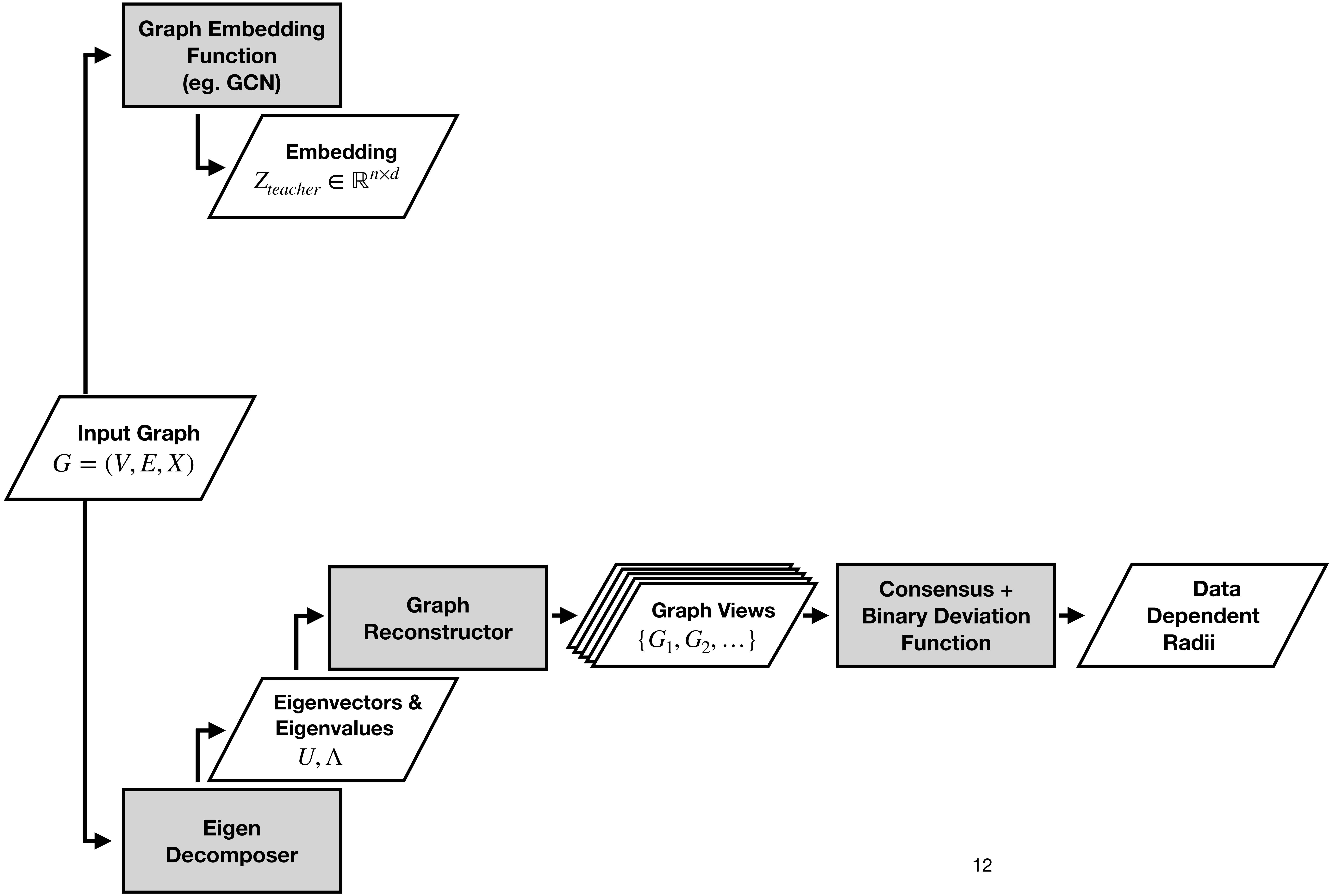

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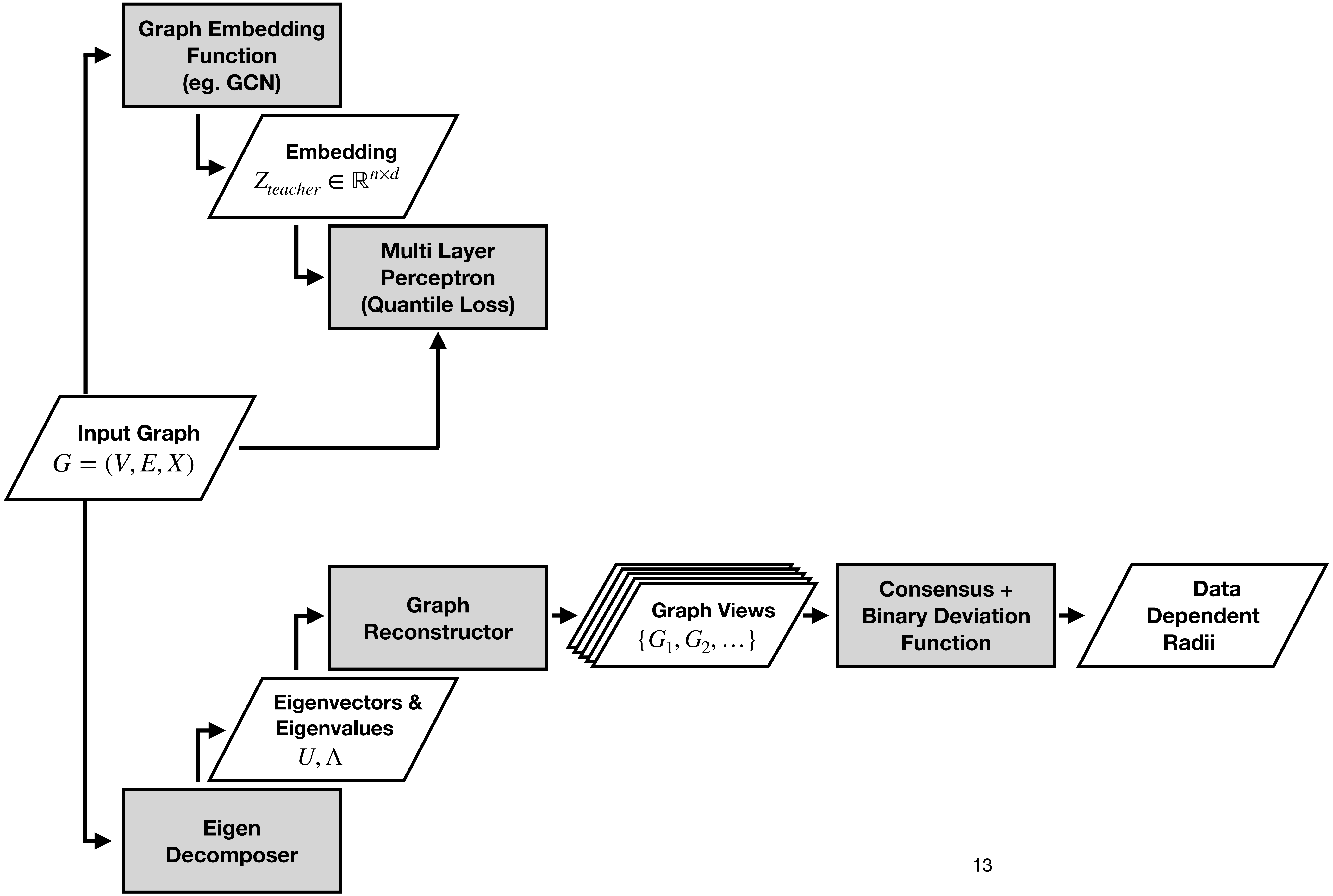

