CVPR 24' Tutorial

Unifying Spectral and Spatial Graph Neural Networks

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Agenda

- **First Half (1 hour 15 min)**
  - *Background*: **unified frameworks for GNN** (35 min)
  - *Preliminary*: **graph convolutions** (40 min)
  - BREAK (15min)
- **Second Half (1 hour)**
  - *Introduction*: **a new unified framework** (40 min)
  - *Future directions* (20min)
  - Q&A (15min)

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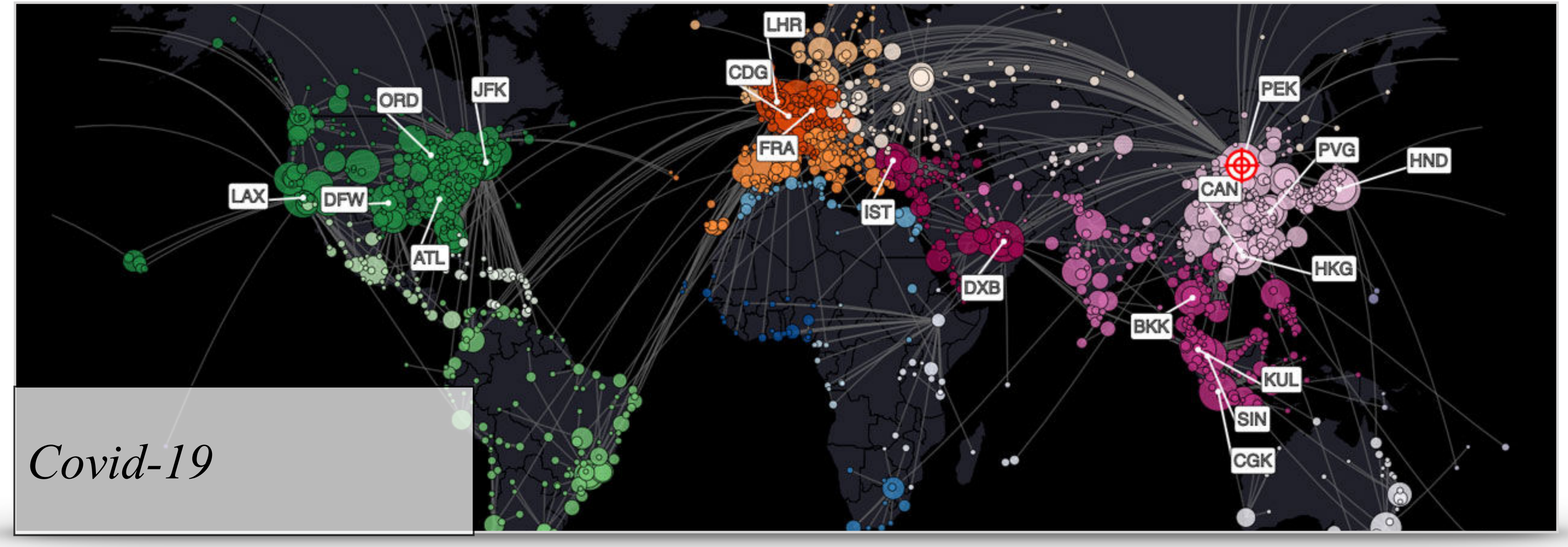
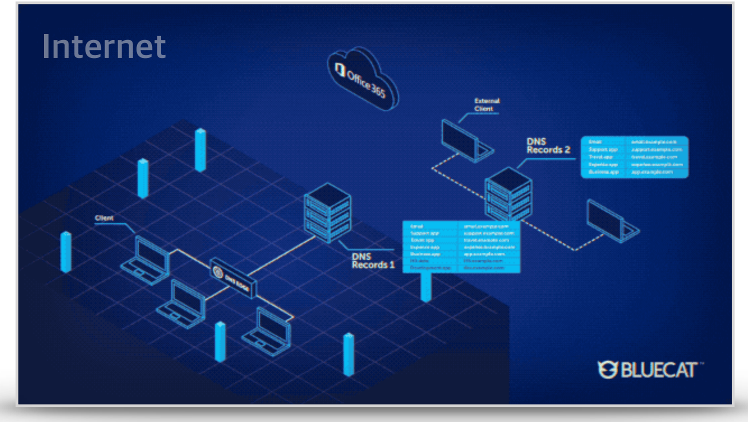
Graph is Pervasive

