FORGE: Foundational Optimization Representations from Graph Embeddings

Zohair Shafi, Serdar Kadioglu

Background

Mixed Integer Programming

$$f(x) = \min\{c^T x \mid Ax \leq b, x \in \mathbb{R}^n, x_j \in \mathbb{Z}\ \forall j \in I\}$$

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Some subset of these decision variables must have integer values

Motivation

- There is an abundance of mixed integer programming (MIP) instances.
    - E.g., vehicle routing, job scheduling, flight scheduling, fibre optic network design
- Can we use these instances without solving them to create a “foundational” model?
- Why?
    - Recent advances in ML for CO problems are problem type or task specific.
    - A lot of training data is needed for current methods.
    - This training data is collected by solving instances which is extremely expensive.

Methodology

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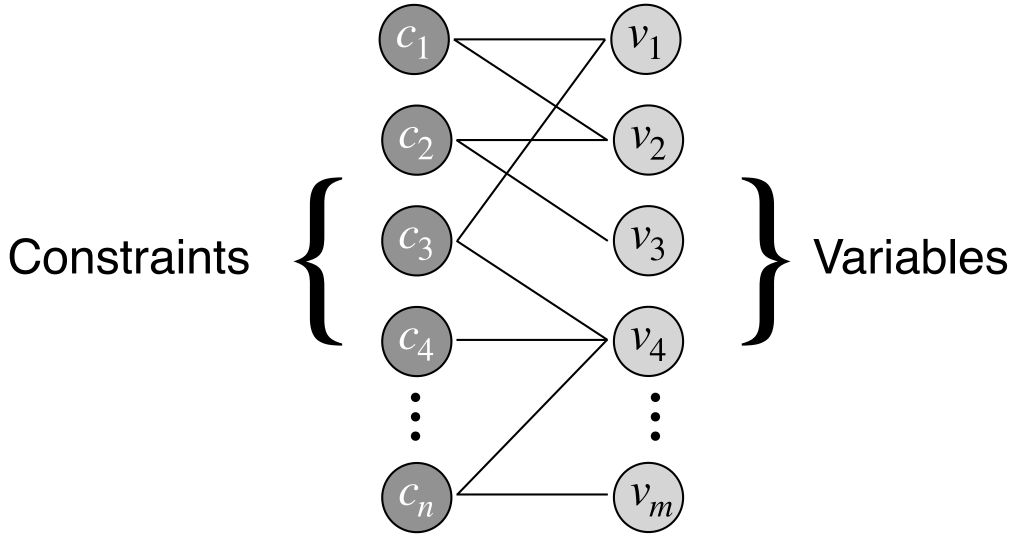
- How?
  As is commonly done, we first represent a MIP instance as a bipartite graph



Input Bipartite Representation of a MIP Instance

Methodology

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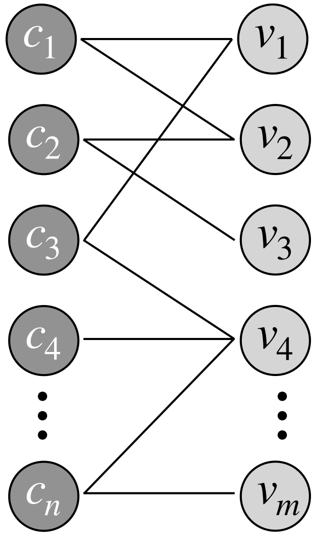
Constraints

Node Features:

Sense $\leftarrow \{ =, <, > \}$

RHS



Variables

Node Features:

Type $\leftarrow$ {*integer*, *binary*, *continuous*}

Upper Bound

Lower Bound

Coefficient in Objective

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Non-zero entries of
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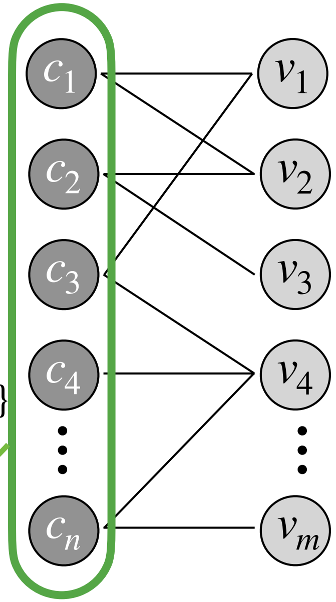

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Edge weights are the magnitude of the non-zero entries of $A \in \mathbb{R}^{\#constraints \times \#variables}$

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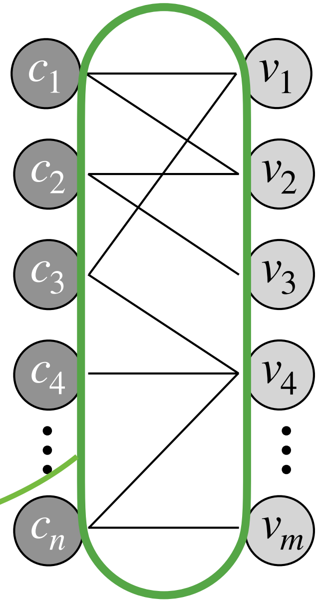

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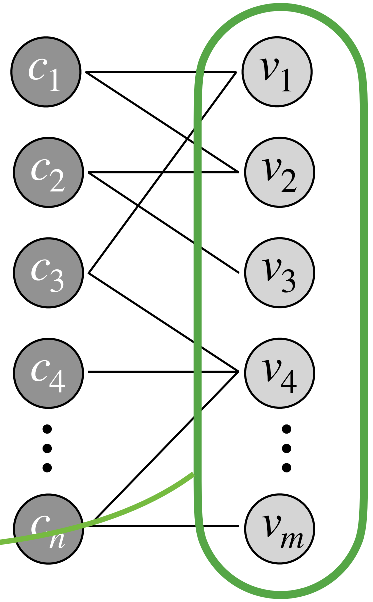

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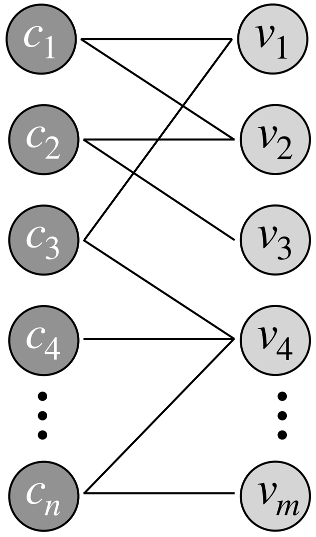

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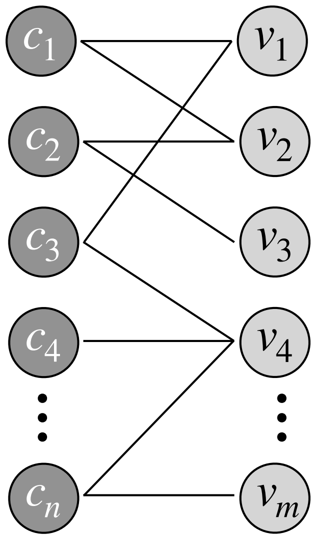

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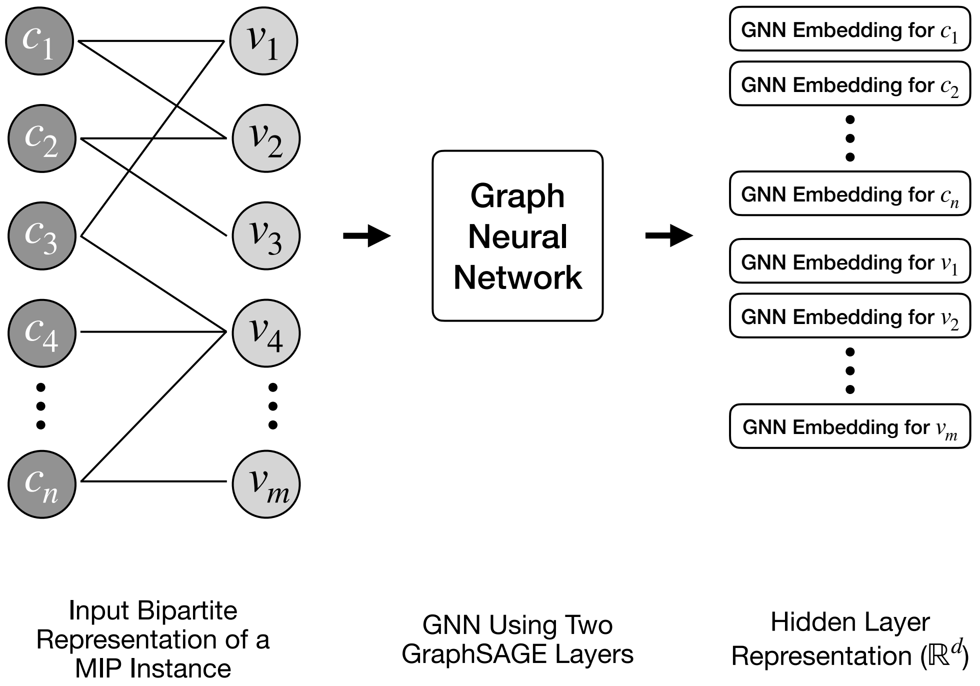
Input Bipartite Representation of a MIP Instance