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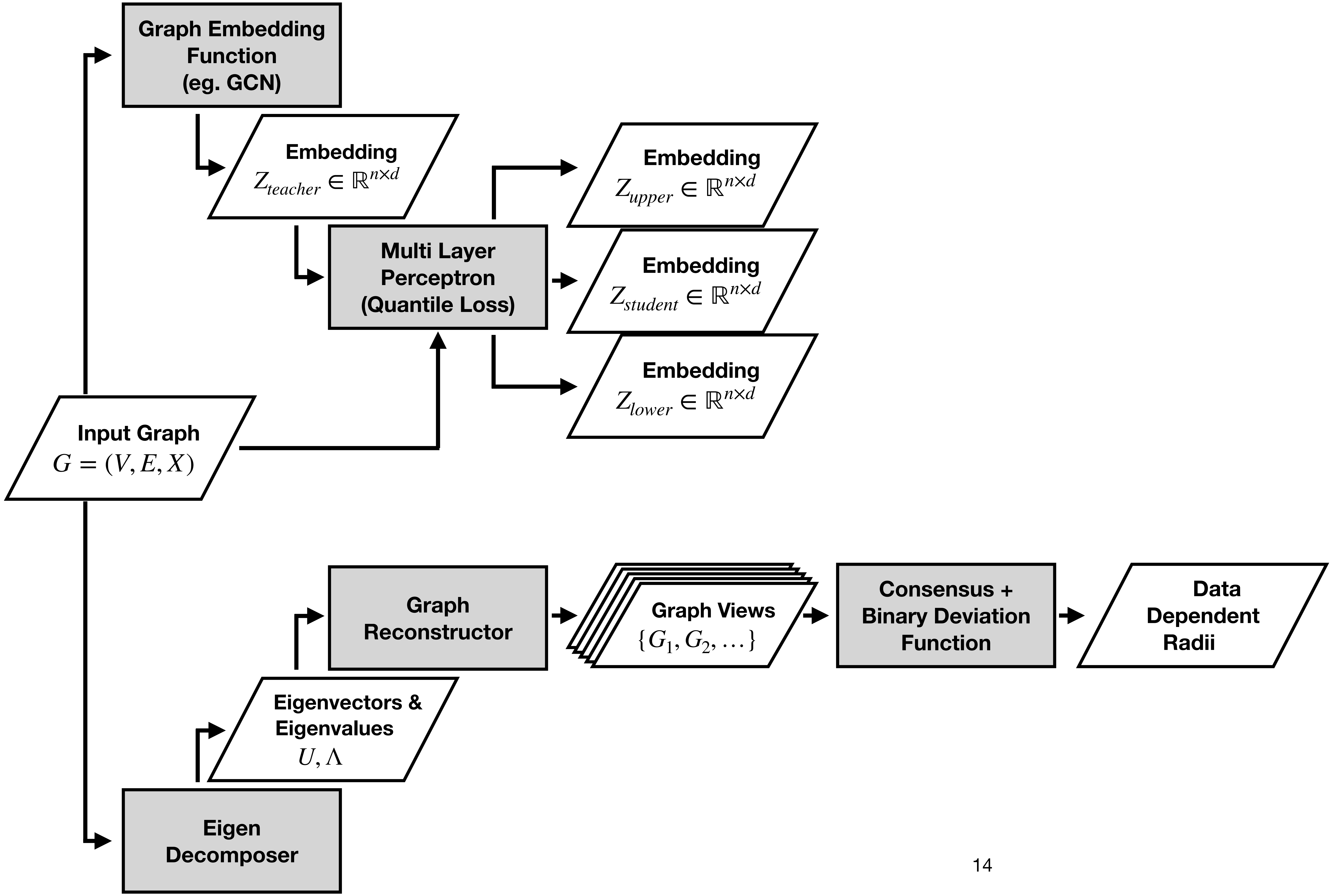