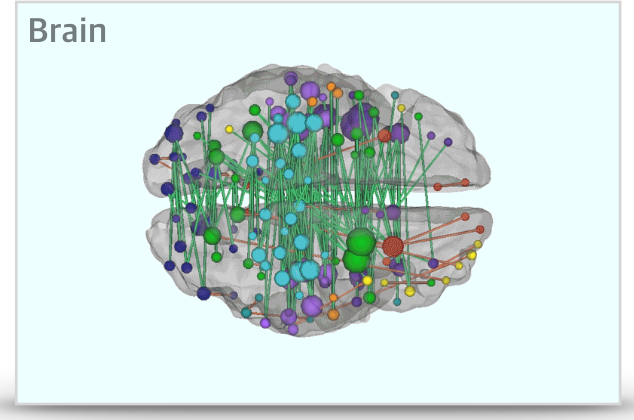


Covid-19

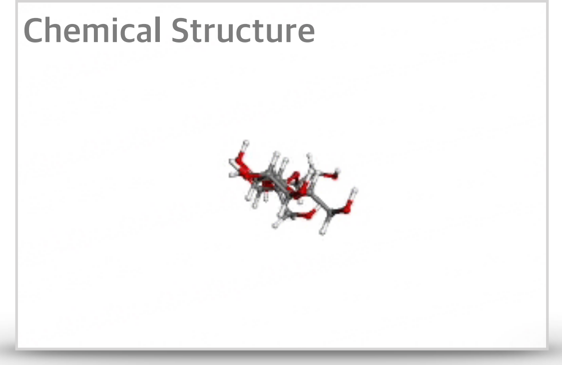
Social Networks



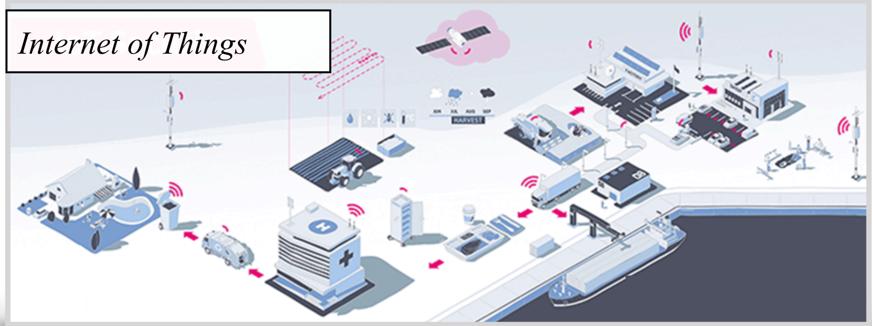
Internet



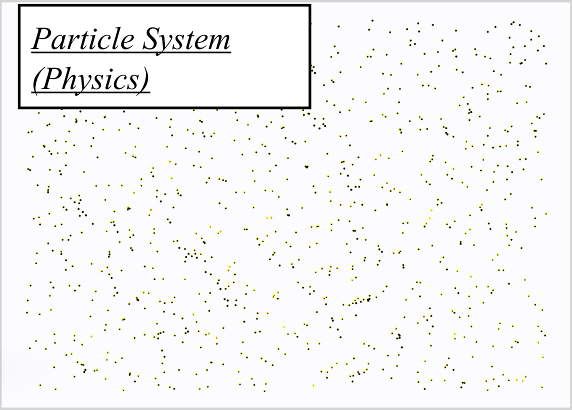
Brain



Chemical Structure

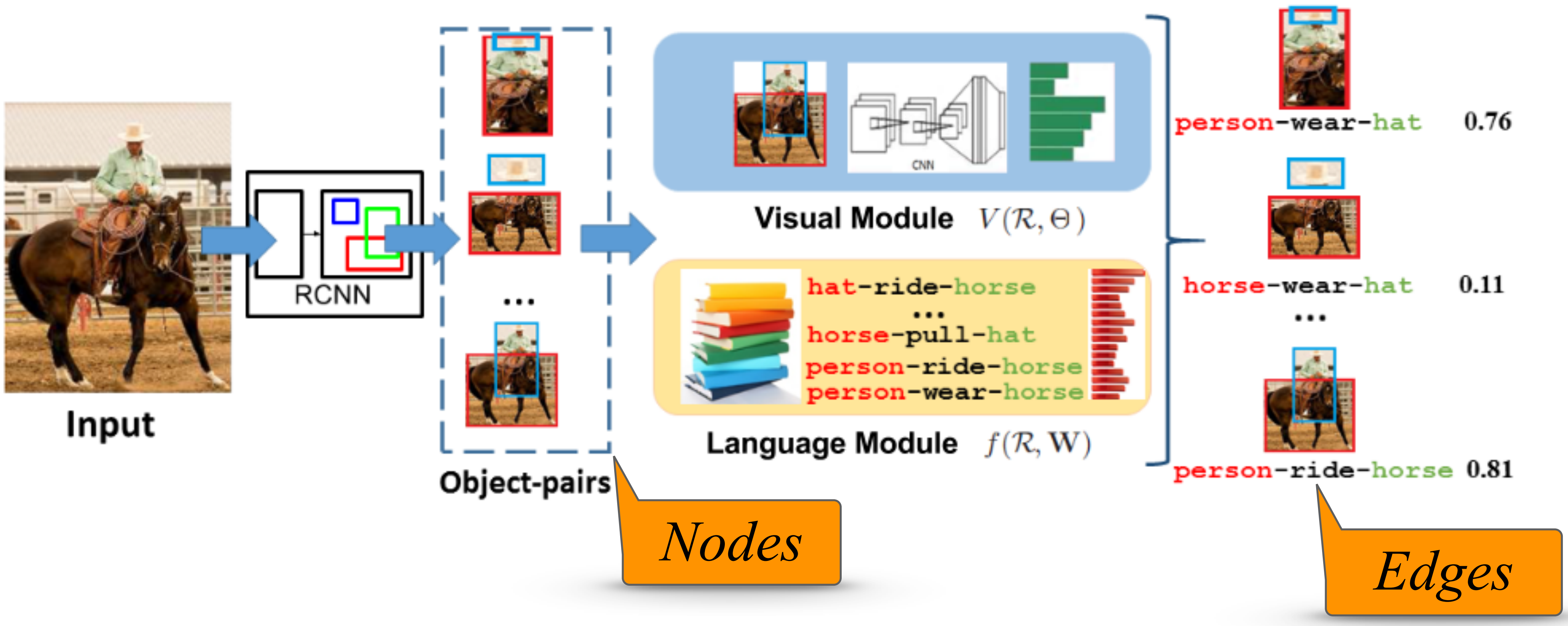


Internet of Things



Particle System (Physics)

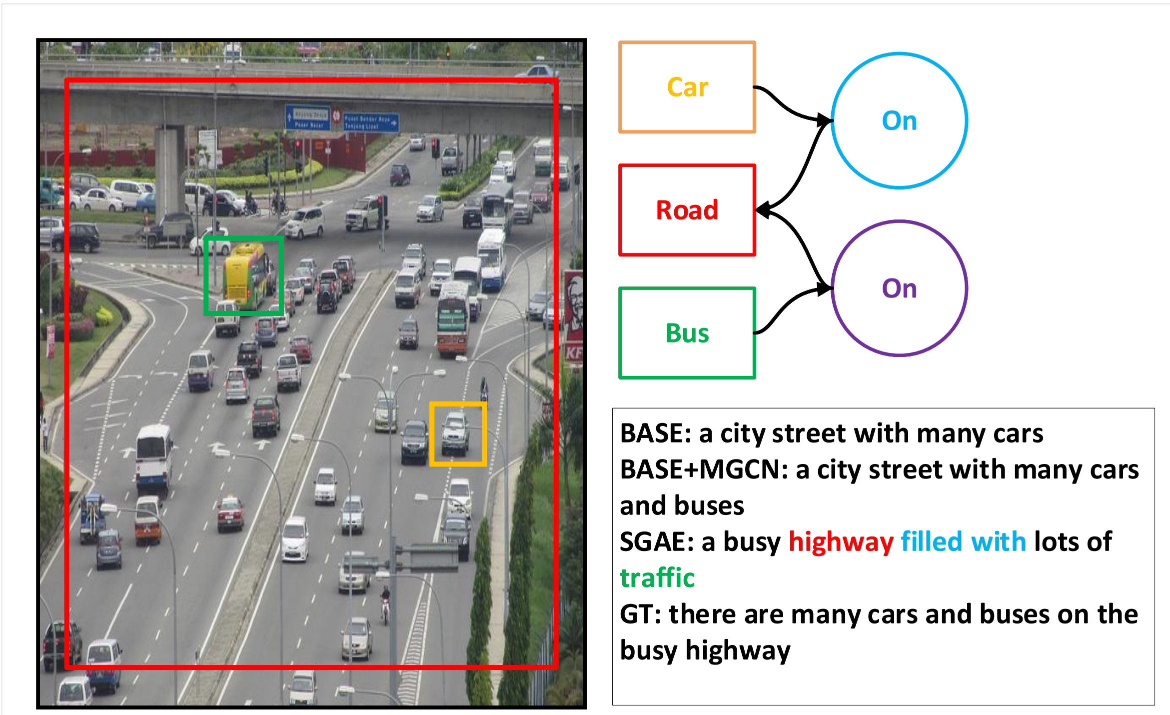
Graphs in CV



Graphs in Image Data:
Scene Graph

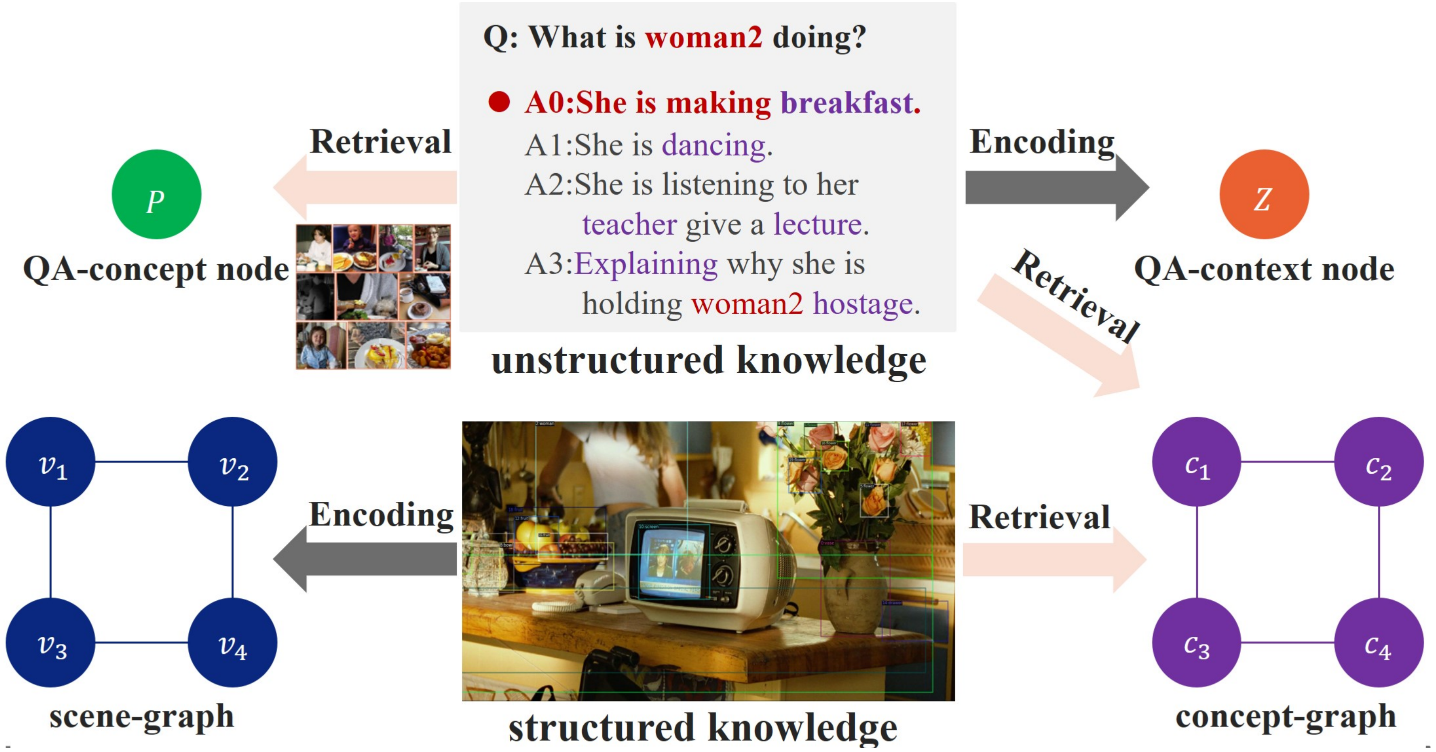
Lu, Cewu, et al. "**Visual relationship detection with language priors.**" ECCV, 2016.