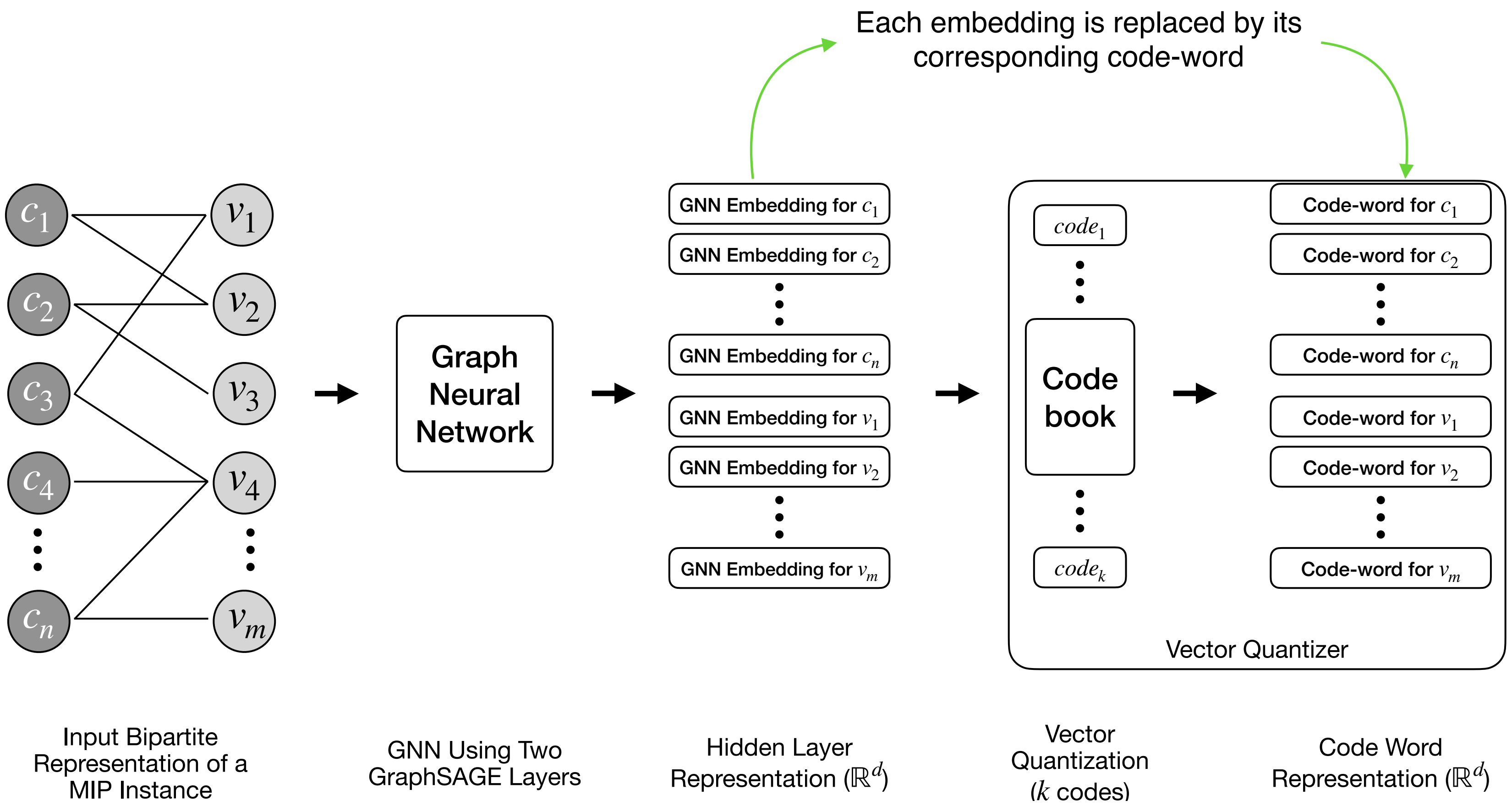
Methodology

- This bipartite graph is then passed into a Graph Neural Network (GNN)
- But GNNs are not very good at preserving global structure due to inherence locality bias.
  - **Preserving global structure is important** in CO problems, especially to generalize across problem types.



Methodology

- This is where Vector Quantization comes in.



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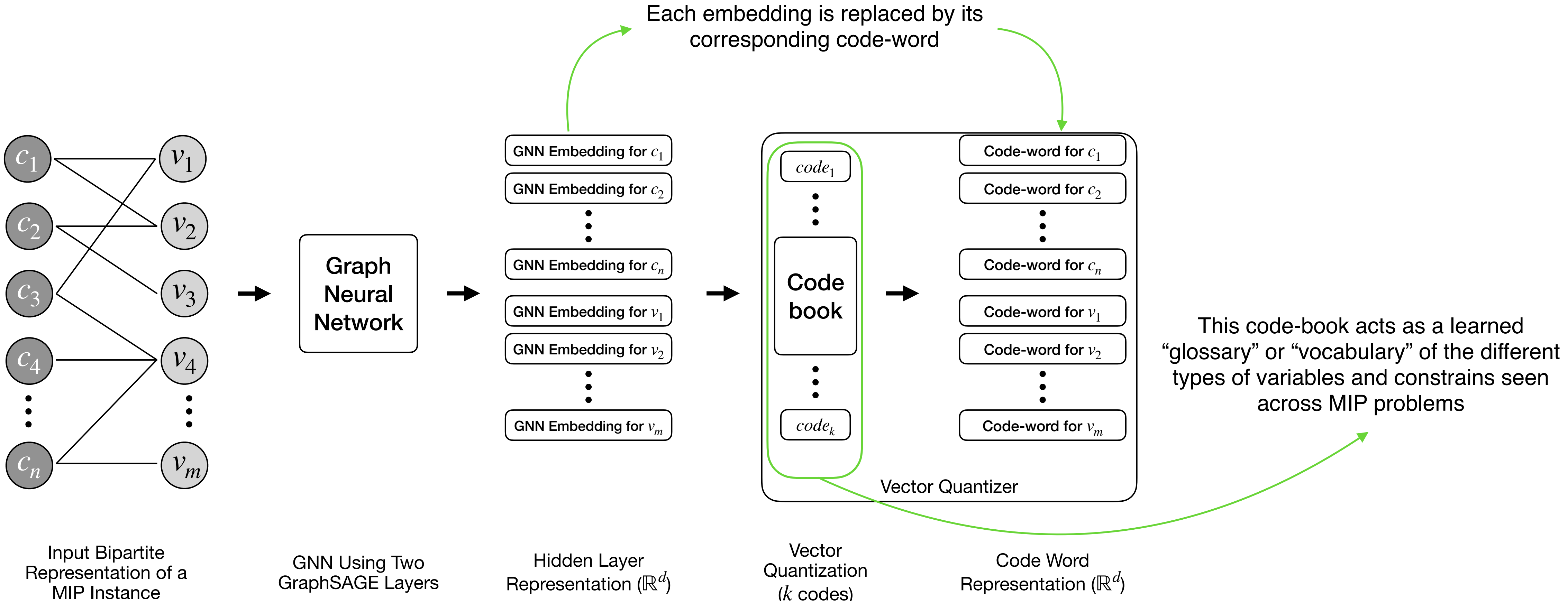