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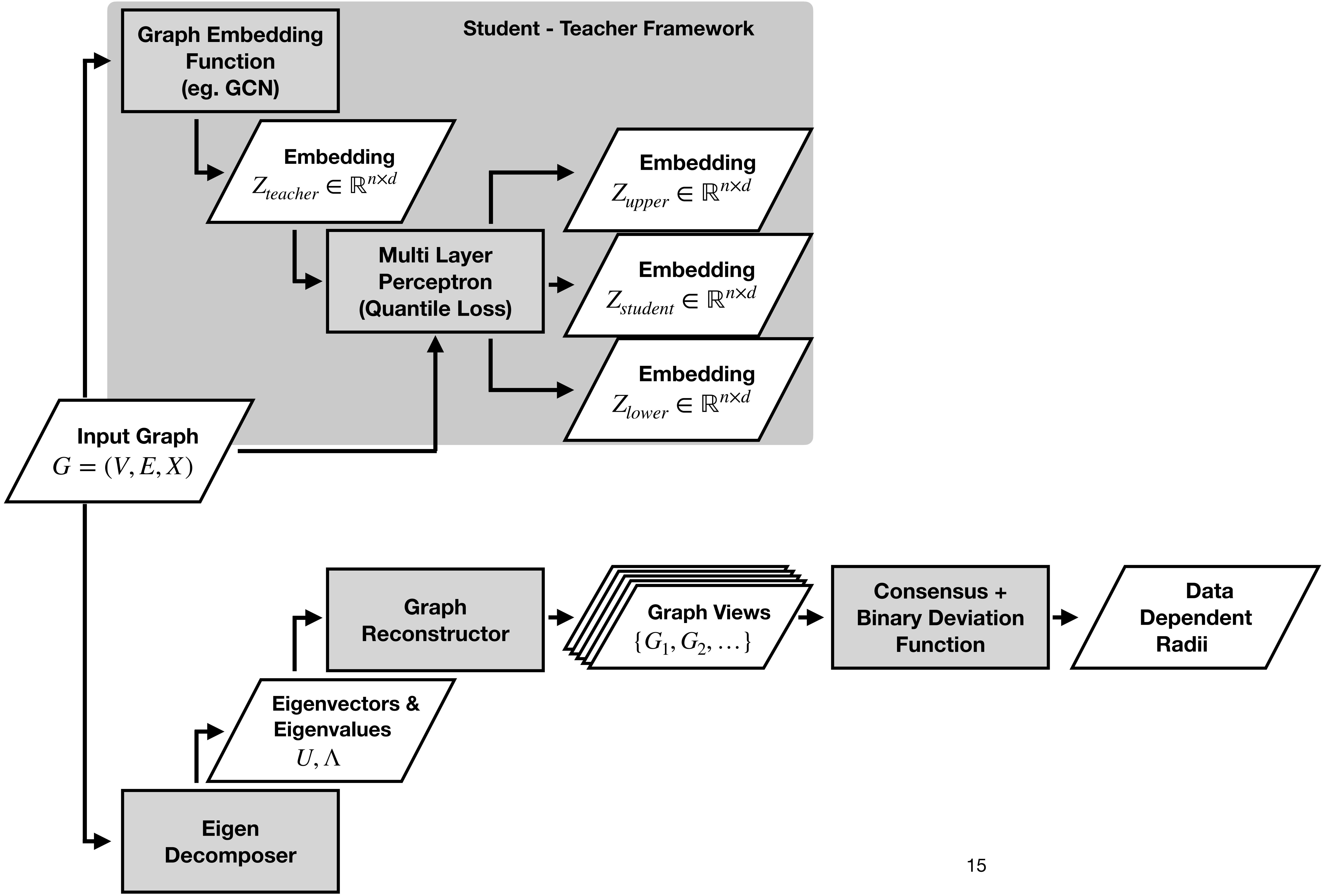