Graphs in CV



Image/Video Captioning

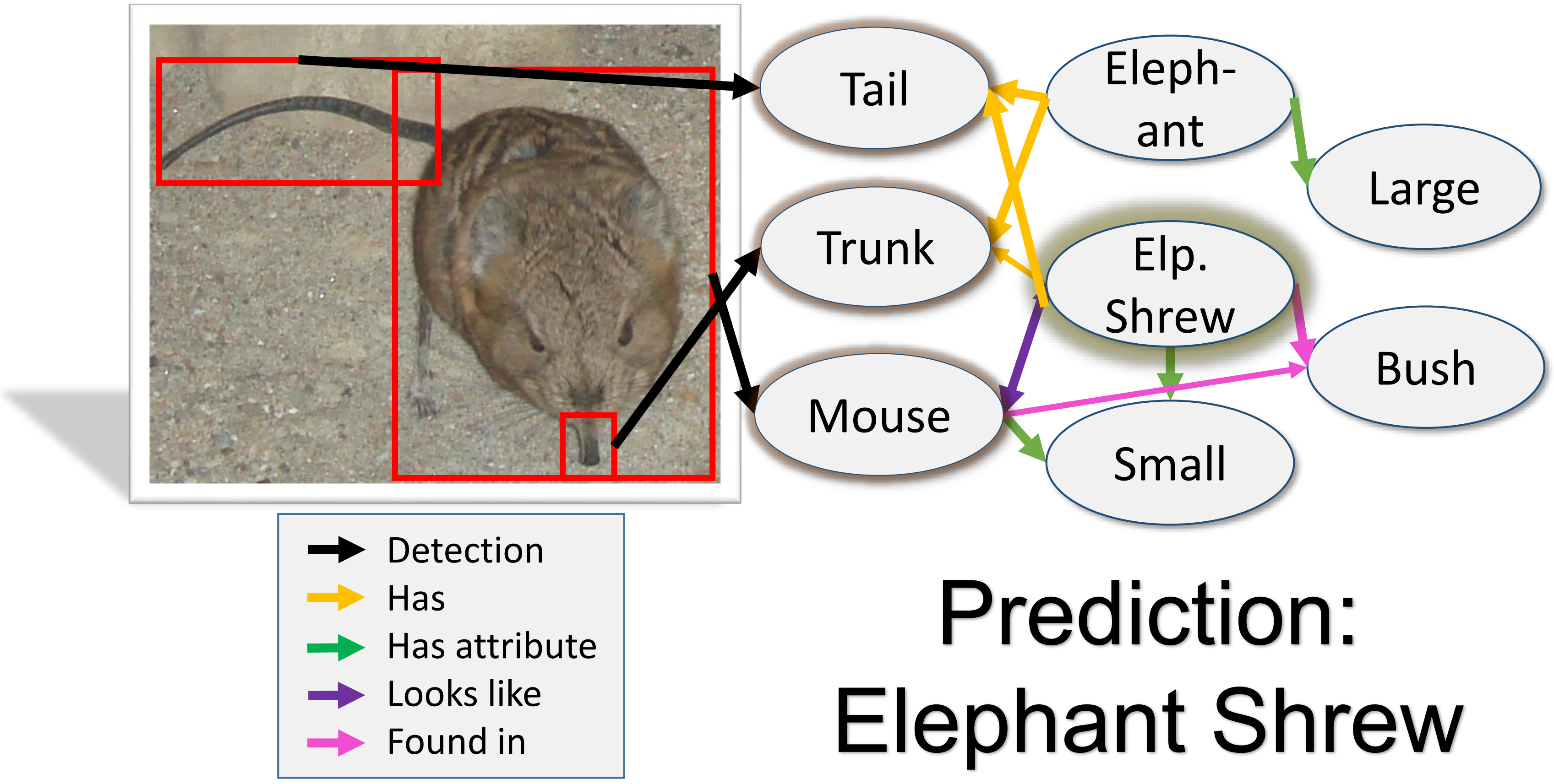
Yang, Xu, et al. "Auto-encoding scene graphs for image captioning." Proceedings of the IEEE/CVF conference on computer vision and pattern recognition. 2019.



Structured reasoning for visual Q&A

Wang, Yanan, et al. "Vqa-gnn: Reasoning with multimodal knowledge via graph neural networks for visual question answering." Proceedings of the IEEE/CVF International Conference on Computer Vision. 2023.

Graphs in CV

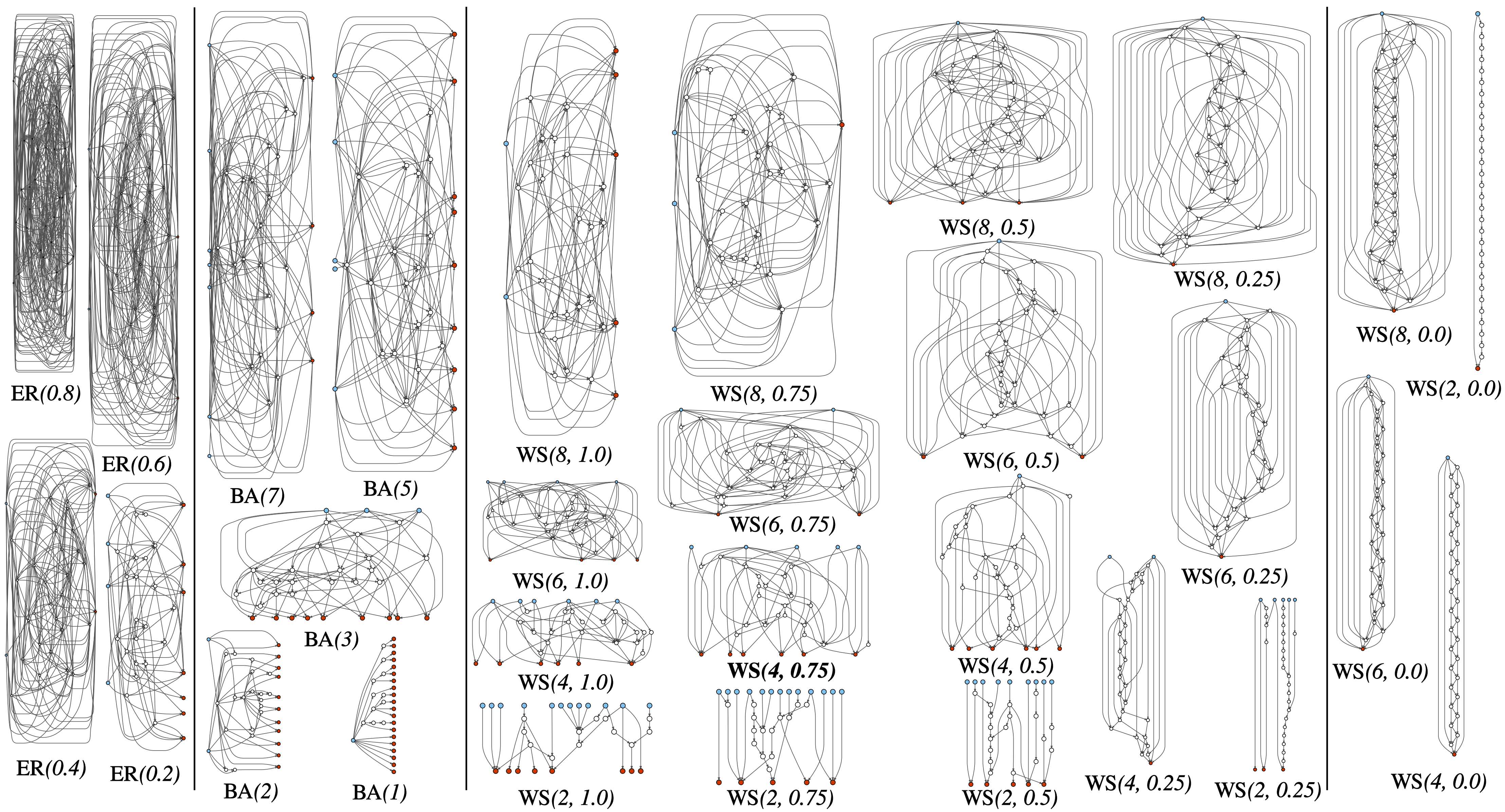


Prediction:
Elephant Shrew

Graph as Auxiliary:
Knowledge graph for image classification

Marino, Kenneth et al. "**The More You Know: Using Knowledge Graphs for Image Classification.**" CVPR 2016

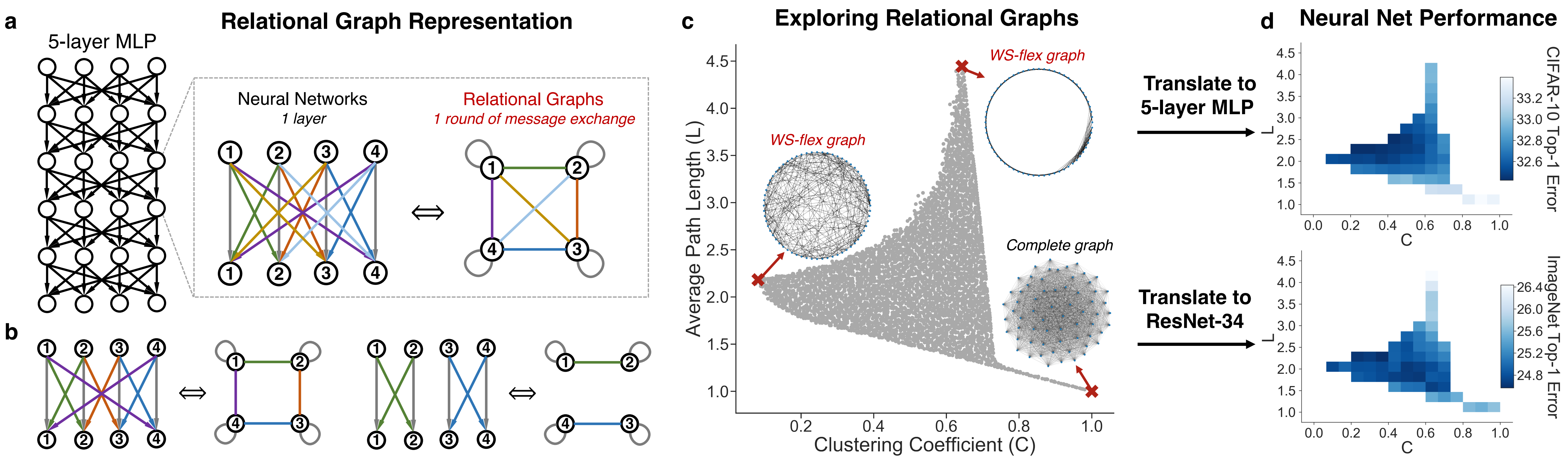
Graphs in CV



Graphs in neural network architecture

Xie, Saining, et al. "**Exploring randomly wired neural networks for image recognition.**" ICCV 2019.