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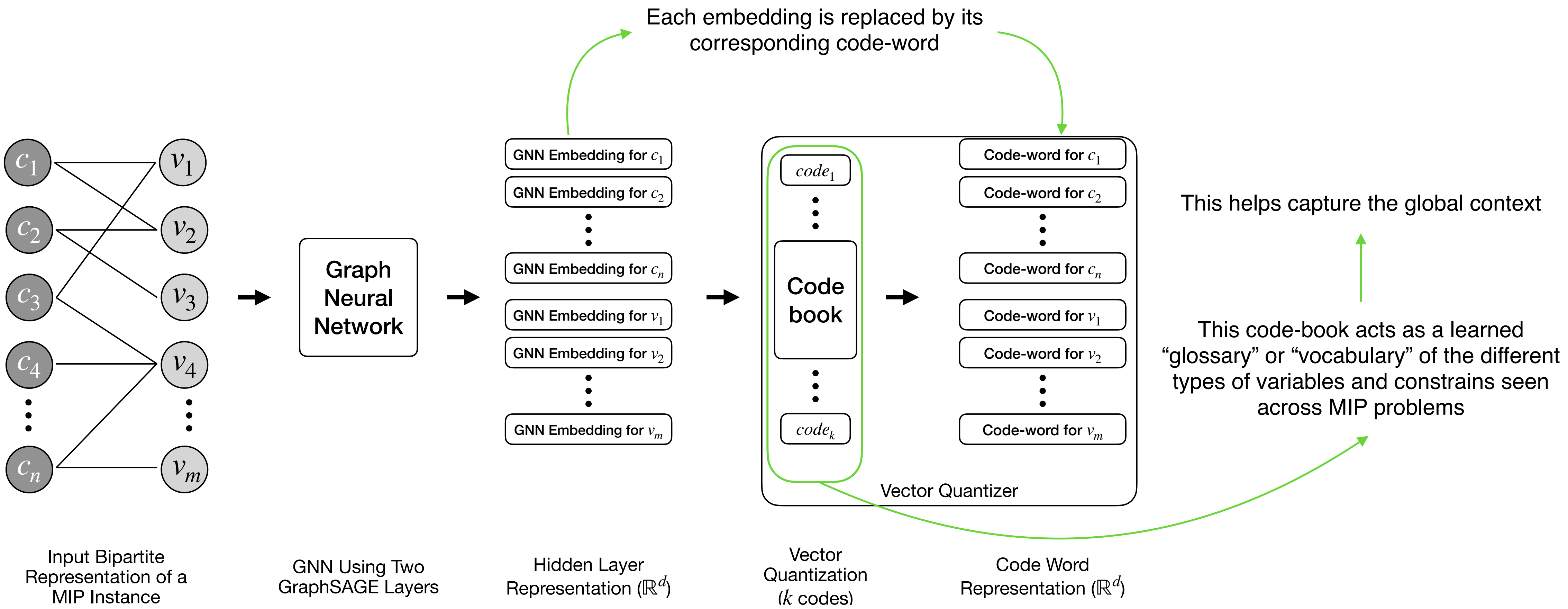

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Vector Quantization Aside

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$$\mathcal{L}_{Rec} = \underbrace{\frac{1}{N}\sum_{i=1}^{N}\left(1 - \frac{\boldsymbol{v}_i{}^T \hat{\boldsymbol{v}}_i}{\|\boldsymbol{v}_i\| \cdot \|\hat{\boldsymbol{v}}_i\|}\right)^{\gamma}}_{\text{node reconstruction}} + \underbrace{\left\|\boldsymbol{A} - \sigma(\hat{\boldsymbol{X}} \cdot \hat{\boldsymbol{X}}^T)\right\|_2^2}_{\text{edge reconstruction}},$$

v_i is the original node feature
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X is the matrix of all $\hat{v}_i$

Methodology

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Codebook Loss

$$\mathcal{L}_{Tokenizer} = \mathcal{L}_{Rec} + \frac{1}{N}\sum_{i=1}^{N} \|\mathrm{sg}[\boldsymbol{h}_i] - \boldsymbol{e}_{z_i}\|_2^2$$

Update codebook embeddings e_{z_i}
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Update encoder weights h_i to be close to chosen code e_{z_i} to **avoid fluctuations in code assignment**

This update is only applied to encoder variables.
Gradients are **not** applied to e_{z_i}

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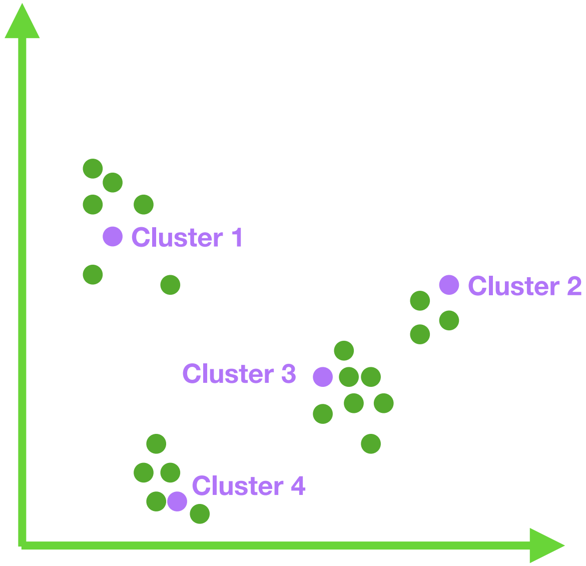
Move cluster centroids only (think standard k-means)

Move data embedding only



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Codebook Loss | Commitment Loss

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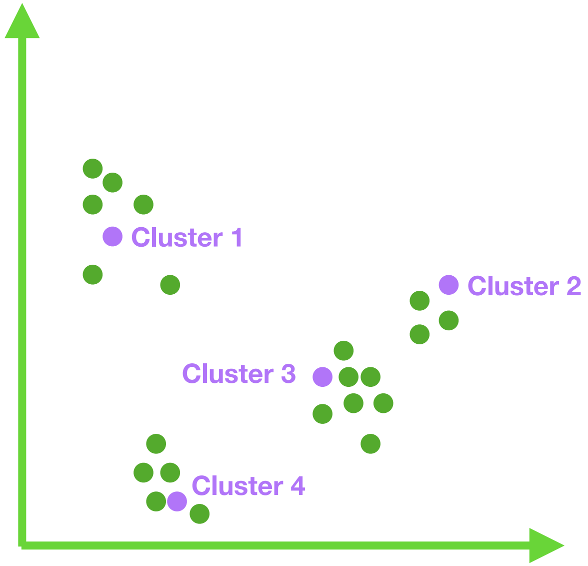

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Codebook Loss: Move cluster centroids only (think standard k-means)

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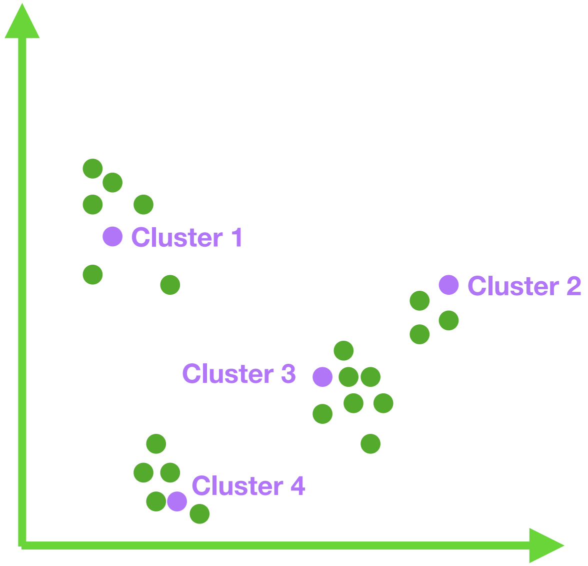