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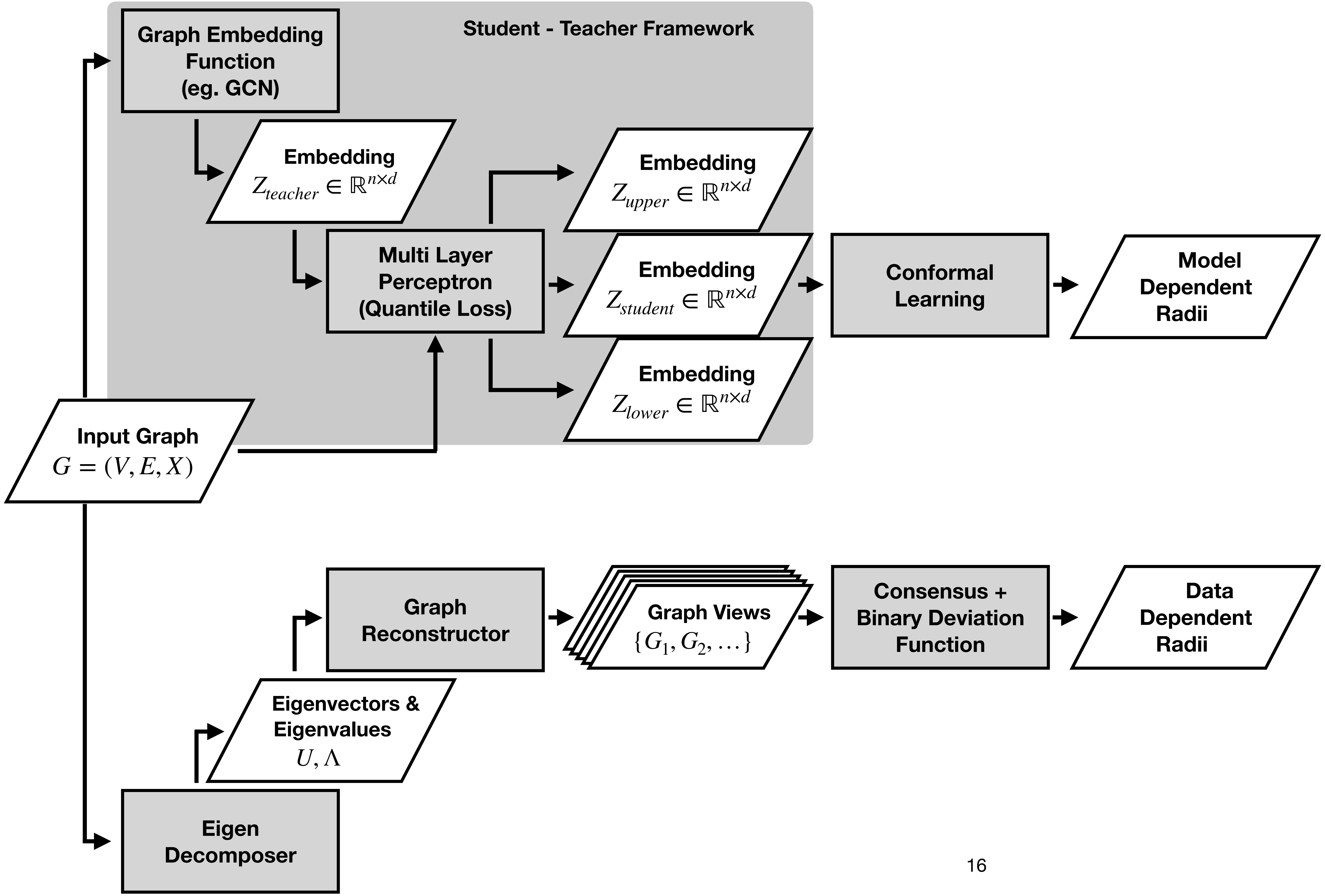
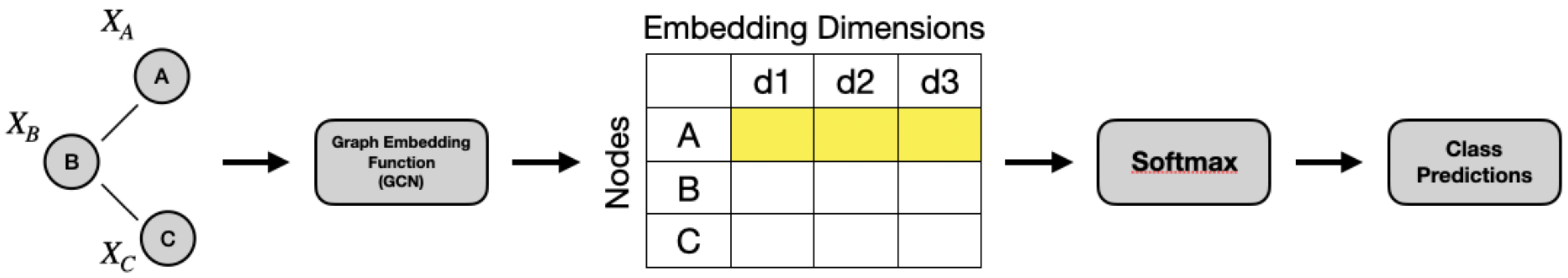


