



Generative Graph Pattern Machine

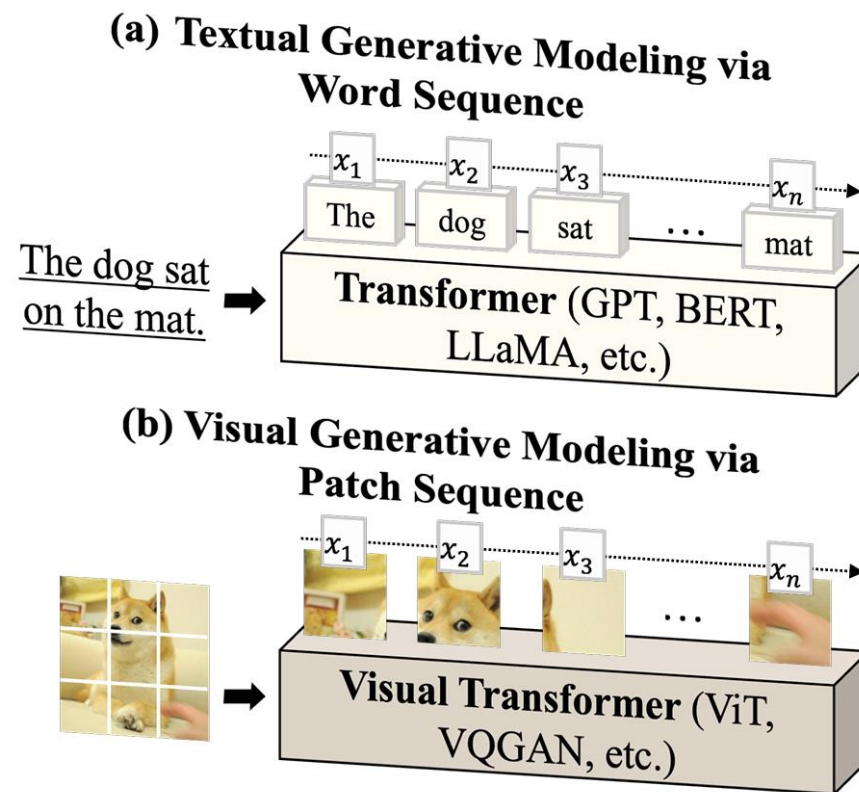
Zehong Wang, Zheyuan Zhang, Tianyi Ma,
Chuxu Zhang, Yanfang Ye

University of Notre Dame, University of Connecticut

Speaker: Zehong Wang

What Are Vocabularies in Text and Image?