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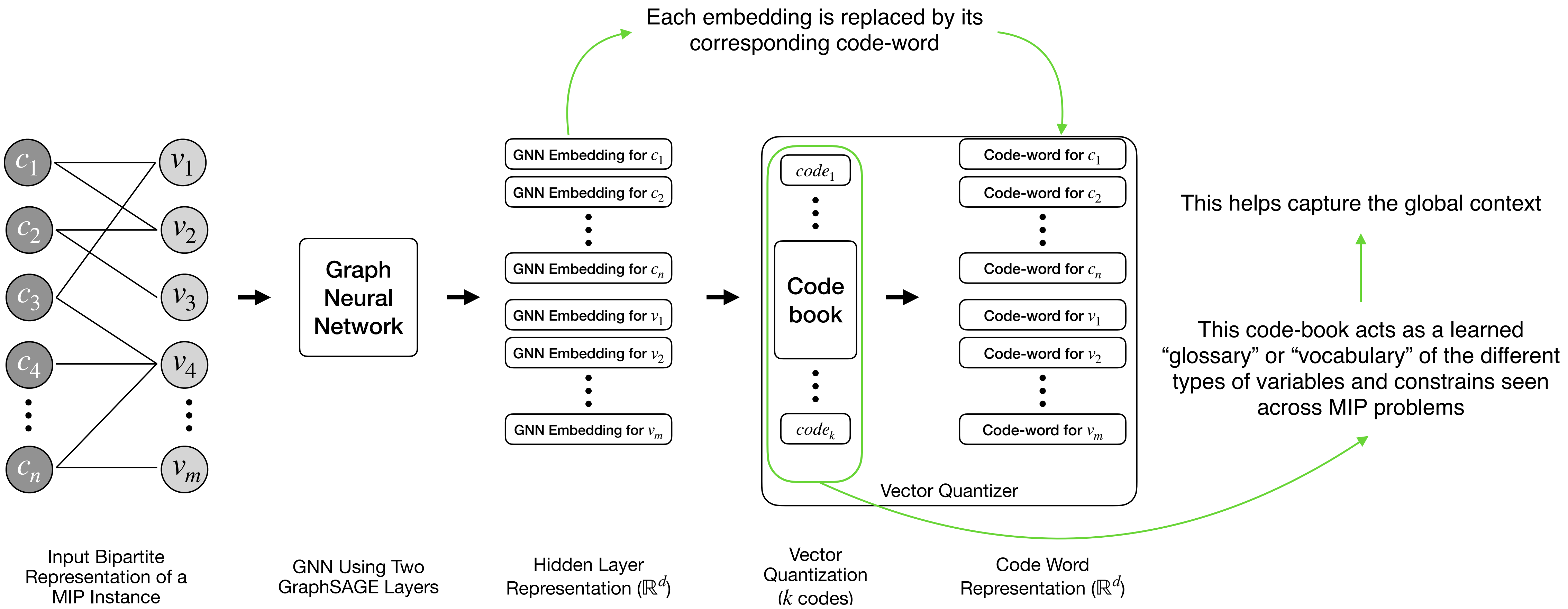
The index of the cluster each data point belongs to is the **discrete index/code** assigned to that data point

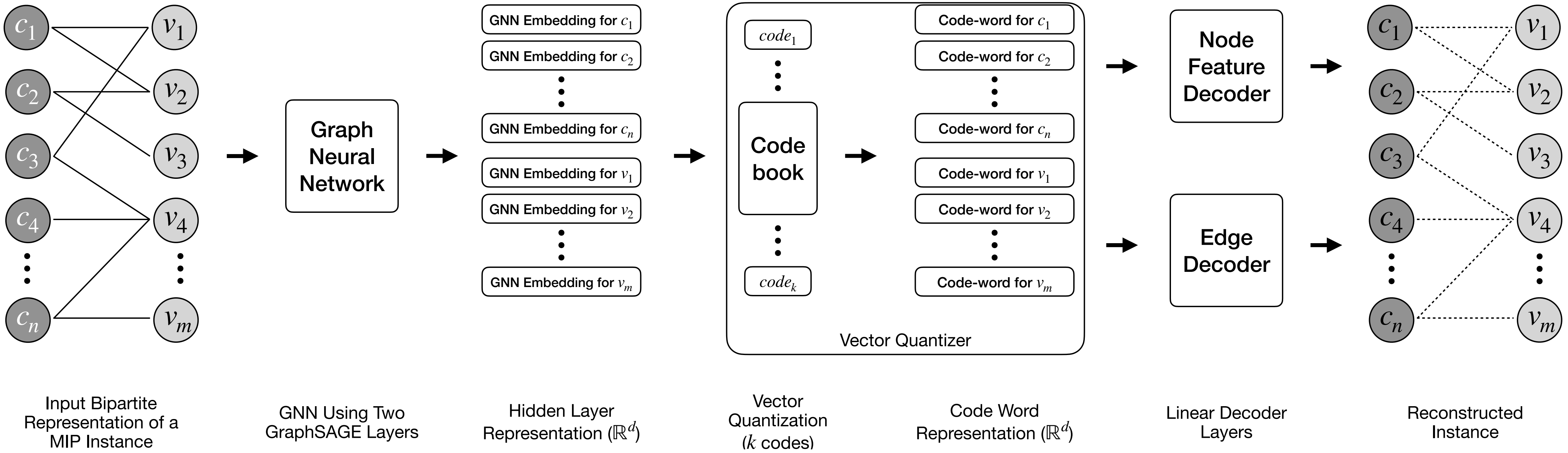
Methodology

- Back to overview



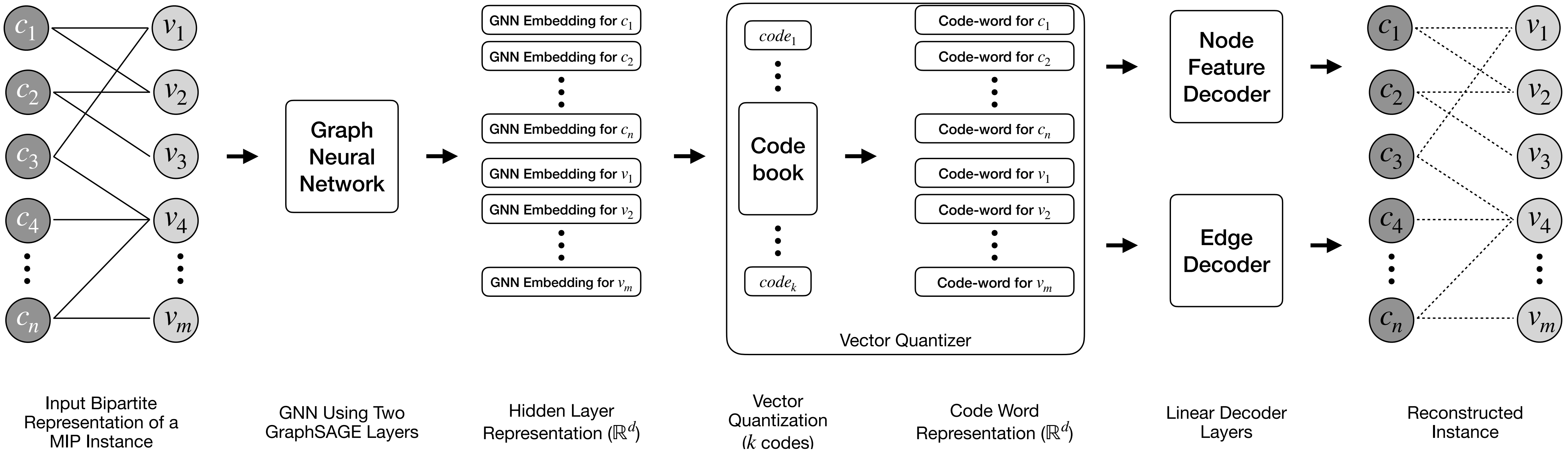
Methodology

- The code-words are then used to reconstruct the input graph structure and node features.



Methodology

Overall Architecture of Unsupervised Pre-training



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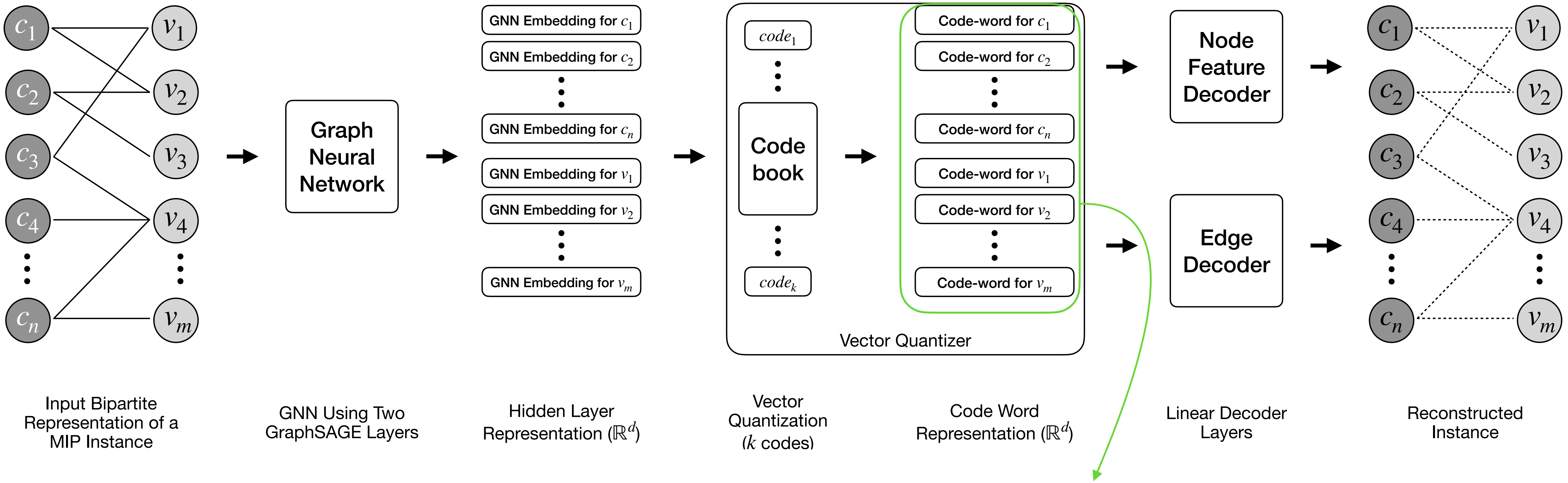
Overall Architecture of Unsupervised Pre-training