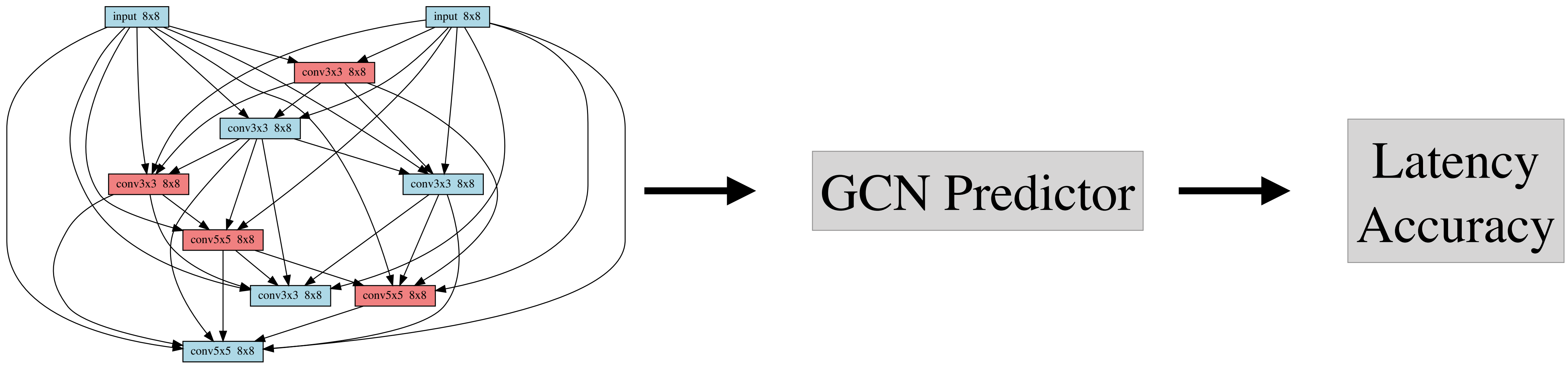
Graphs in CV



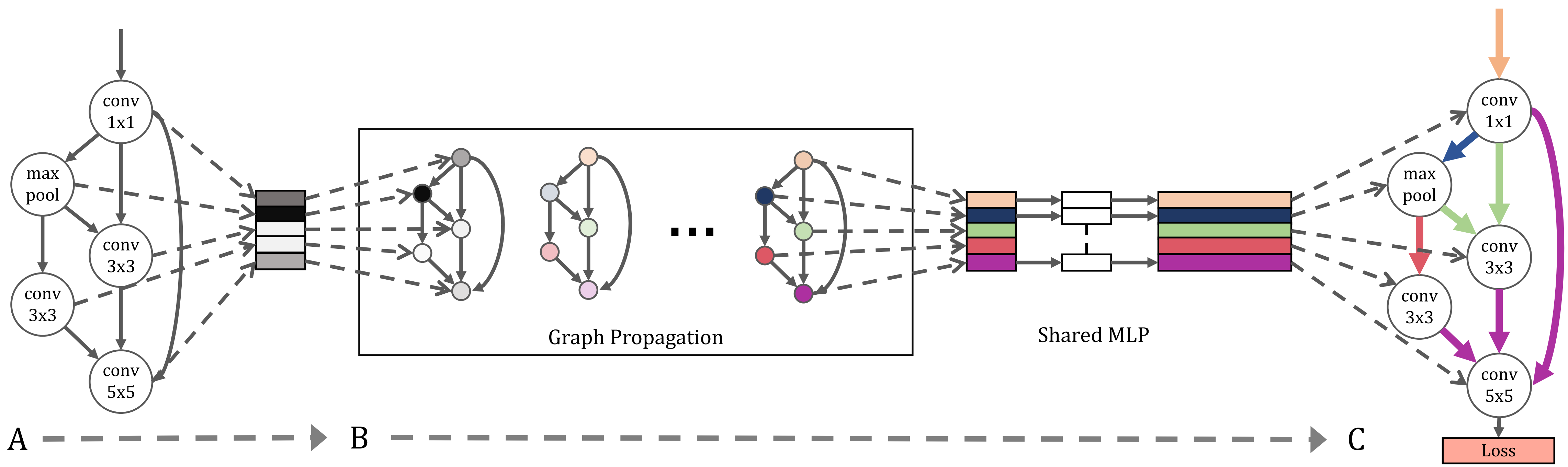
Graph topology and neural network architectures

You, Jiaxuan, et al. "**Graph structure of neural networks.**" International Conference on Machine Learning. PMLR, 2020.

Graphs in CV



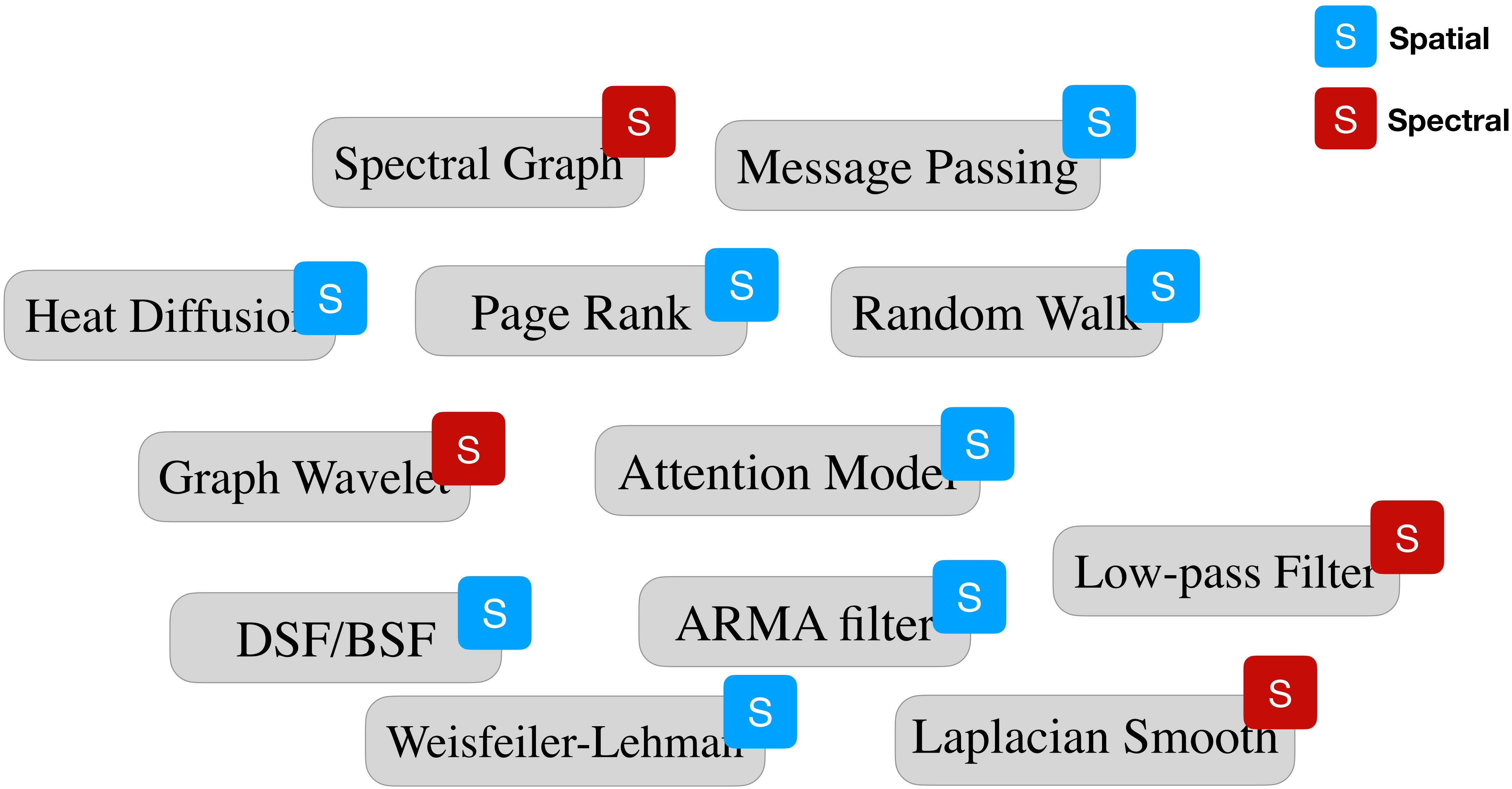
Dudziak, Lukasz, et al. "**Brp-nas: Prediction-based nas using gcns.**" Advances in Neural Information Processing Systems 33 (2020): 10480-10490.



Zhang, C., et al,. ***Graph hypernetworks for neural architecture search****. ICLR 2019*

Motivation: A Unified View

A large number of graph neural networks, with different mechanisms



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A large number of graph neural networks, with different mechanisms

Challenge

no uniform theoretical framework to compare them

...

