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A Comprehensive Benchmark on Spectral GNNs: The Impact on Efficiency, Memory, and Effectiveness

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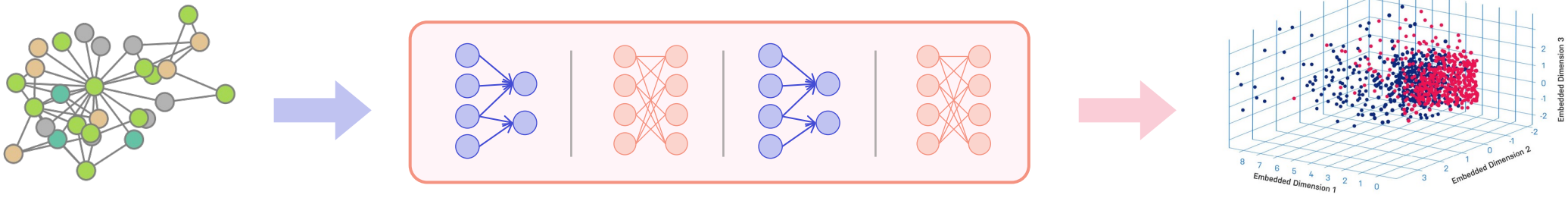
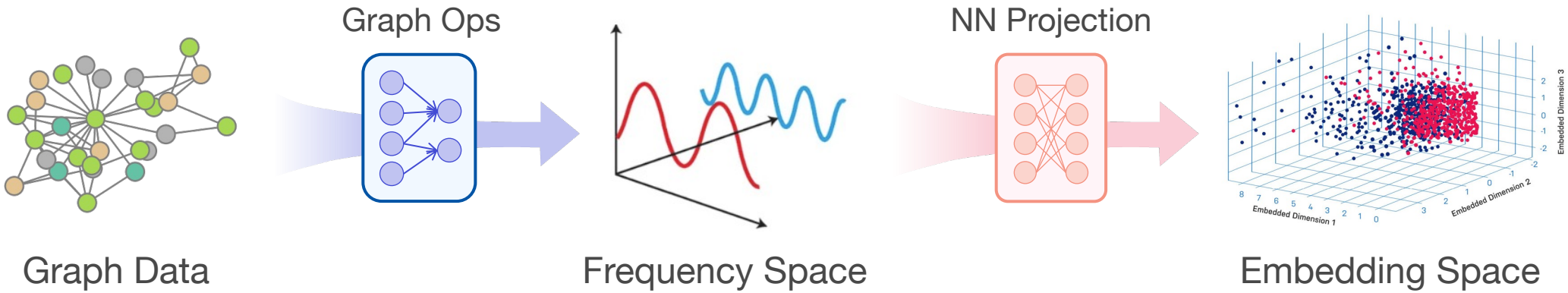
UBC