Observe that we get 2 types of embeddings



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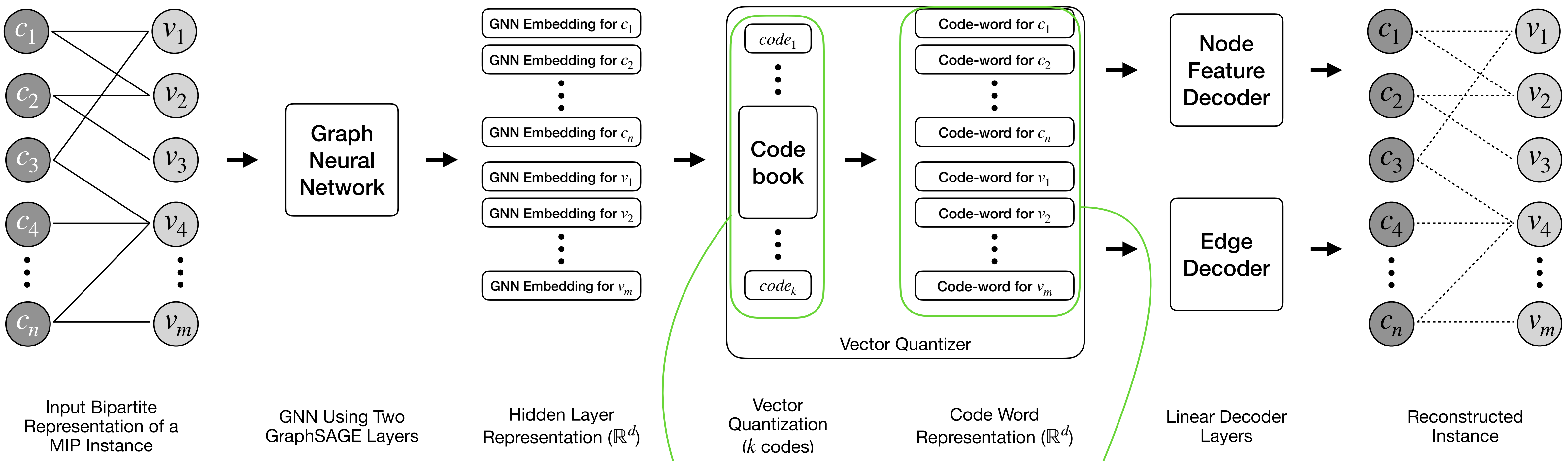
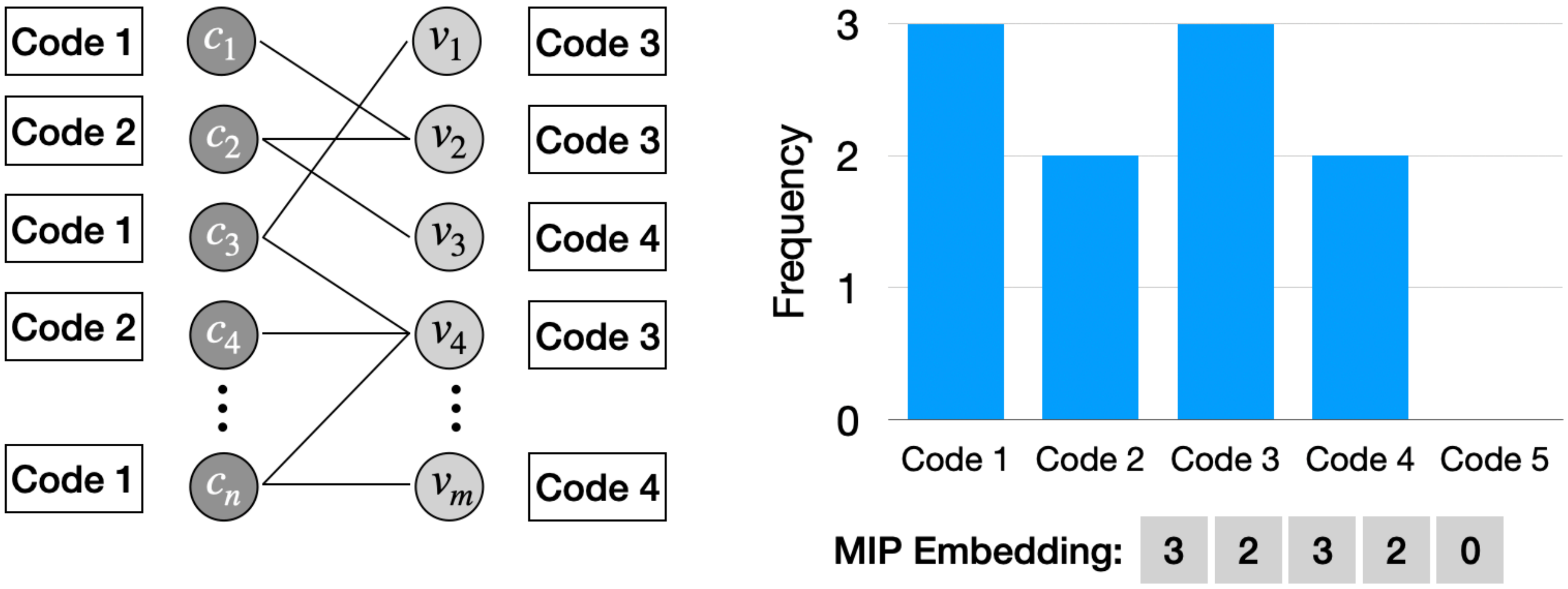


1. Embedding vector per variable and constraint
2. Distribution of codes assigned to get one vector per instance

Methodology

MIP Embedding Aside



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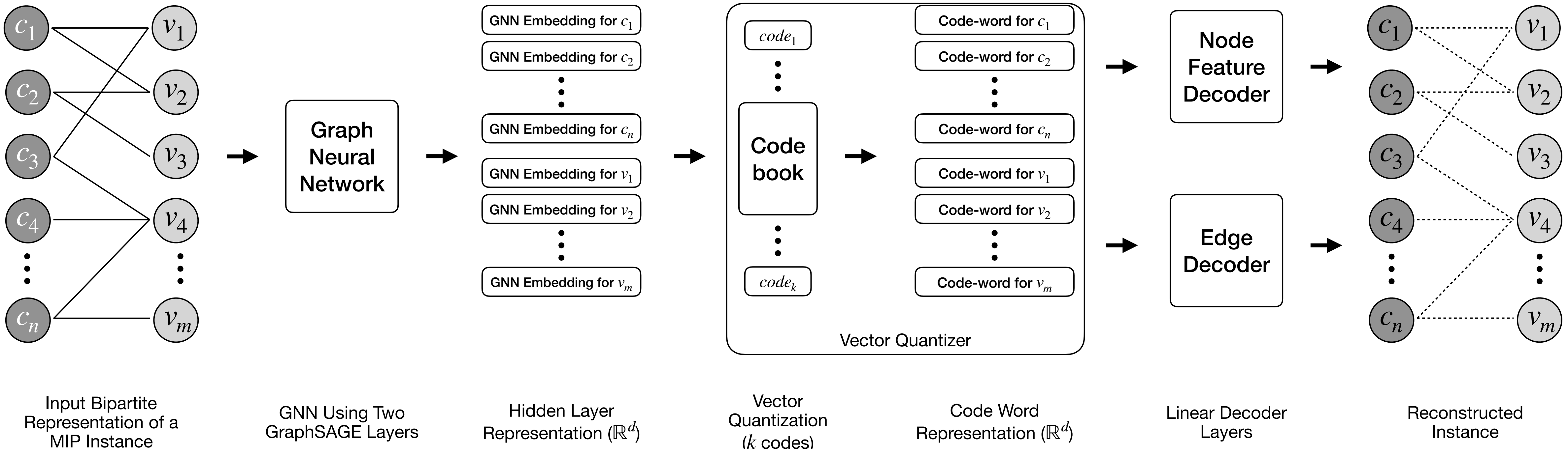