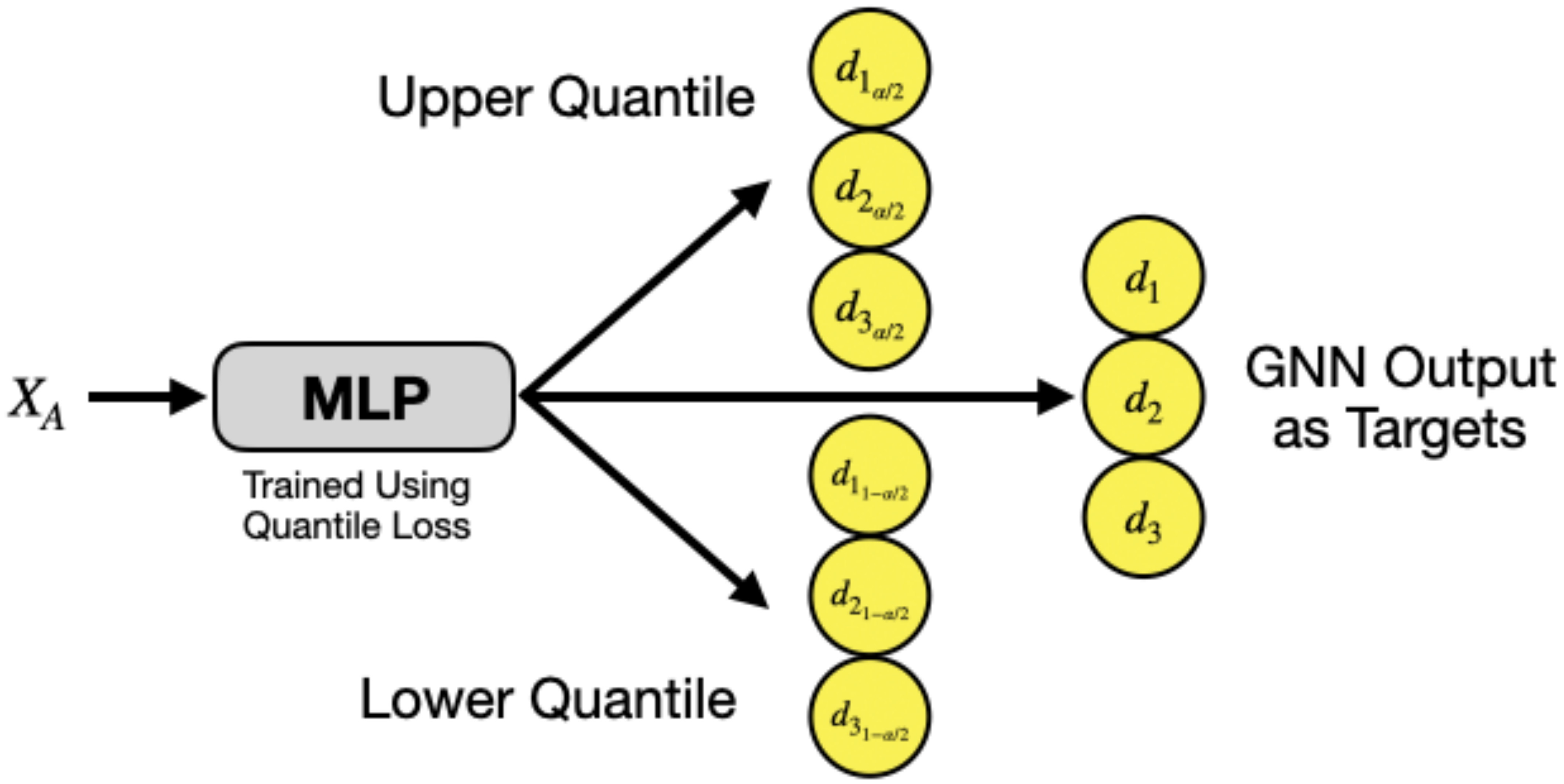
Model-dependent Radii

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

Teacher Model - A Standard GNN