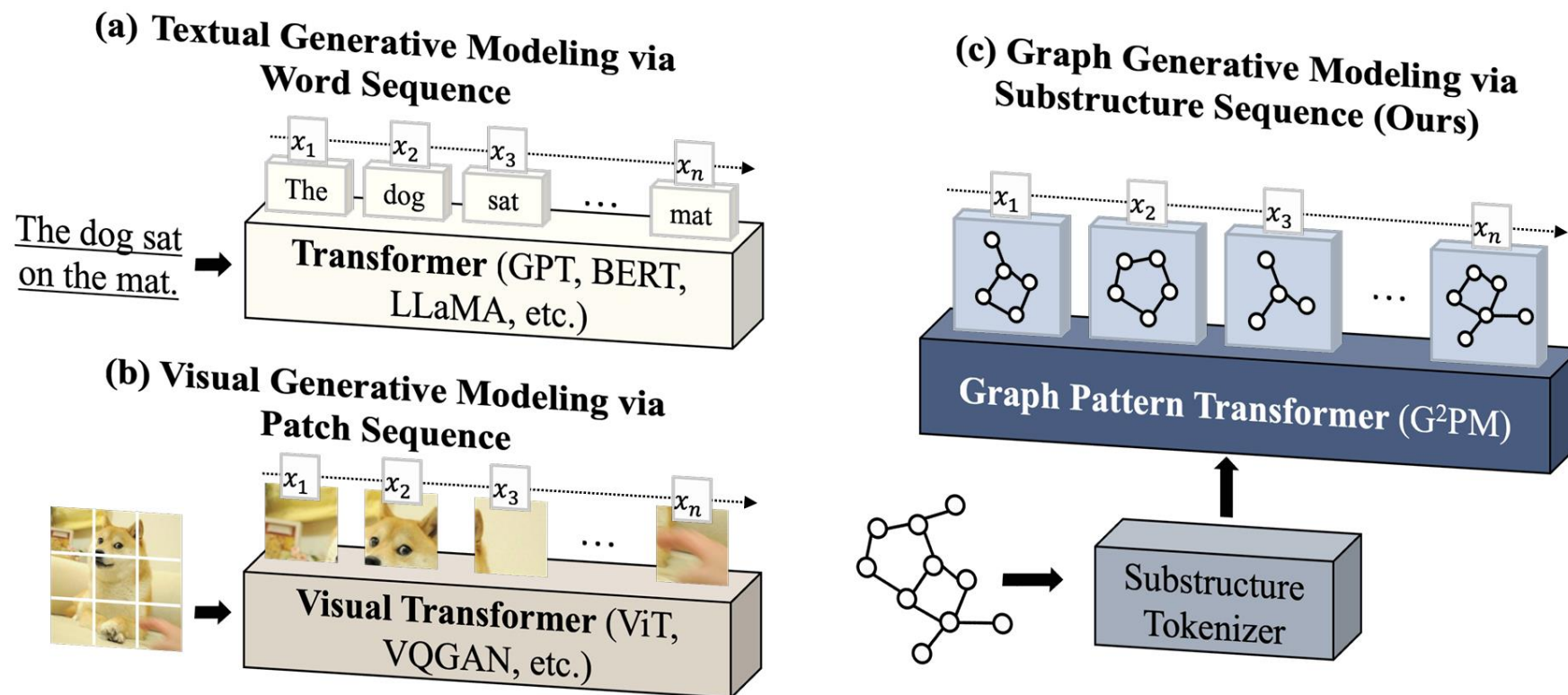
- Text vocabulary preserves textual tokens
- Image vocabulary preserves image concepts.



Extending Vocabulary to Graphs

- **Graph vocabulary preserves substructure information.**

- ✧ Social network: triangle structure, star-like structure
- ✧ Molecule graph: ring-like structure, like benzene rings.



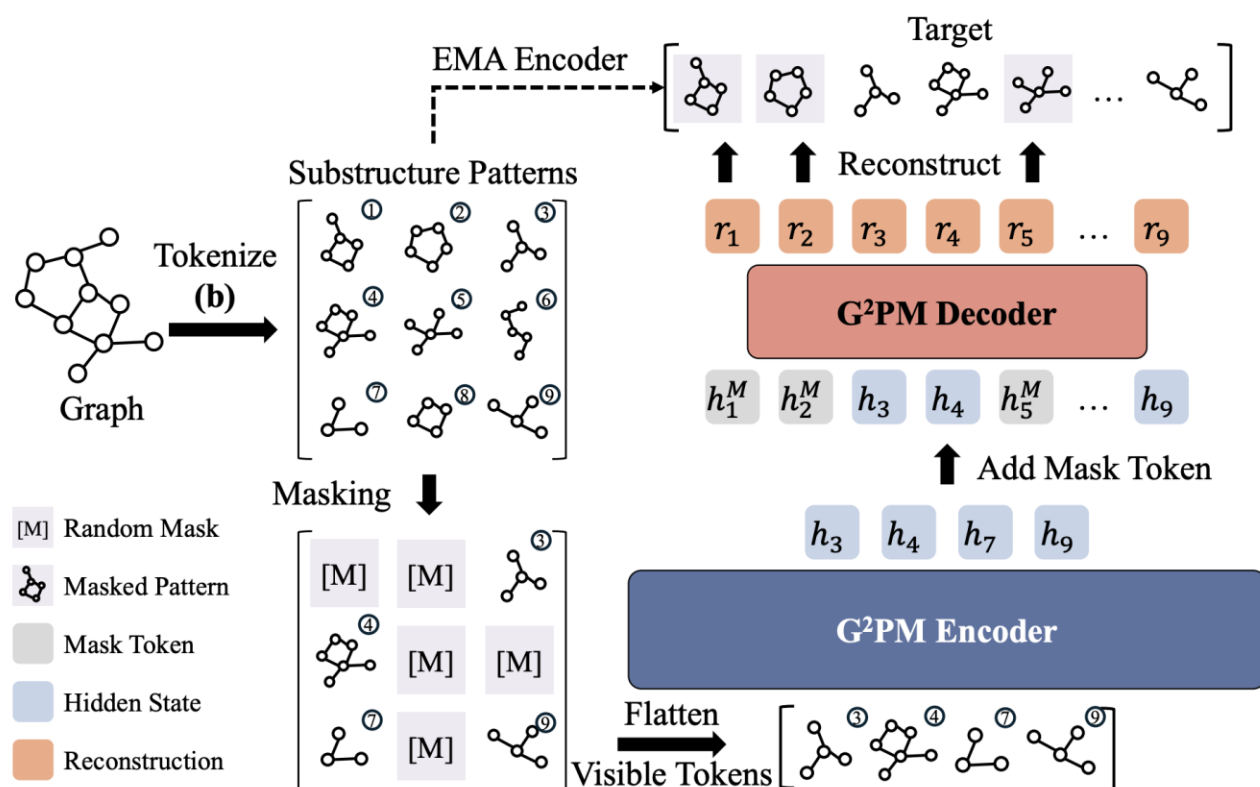
Wang, Z., Zhang, Z., Ma, T., Chawla, N. V., Zhang, C., & Ye, Y. Beyond Message Passing: Neural Graph Pattern Machine. In Forty-second International Conference on Machine Learning.