Datasets

- MIPLIB
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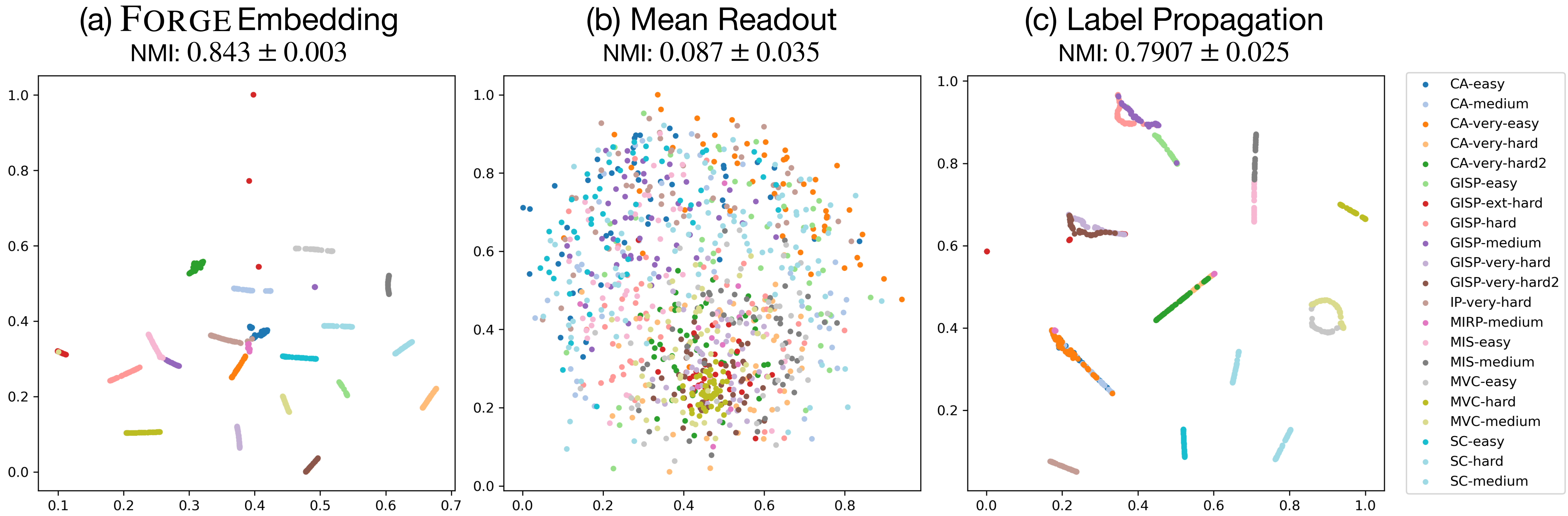
- Distributional MIPLIB
  - Set Cover (easy, medium, hard)
  - Maximum Independent Set (easy, medium)
  - Minimum Vertex Cover (easy, medium, hard)
  - Generalized Independent Set (easy, medium, hard, very-hard, very-hard2, ext-hard)
  - Combinatorial Auction (very-easy, easy, medium, very-hard, very-hard2)
  - Item Placement (very-hard)
  - Maritime Inventory Routing Problem (medium)
- 50 instances from each category - 1050 instances used as the test set

Visualizing MIP Instances from Unsupervised Pre-training



Takeaway:
FORGE can cleanly cluster out previously unseen MIP instances with the highest NMI

Supervised Fine-tuning - Integrality Gap

- Can we fine tune FORGE to predict the integrality gap?

Supervised Fine-tuning - Integrality Gap

- What is an *integrality gap*?

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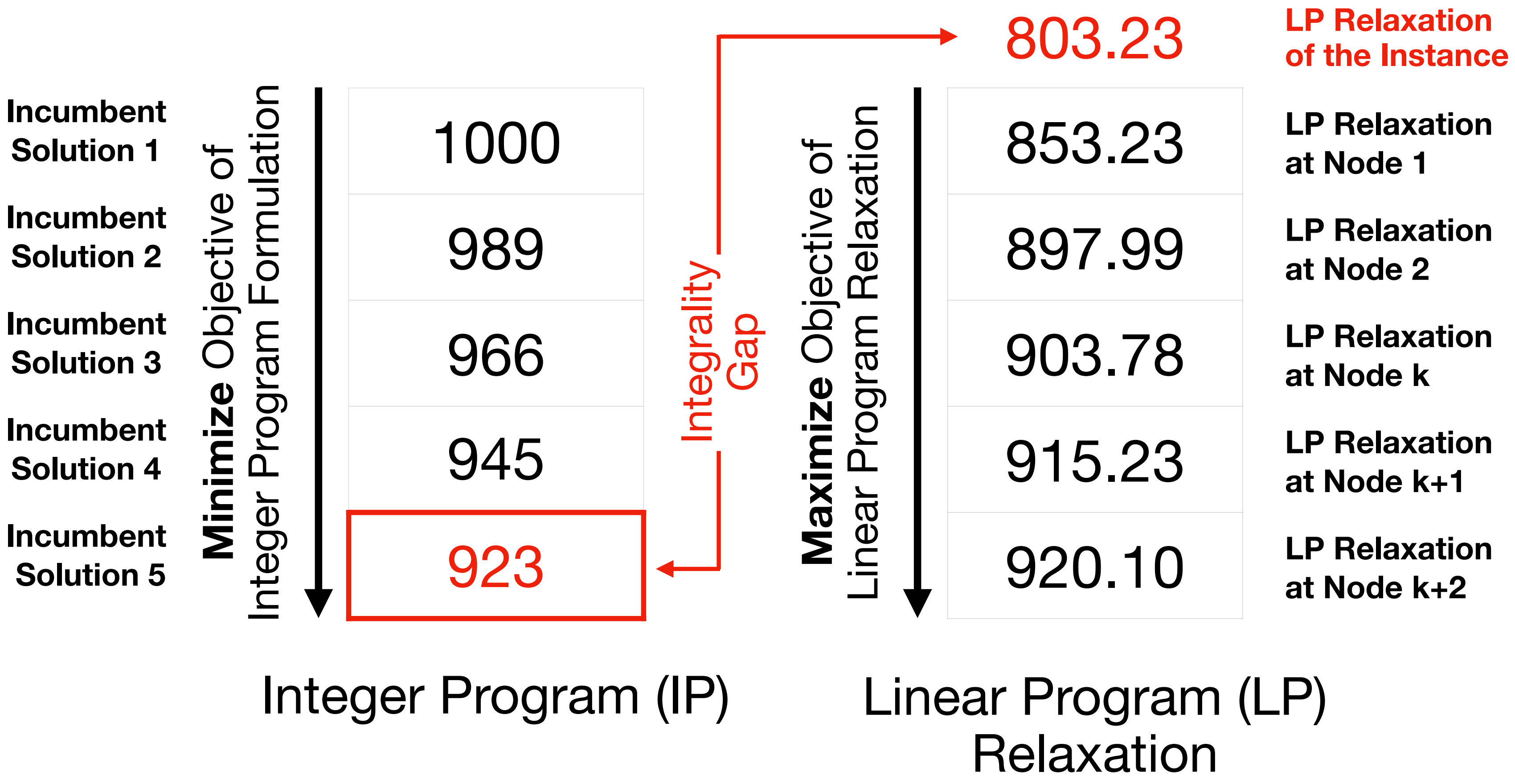

Supervised Fine-tuning - Integrality Gap

- We add a simple single layer prediction head to predict the integrality gap.
- The predicted gap is then used to compute a “pseudo-cut”.
    - This pseudo-cut is added as a constraint to a solver.
    - Note that a overestimation of the pseudo-cut would lead to a suboptimal solution.
- FORGE is pre-trained to learn the structures of all 1800 MIPLIB instances as well as 1050 Distributional MIPLIB instances.