Student Model - Multi-layer Perceptron



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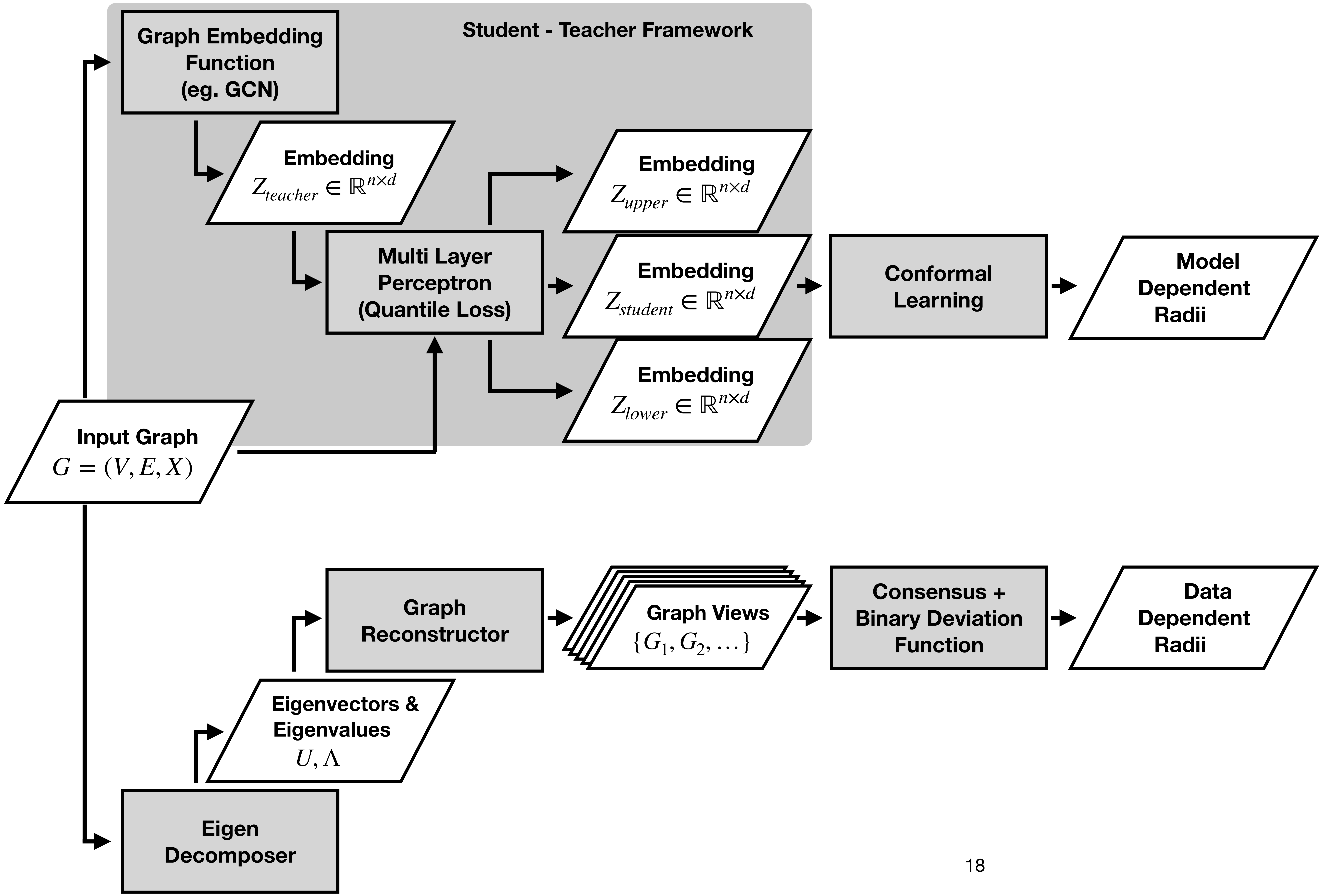