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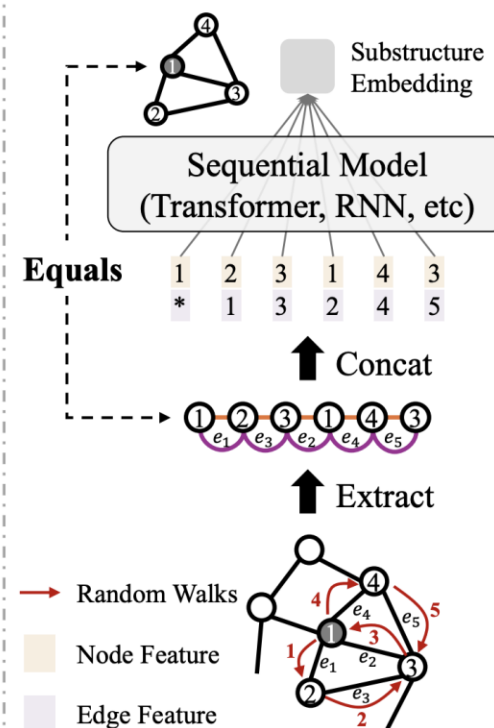
- Learning from graph vocabularies

Masked token prediction enables self-supervised learning.

(a) Pre-Training Generative Graph Pattern Machine (G²PM)



(b) Tokenizing Substructures via Random Walks

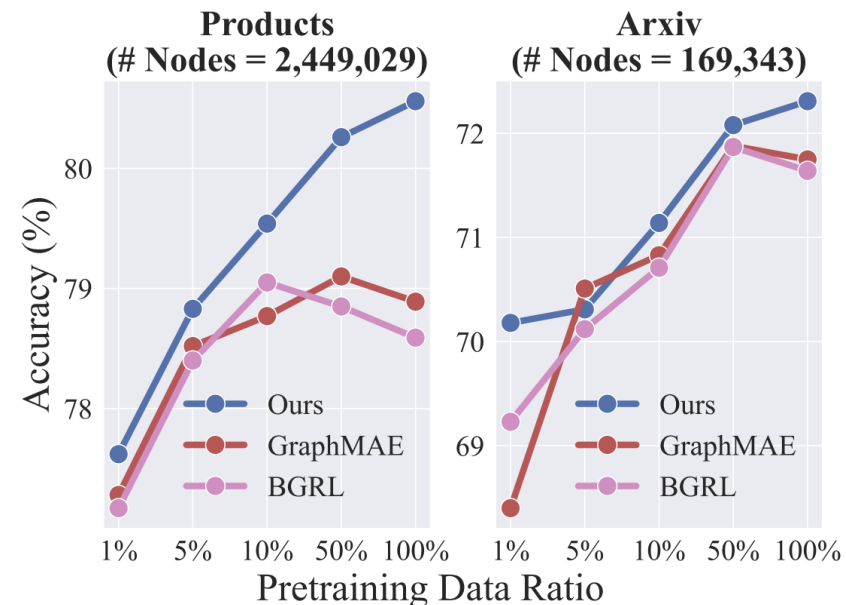
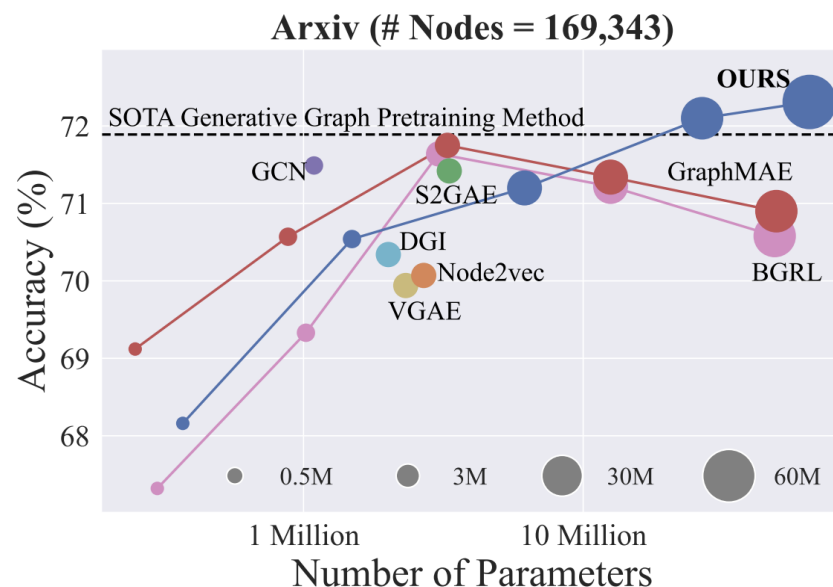