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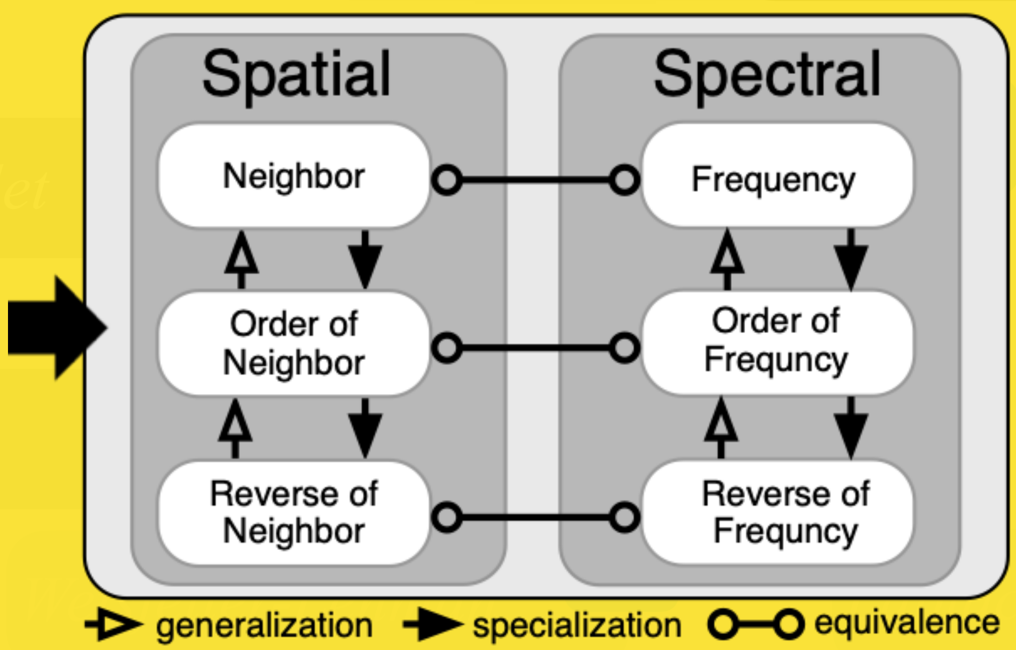
This Tutorial



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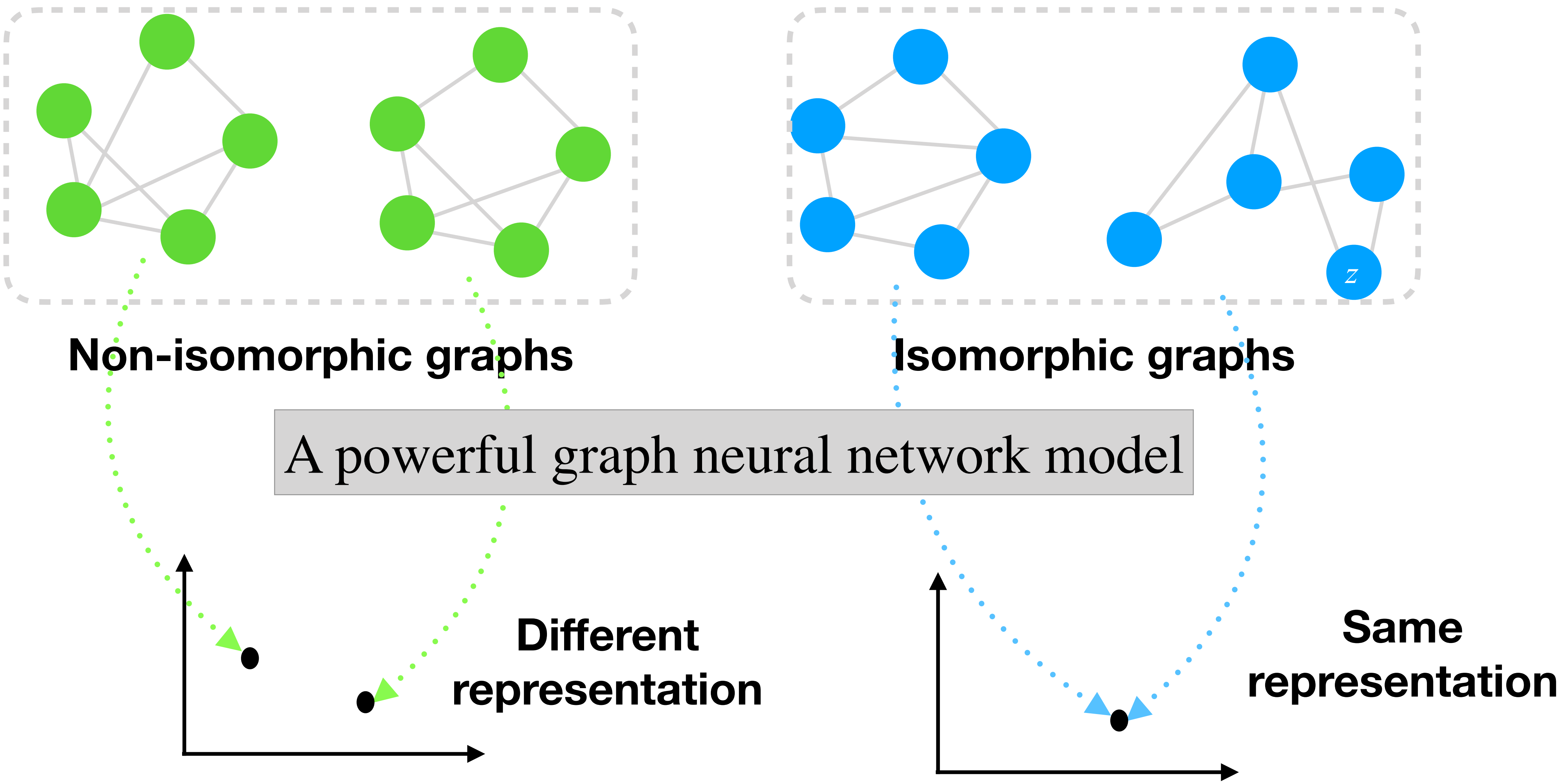
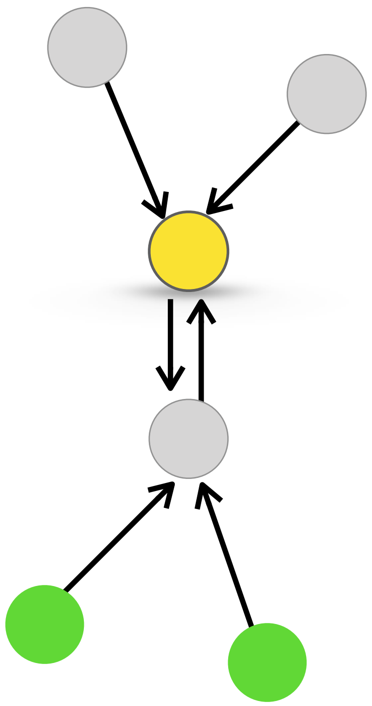
Attempts to Unify GNNs



Compare GNNs with respect to their **expressive power** (ability to distinguish different graph structures)

WL-Test: on Spatial GNNs



GNNs are defined as a composition of

- AGGREGATE functions and
- READOUT functions

$$h_u^{(k)} = \boxed{\mathrm{AGGREGATE}}^{(k)}\left(\left\{\left(h_v^{(k-1)}, h_u^{(k-1)}\right)\right\} \mid v \in \mathcal{N}(u)\right)$$

$$h_G = \boxed{\mathrm{READOUT}}\left(\{h_u^{(K)}\} \mid u \in V\right)$$

*GNNs are at most as powerful as a **Weisfeiler-Lehman** graph isomorphism test.*

Xu, K. et al., ***How powerful are graph neural networks?*** *In International Conference on Learning Representations, 2019.*

WL-Test: on Spatial GNNs

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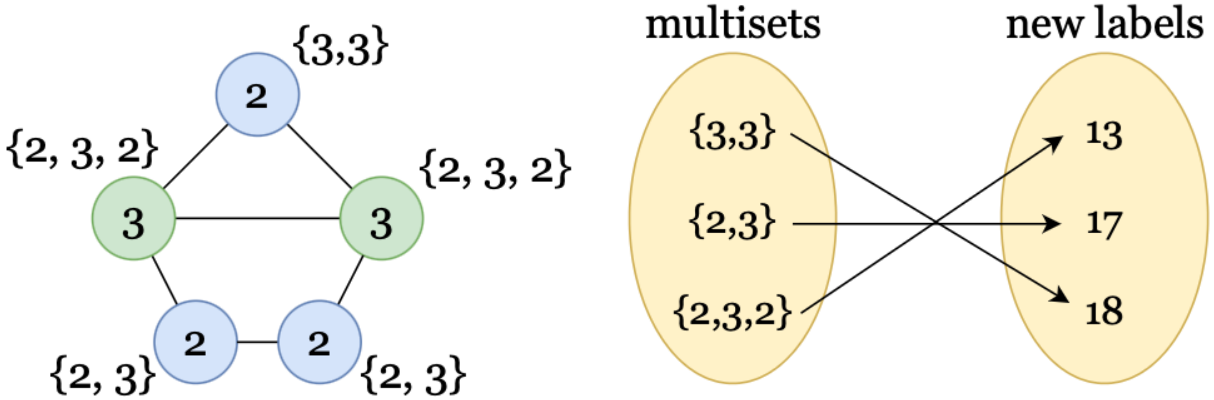
$$h_G = \boxed{\mathrm{READOUT}}\left(\left\{h_u^{(K)}\right\} \mid u \in V\right)$$

This upper bound is achieved if ***AGGREGATE*** *and* ***READOUT*** *are* ***Injective Multiset Functions***

Example GNNs that are ***LESS*** *powerful than WL test: GCN, GraphSage*



Every possible output has at most one associated input

$$h_v^{(k)} = \mathrm{ReLU}\left(W \cdot \mathrm{MEAN}\left\{h_u^{(k-1)}, \forall u \in \mathcal{N}(v) \cup \{v\}\right\}\right).$$

GCN has mean AGGREGATE, so it is not an injective function. As a result, it is less powerful. *

Xu, K. et al., ***How powerful are graph neural networks?*** *In International Conference on Learning Representations, 2019.*

Spectral GNNs and Isomorphism Test

Spatial GNNs

AGGREGATE + READOUT ⟷ Isomorphism Test

What is the connection?