Background: Spectral GNN

(Spatial) GNN



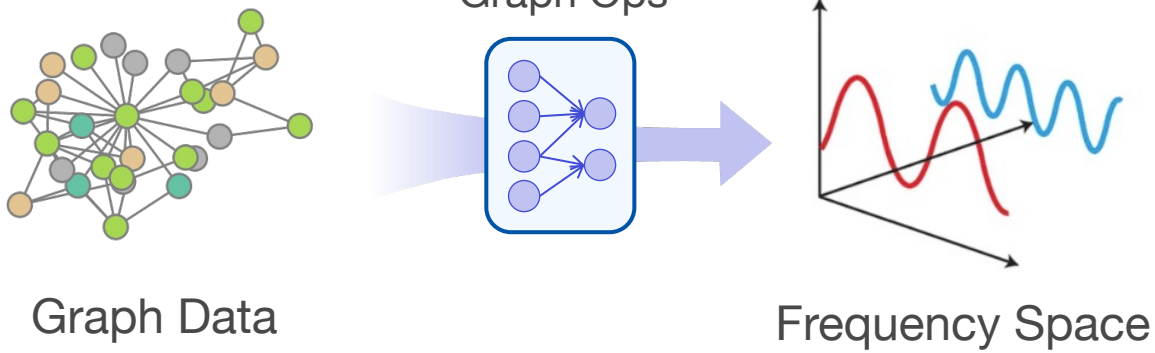
Spectral GNN



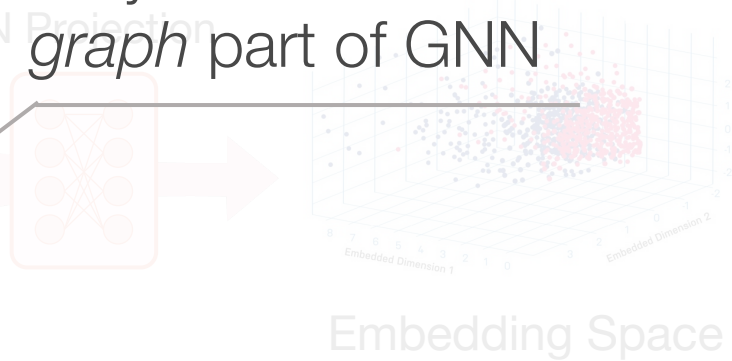
Chen et al. “Bridging the Gap between Spatial and Spectral Domains: A Unified Framework for Graph Neural Networks”. *ACM Comput. Surv.*. 2023.

Background: Spectral GNN

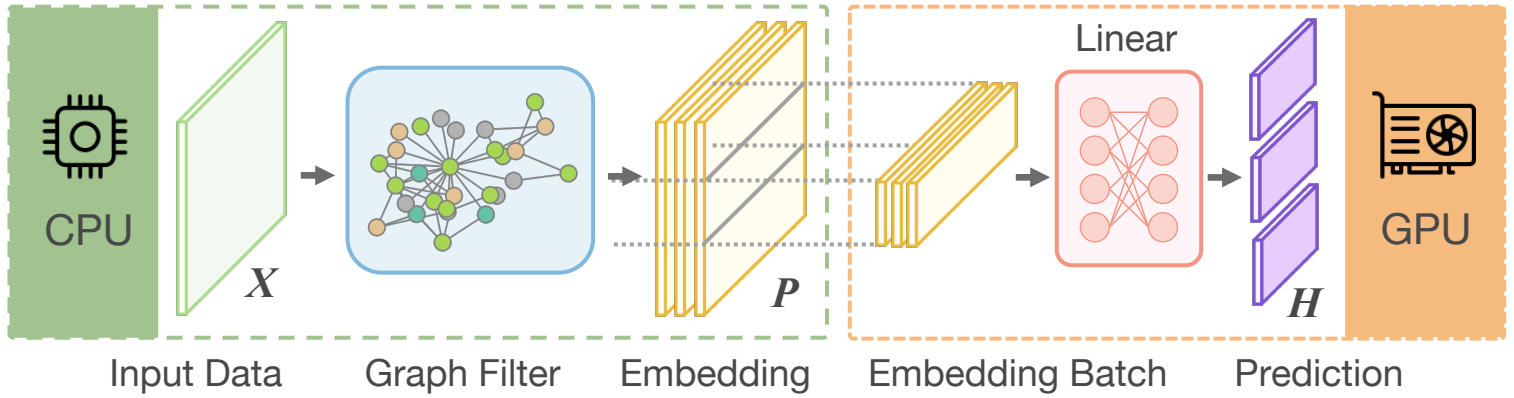
Spectral GNN



Only focus on the *graph* part of GNN



Decoupled Pipeline



Fast computation
& Memory-efficient

Taxonomy: Graph Filters

GCN $\quad H = (I + \tilde{A})^K \cdot X$

APPNP $\quad H = \sum_{k=0}^{K} \alpha(1-\alpha)^k \tilde{A}^k \cdot X$

GIN $\quad H = (\theta I + \tilde{A})^K \cdot X$

ChebNet $\quad H = \sum_{k=0}^{K} \theta_k T_{\text{Cheb}}^{(k)}(\tilde{A}) \cdot X$