Generative Graph Pattern Machine (G²PM) [NeurIPS'25]

- G²PM Enable Scalability on Graphs

- ⌘ **Model Scaling:** G²PM achieves scalability up to 60M parameters, whereas existing methods saturate on 3M parameters.

- ⌘ **Data Scaling:** G²PM shows robust improvements with more training data, whereas existing methods peak at small data ratios.



Generative Graph Pattern Machine (G²PM) [NeurIPS'25]

- G²PM Enable Scalability on Graphs
- **G²PM Enable Transferability Across Graphs**
 - ⌘ Cross-domain transfer learning.
 - ⌘ Cross-domain pre-training.

Table 4: **Cross-domain transferability** performance across diverse source and target datasets. Parentheses indicate the performance gap compared to training from scratch on the target graph.

Source	Arxiv		HIV	
Target	Products	HIV	Arxiv	PCBA
GNN [55, 68]	78.3 (1.2 ↓)	70.1 (5.7 ↓)	71.1 (1.0 ↓)	71.9 (1.6 ↑)
GPM [63]	82.0 (0.6 ↓)	74.3 (2.7 ↓)	71.4 (1.5 ↓)	76.4 (1.3 ↑)
BGRL [48]	78.8 (0.2 ↑)	72.5 (3.8 ↓)	68.6 (1.9 ↓)	72.9 (0.6 ↓)
GraphMAE [21]	77.5 (1.4 ↓)	74.7 (3.1 ↓)	69.9 (1.9 ↓)	73.4 (0.2 ↑)
G ² PM	81.3 (0.7 ↑)	76.8 (1.9 ↓)	72.6 (0.3 ↑)	77.9 (2.3 ↑)

Table 5: **Cross-domain pre-training** results on text-attributed graphs processed by [32], where node features are aligned via a textual encoder.

Pretrain	Arxiv + FB15K237 + ChemBL		
Downstream	Arxiv (Academia)	FB15K237 (Knowledge Graph)	HIV (Molecule)
BGRL [48]	70.8 ± 0.2	86.5 ± 0.3	68.5 ± 1.6
GraphMAE [21]	70.3 ± 0.3	87.8 ± 0.4	64.1 ± 0.5
OFA [32]	71.4 ± 0.3	84.7 ± 1.3	72.0 ± 1.6
GFT [60]	71.9 ± 0.1	89.3 ± 0.2	72.3 ± 2.0
G ² PM	72.5 ± 0.1	88.9 ± 0.5	74.1 ± 1.3

Wang, Z., Zhang, Z., Ma, T., Zhang, C., & Ye, Y. (2025). Scalable Graph Generative Modeling via Substructure Sequences. NeurIPS 25.