Spectral GNNs

Spectral Filters ⟷ Isomorphism Test

Xu, K., et al., ***How powerful are graph neural networks?*** *In International Conference on Learning Representations, 2019.*
Wang, X et al.,. ***How powerful are spectral graph neural networks.*** *International Conference on Machine Learning. PMLR, 2022.*

Spectral GNNs and Isomorphism Test

Spatial GNNs

AGGREGATE + READOUT ⟷ Isomorphism Test

*Doesn't work on GNNs with **Continuous** features.*
WL-test (1-WL test) is not perfect.

Spectral GNNs

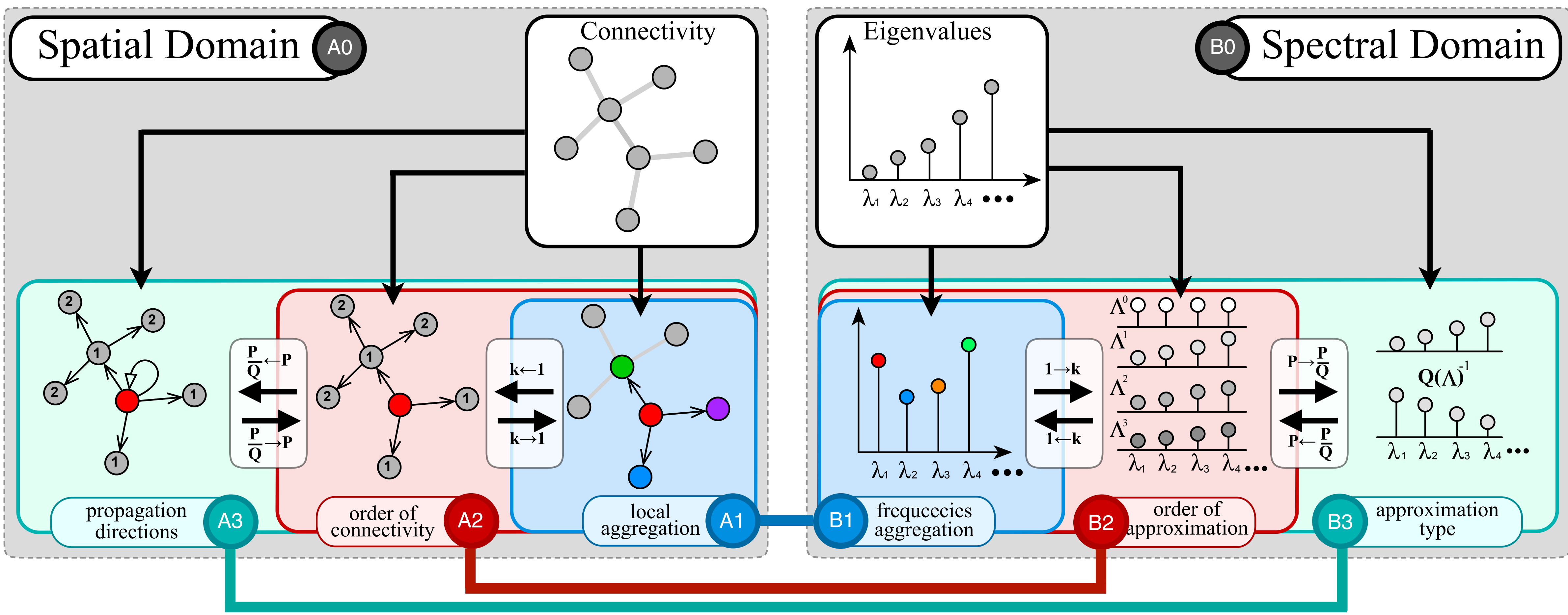
Spectral Filters ⟷ Isomorphism Test

Spectral filters are universal approximators when satisfying two conditions.
*The analysis is **limited to Spectral** GNNs without nonlinearity.*

Xu, K., et al., **How powerful are graph neural networks?** In International Conference on Learning Representations, 2019.
Wang, X et al.,. **How powerful are spectral graph neural networks.** International Conference on Machine Learning. PMLR, 2022.

Comparison

- Existing surveys and theoretical analyses focus on either the spatial or the spectral GNNs, not all of them.
- Here is the framework we will introduce later



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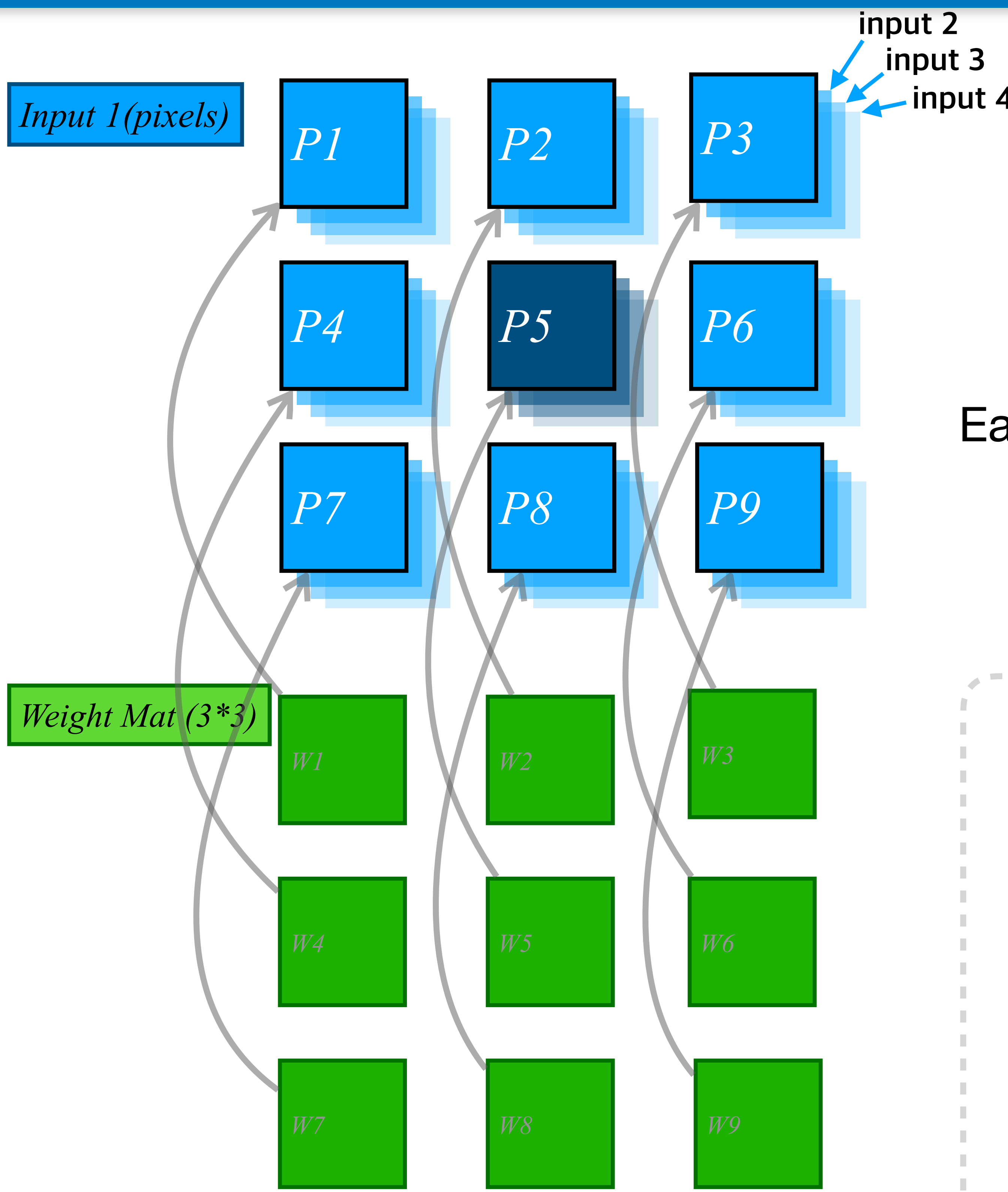
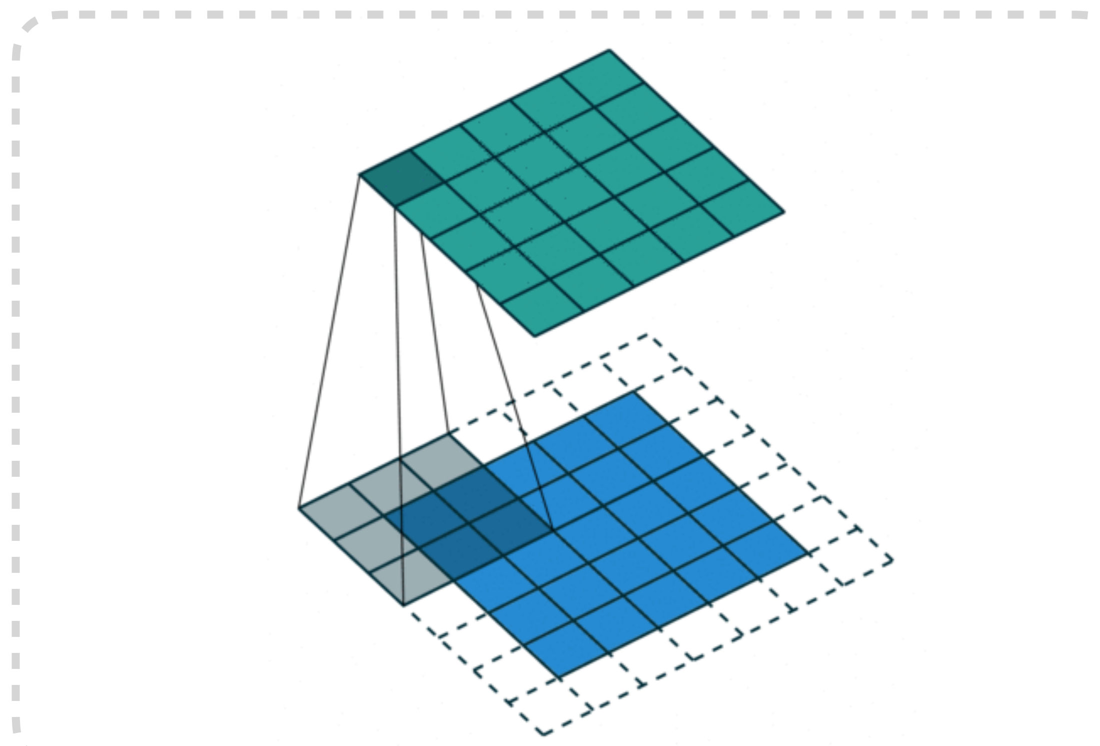
ConvNet