BernNet $\quad H = \sum_{k=0}^{K} \frac{\theta_k}{2^K} \binom{K}{k} (2I - \tilde{L})^{K-k} \tilde{L}^k \cdot X$

AdaGNN $\quad H = (I + \Theta_k \tilde{A})^K \cdot X$

Spectral Filter:

$$g(\tilde{\mathbf{L}}) = \sum_{k=0}^{K} \theta_k T^{(k)}(\tilde{\mathbf{L}})$$

Filter — Graph

Taxonomy: Graph Filters

Fixed Filters

GCN APPNP

SGC G^2CN ...

Variable Filters

GIN ChebNet ...

BernNet GPRGNN

Composed Filters

AdaGNN ACMGNN

FAGNN FiGURe ...

Spectral Filter:

$$g(\tilde{\mathbf{L}}) = \sum_{k=0}^{K} \theta_k T^{(k)}(\tilde{\mathbf{L}})$$

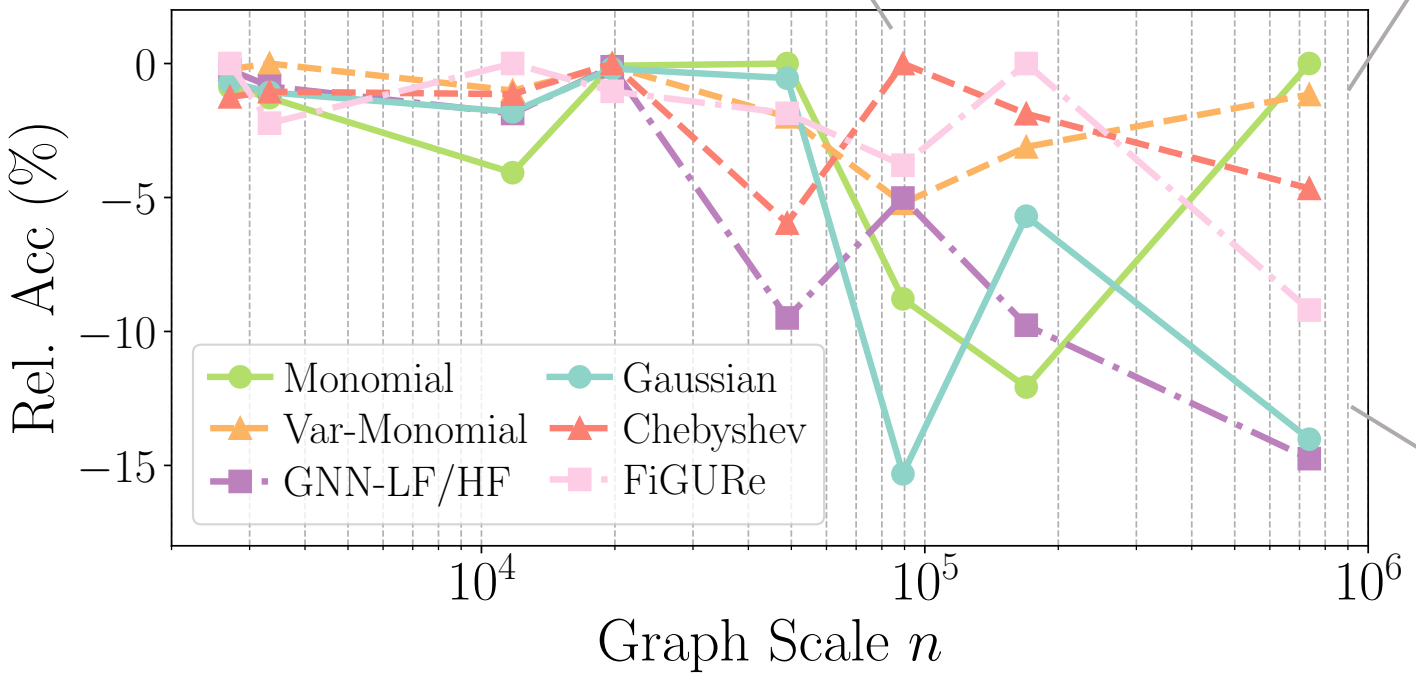
35 Covered GNNs

3 Filter Types

Results: Effectiveness & Scalability

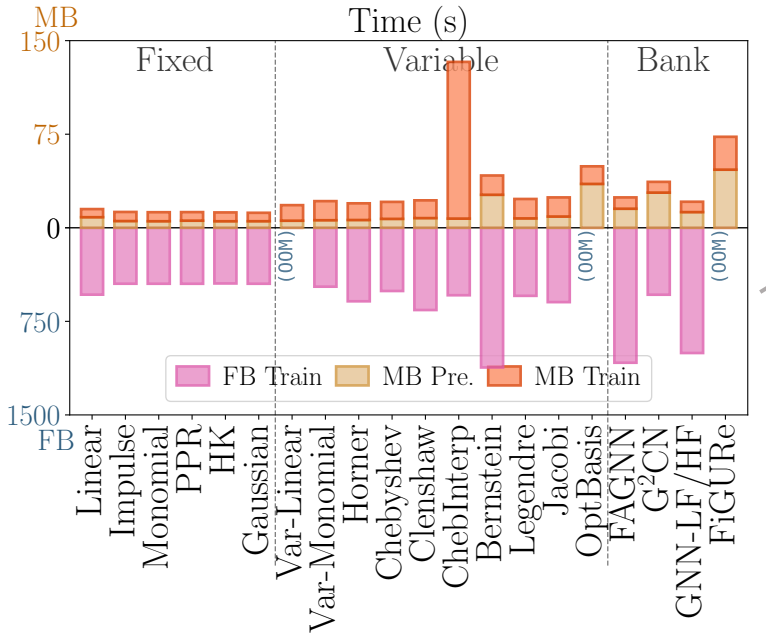
Efficacy and efficiency are not mutually exclusive.

Simple, invariable filters can also capture global view.



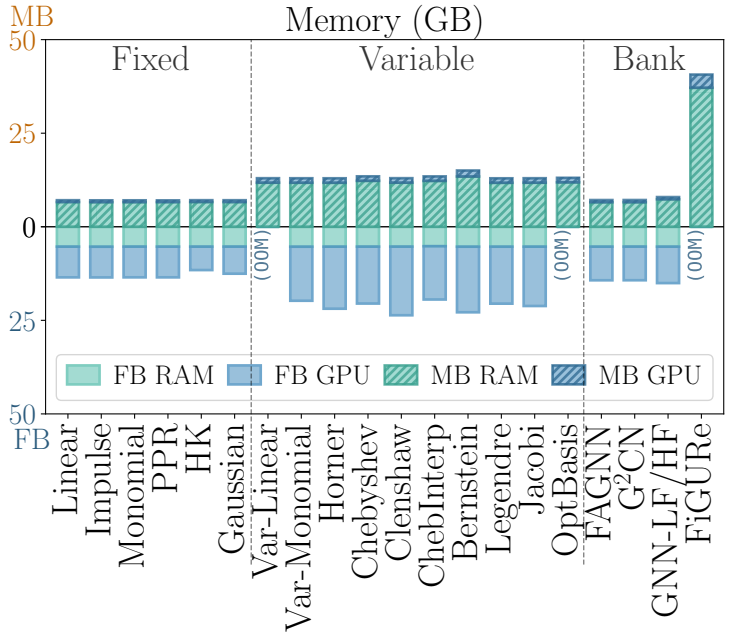
Global view is important for large-scale prediction.

Results: Efficiency & Memory



Time Efficiency: graph operation bottleneck shifts across data scale.

Memory Overhead: Mini-batch training facilitates device utilization.



THANK YOU

Paper

Code