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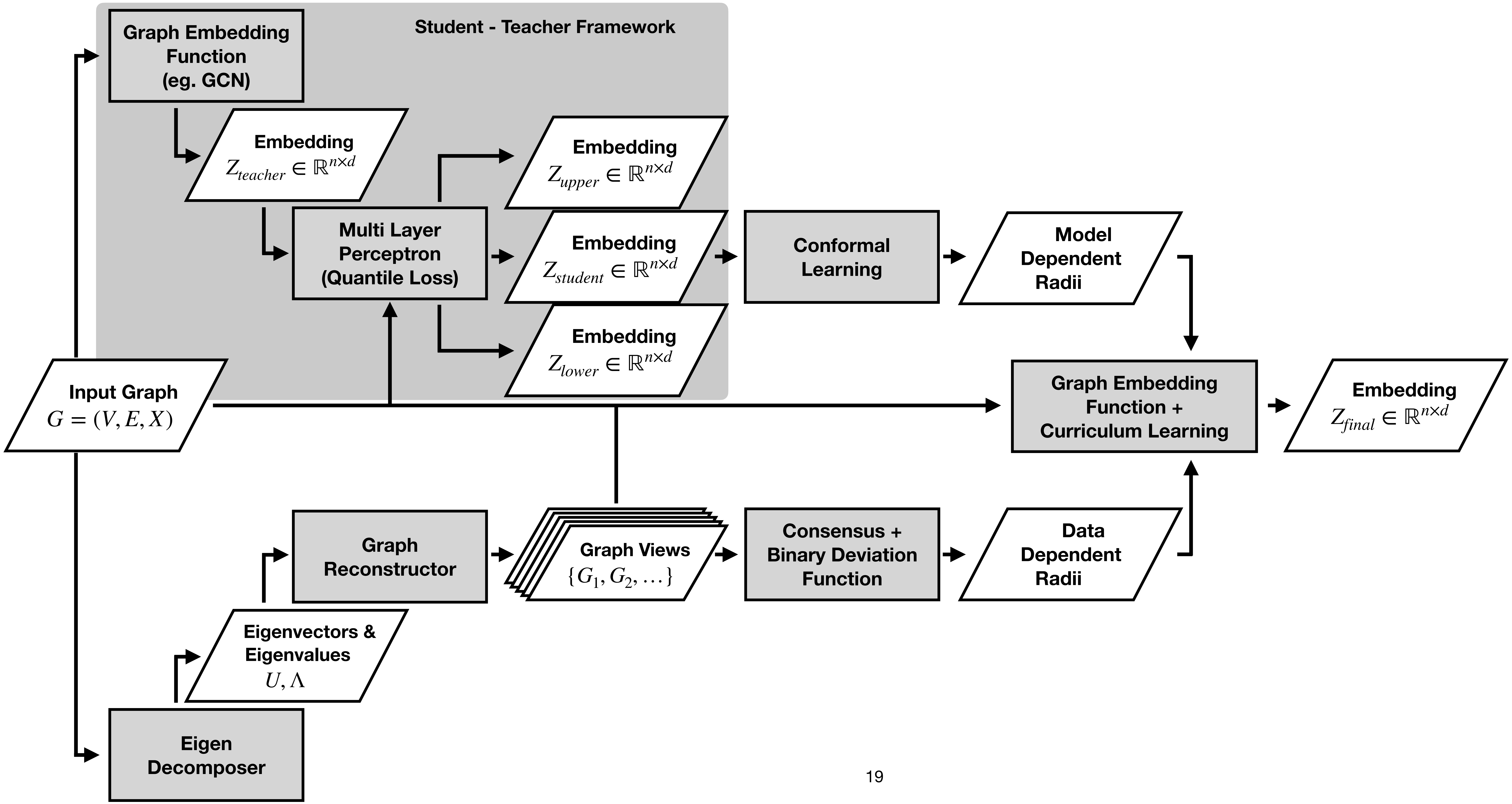

How does REGE incorporate uncertainty?