$$\hat{P}_5 = \sum_{i=1}^{9} P_i \cdot W_i$$

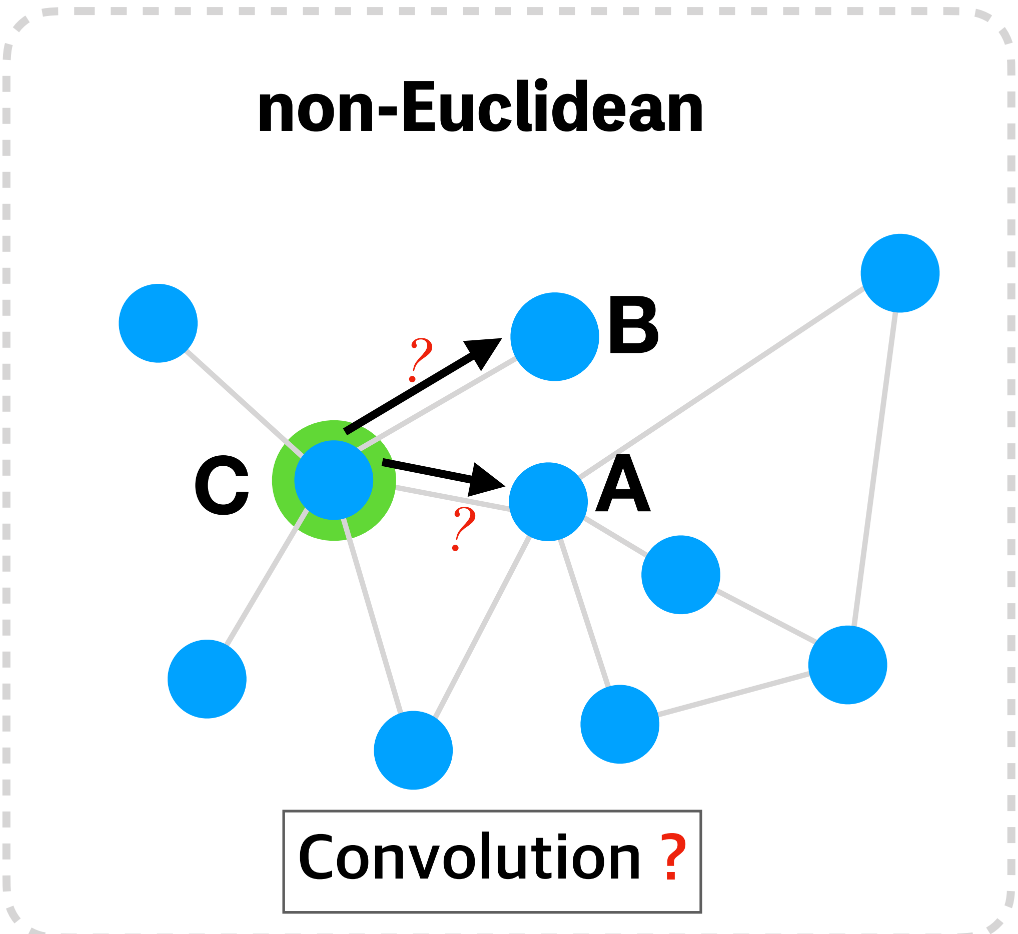
Each pixel has **fixed** number of neighbors

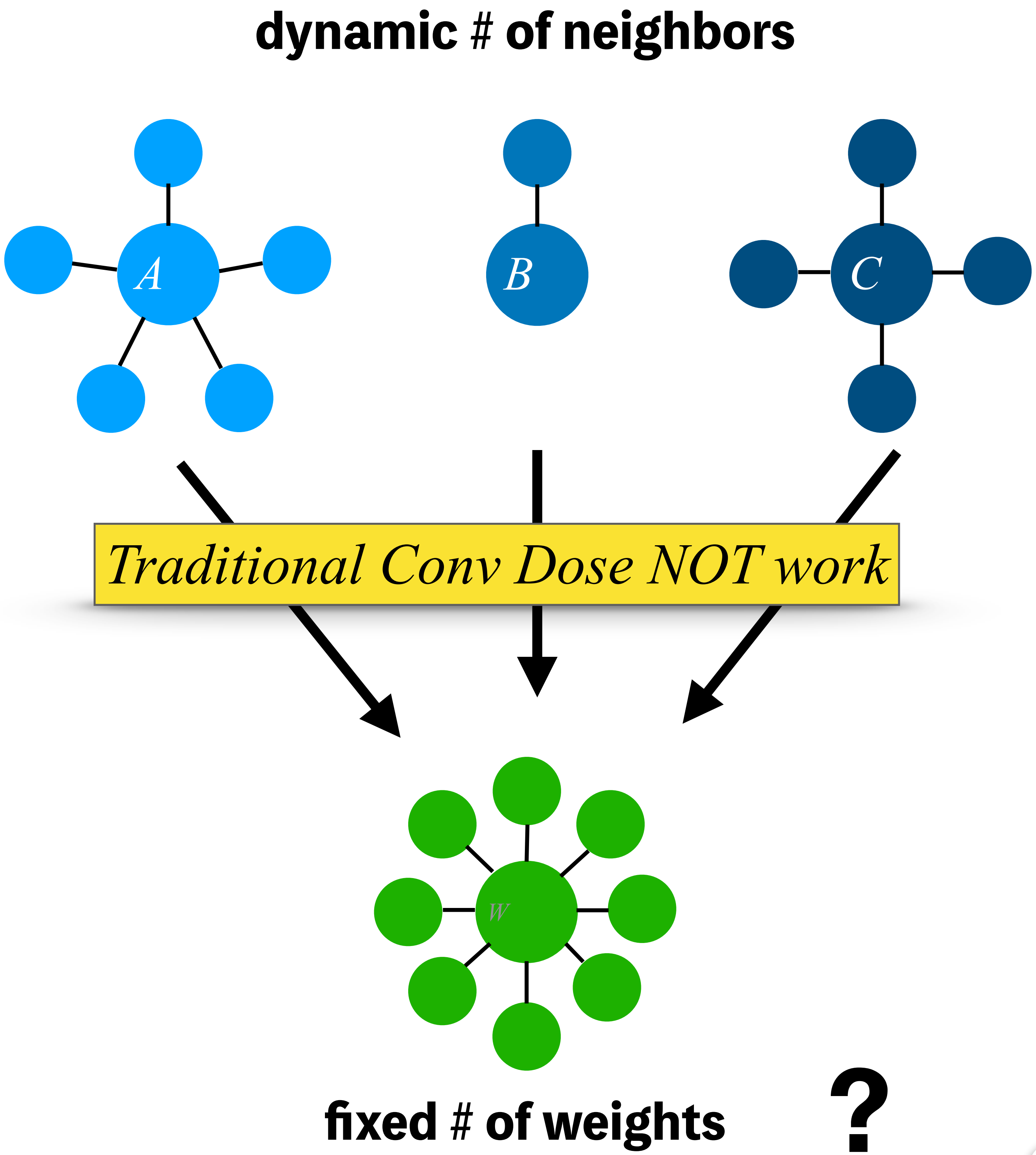
Convolution



Credit: Prof. Dr. Johannes Maucher

Challenge for ConvNet on Graphs





What is Graph Convolution

- **Convolution Theorem**
  - Fourier transform of the convolution of two functions is equal to the point-wise multiplication of their Fourier transforms.