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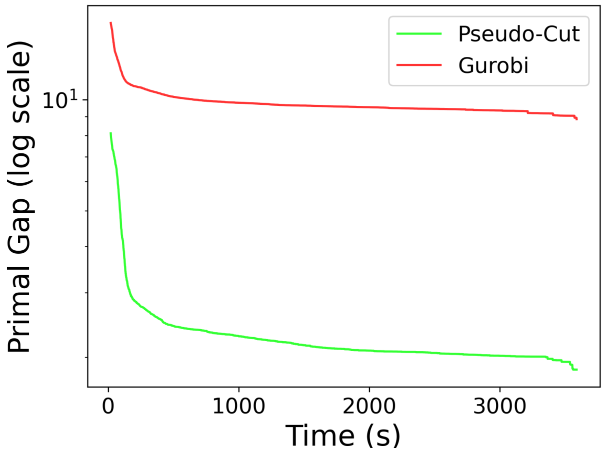
- FORGE is pre-trained to learn the structures of all 1800 MIPLIB instances as well as 1050 Distributional MIPLIB instances.
- **Fine Tuning Training Data**: CA (very-easy, easy, medium), SC (easy, medium, hard), and GIS (easy, medium, hard) with 50 instances for each. In total, we obtain a total of 450 training instances.

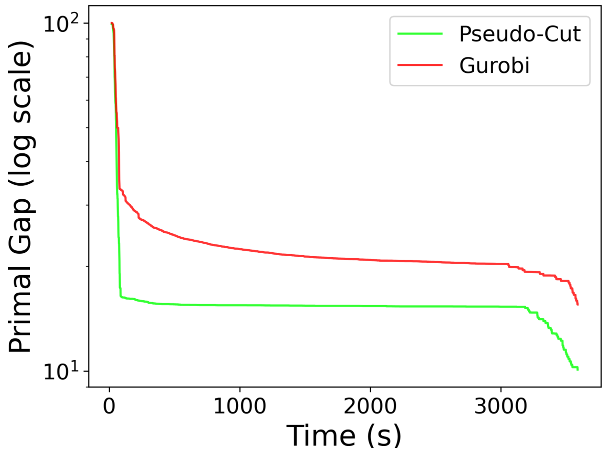
Results - Integrality Gap

Tests are run on 50 'very-hard' unseen instances from Distributional MIPLIB.

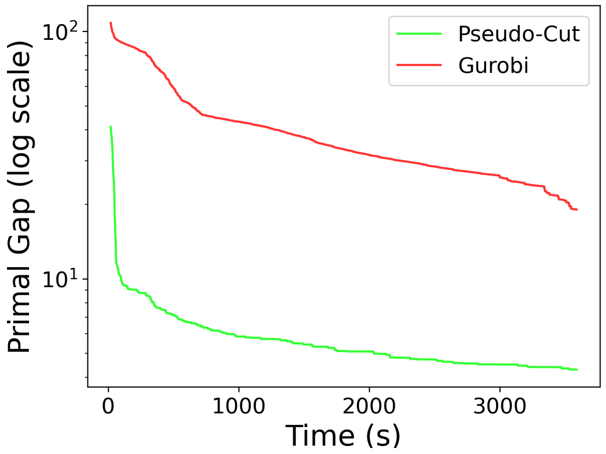
(a) Combinatorial Auction
Primal Gap Gain: 76.77%



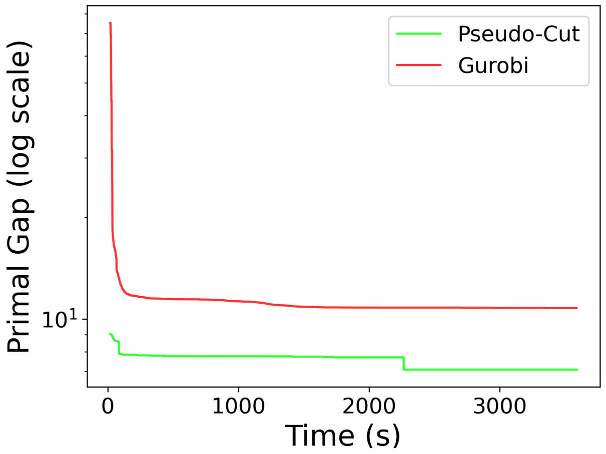
(b) Set Cover
Primal Gap Gain: 29.59%



(c) Generalized Ind. Set
Primal Gap Gain: 84.52%



(d) Minimum Vertex Cover
Primal Gap Gain: 32.38%



Takeaway:
FORGE generated pseudo-cuts lead to a significant decrease in primal gaps.

Supervised Fine-tuning - Warm Start

- Can we predict which variables will be part of the solution?
- How do we train this?
    - Binary Cross Entropy - commonly used approach but has a large class imbalance issue

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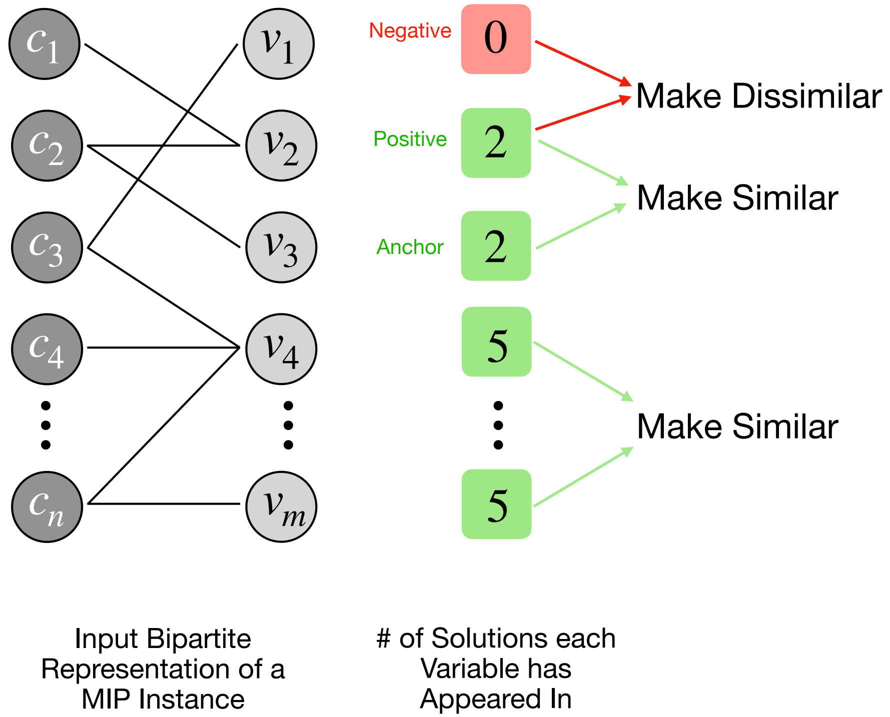
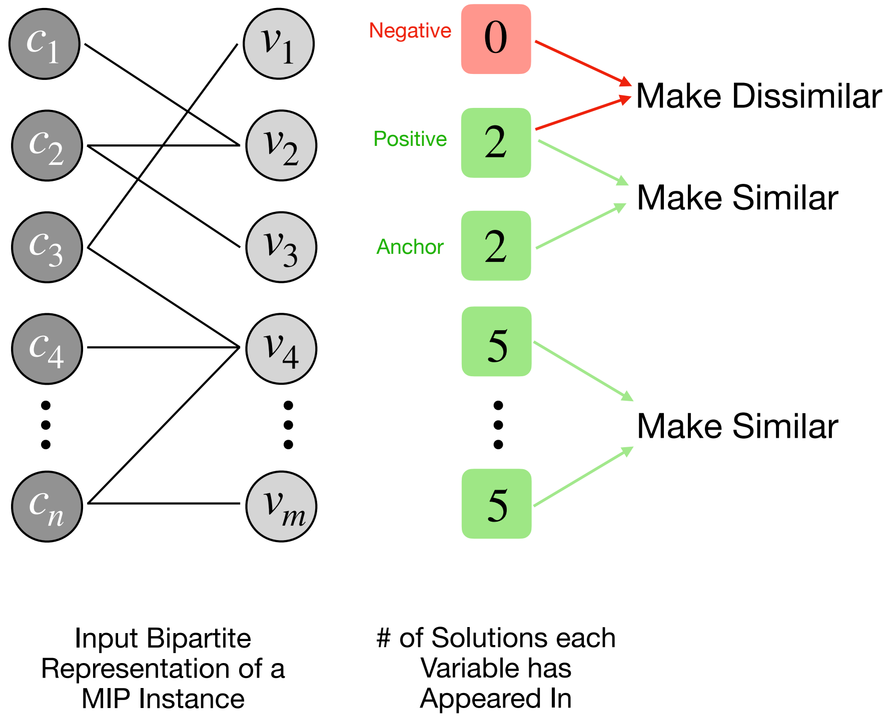
- How do we train this?
  - Binary Cross Entropy - commonly used approach but has a large class imbalance issue
  - Triplet Loss:
    - Generate 5 solutions
    - Make variables appearing in solutions similar to each other
    - Variables appearing in **none** of the solutions are used as negative variables
    - Negative variables are further filtered as variables that don't appear in any solution but are closest to positive variables in **unsupervised embedding space**



Supervised Fine-tuning - Warm Start

- **Fine Tuning Training Data**: 100 instances each from CA (easy, medium), SC (easy, medium, hard) and GIS (easy, medium) for a total of 700 training instances.