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. Mitrovi´c and B. Tadi´c, "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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- REGE (D): Data-dependent Radii
- REGE (M): Model-dependent Radii

Evaluation on PolBlogs

(See paper for more results.)

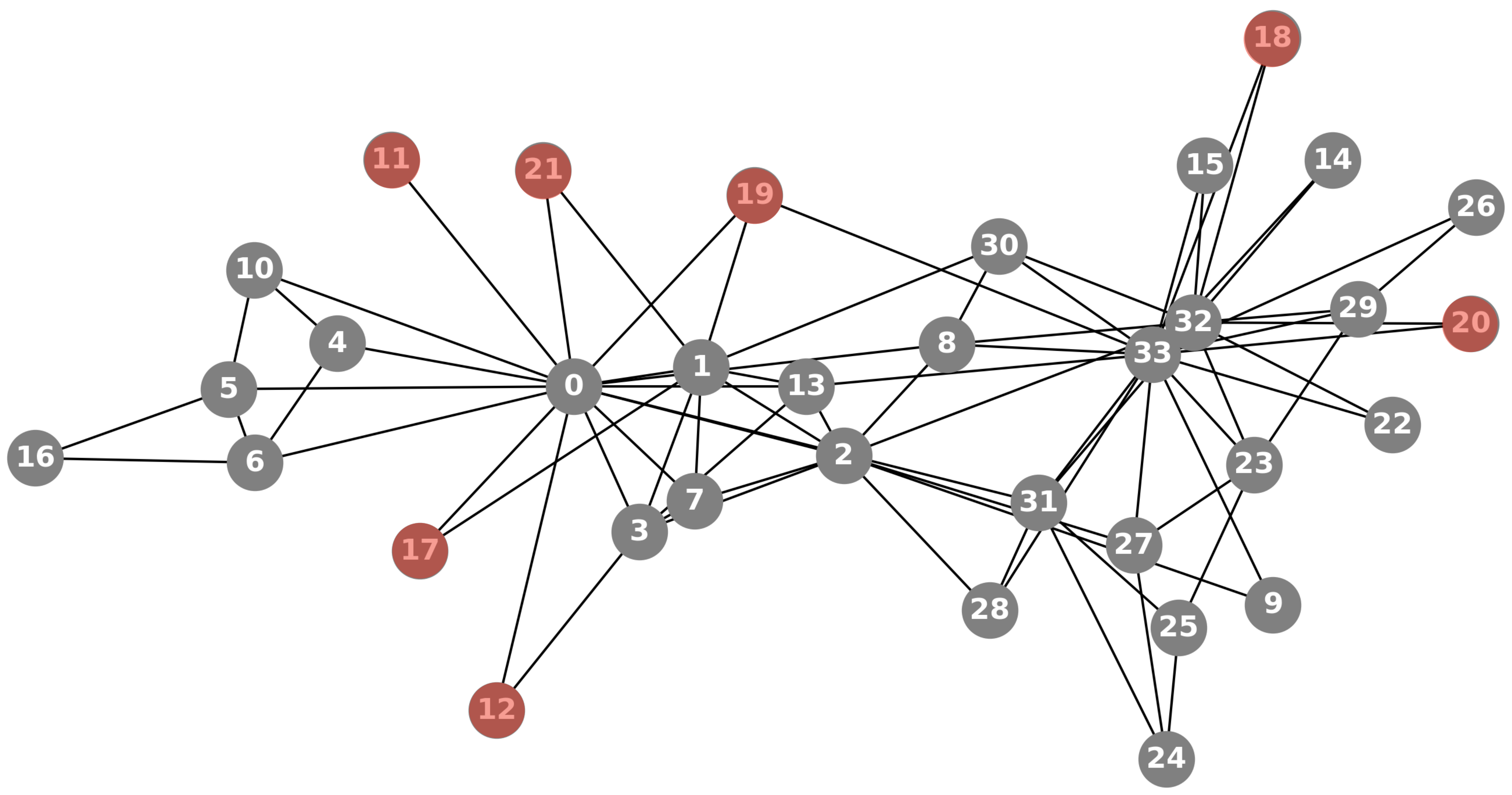
- Methods in the red box are some of the well-established defense methods
- Highlighted in blue are recent methods
- Best results are shown in **bold**, with second best underlined.

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

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.