Results - Warm Start

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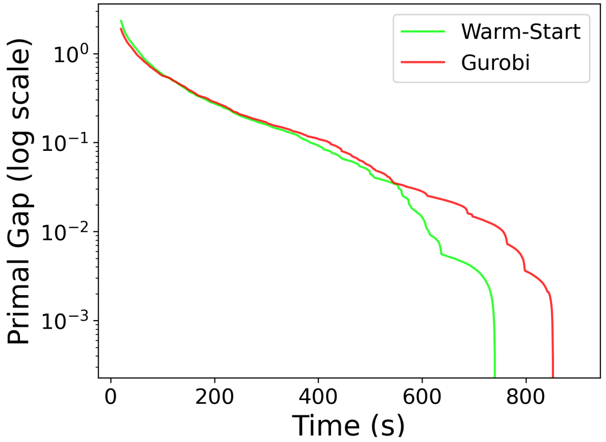
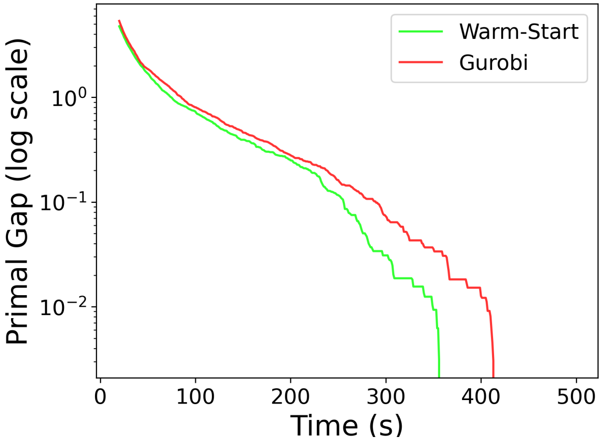
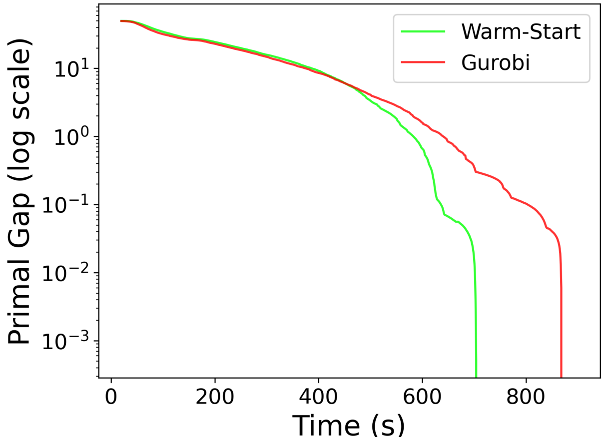
(a) Combinatorial Auction
Primal Gap Gain: 31.16%



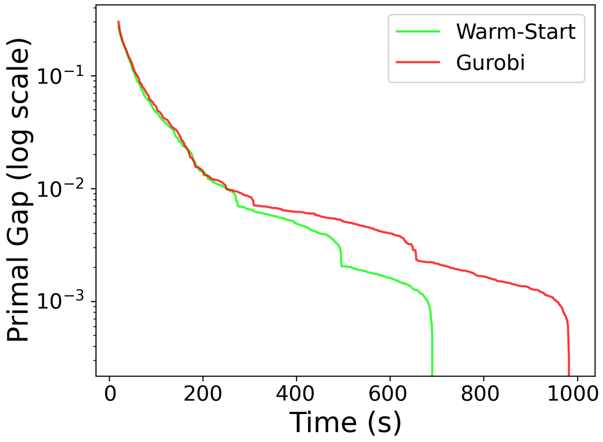
(b) Set Cover
Primal Gap Gain: 39.17%



(c) Generalized Ind. Set
Primal Gap Gain: 31.62%



(d) Minimum Vertex Cover
Primal Gap Gain: 48.75%



Takeaway:
Gurobi with FORGE generated warm starts leads to a significant decrease in primal gaps and faster run times.

Additional Results

Integrality Gaps

- Li et al. [1] train a GNN on 38,256 instances from 643 generated problem types and test on 11,584 instances spanning 157 problem types.
- We train on **no additional data** and test on 17,500 previously unseen instances spanning 400 problem types, from the dataset in [1].
- FORGE achieves a mean deviation of 18.63% in integrality gap prediction, outperforming the 20.14% deviation reported.

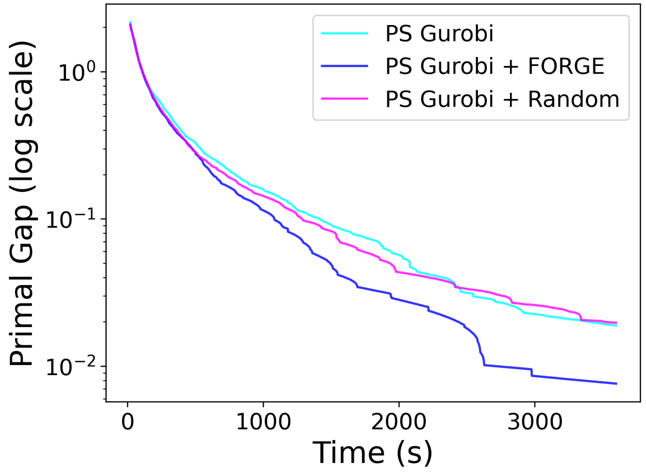
[1] Li, S., Kulkarni, J., Menache, I., Wu, C. and Li, B., Towards Foundation Models for Mixed Integer Linear Programming. In *The Thirteenth International Conference on Learning Representations*.

Additional Results

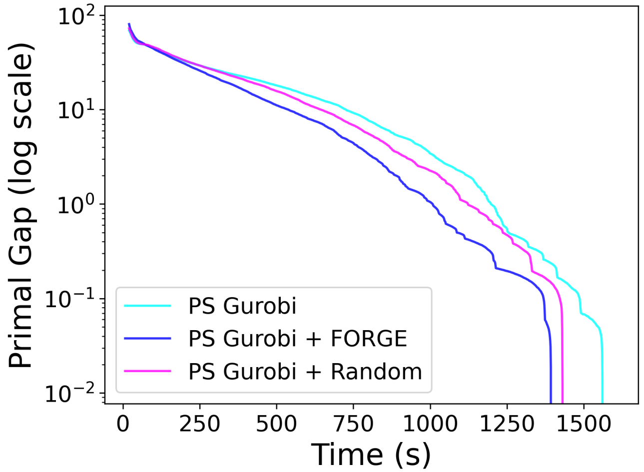
Warm Starts

- We also compare warm starts with PS-Gurobi [2].
    - FORGE embeddings for each variable and constraint are added to PS-Gurobi.
    - Since adding these embeddings increases model complexity significantly, we also add random embeddings of the same size to ensure any gains are **not due to larger model size**.
    - FORGE + PS-Gurobi outperforms the original variant in terms of primal gap and run time.

(a) Combinatorial Auction
Primal Gap Gain: 41.07%



(b) Generalized Ind. Set
Primal Gap Gain: 50.51%



[2] Han, Q., Yang, L., Chen, Q., Zhou, X., Zhang, D., Wang, A., Sun, R. and Luo, X., A GNN-Guided Predict-and-Search Framework for Mixed-Integer Linear Programming. In The Eleventh International Conference on Learning Representations.

FORGE in Practice

- Integrality Gap
    - Easiest to use
    - Pass in a .lp or a .mps file - get back a real number
    - Add constraint that the integer solution is greater than the real number generated
- Warm Starts
    - Pass in a .lp or a .mps file - get back a list of variables
    - Set initial values of variables - solver specific - for example, hint values in Gurobi

Summary

- FORGE uses a **single** model with **~3.25M parameters**.
- FORGE can generate one embedding vector per MIP instance and can effectively cluster unseen instances and place them within the space of all MIP instances.
- FORGE can be fine tuned on a variety of tasks for multiple problem types.
  - A single FORGE model can be used to predict **both** warm-starts as well as integrality gaps for a variety of problem type and difficulty pairs.

arXiv Paper

Thank you!
Questions?