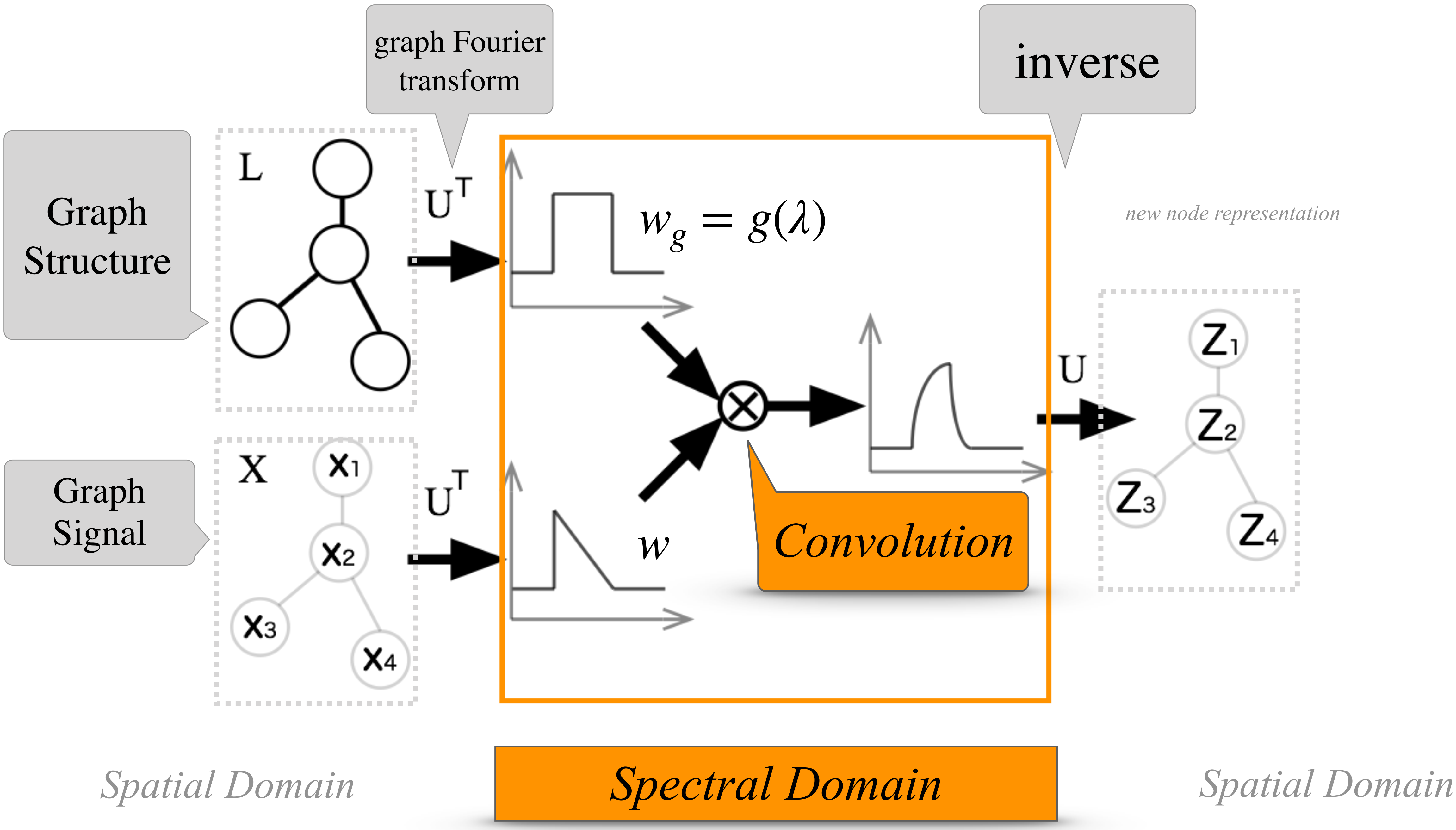
$$\mathcal{F}\{f * g\} = \mathcal{F}\{f\} \cdot \mathcal{F}\{g\}$$

Space convolution = frequency multiplication

$$f * g = \mathcal{F}^{-1}\{\mathcal{F}\{f\} \cdot \mathcal{F}\{g\}\}$$

We can do the convolution in the spectral domain, such that avoiding the issues.

Convolution on Graph Data



$$f * g = \mathcal{F}^{-1}\{\mathcal{F}\{f\} \cdot \mathcal{F}\{g\}\}$$

Chung, Fan RK. ***Spectral graph theory****. Vol. 92. American Mathematical Soc., 1997.*

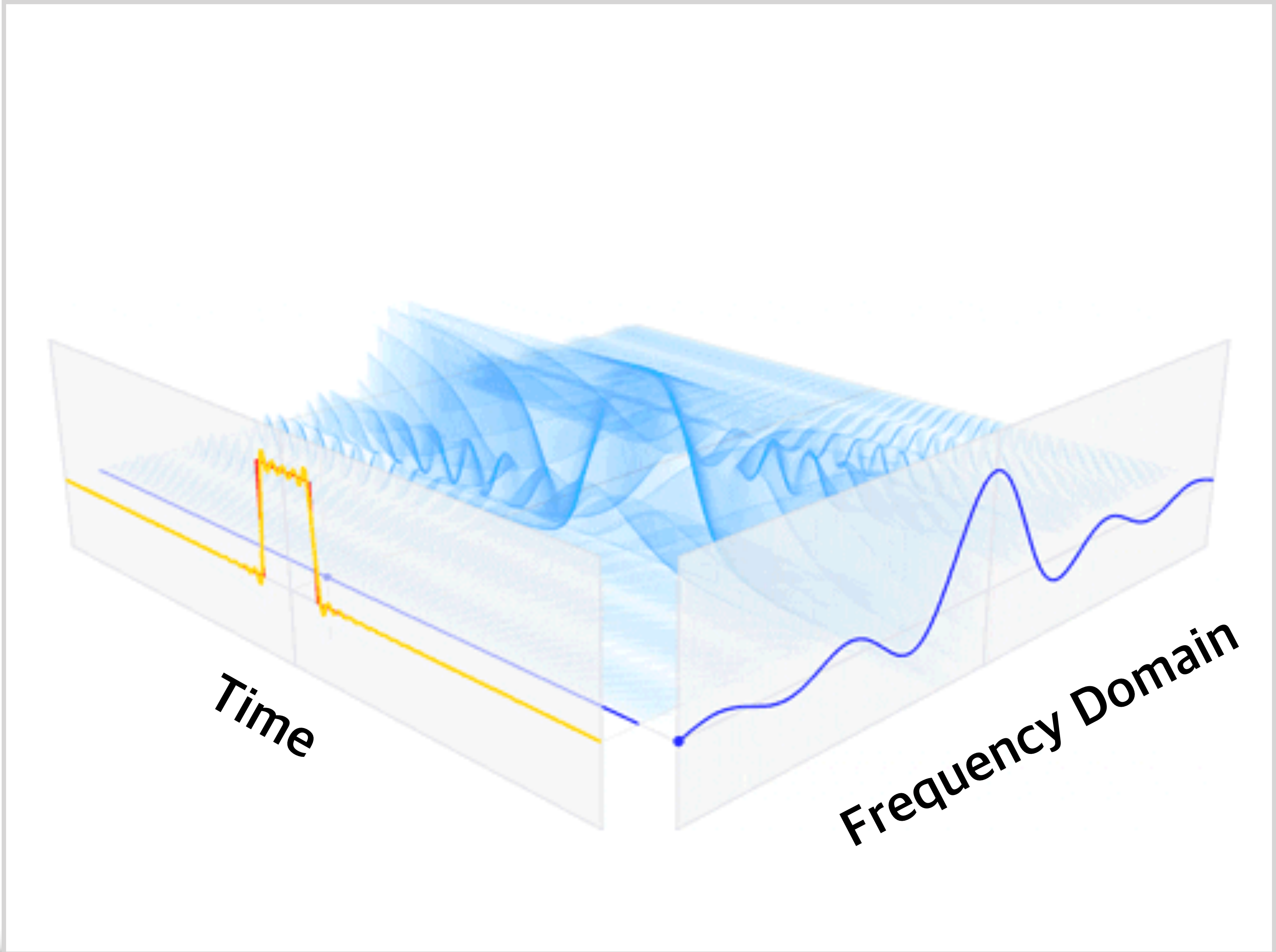
Convolution on Graph Data

Convolution theorem: $f * g = \mathcal{F}^{-1}\{\mathcal{F}\{f\} \cdot \mathcal{F}\{g\}\}$

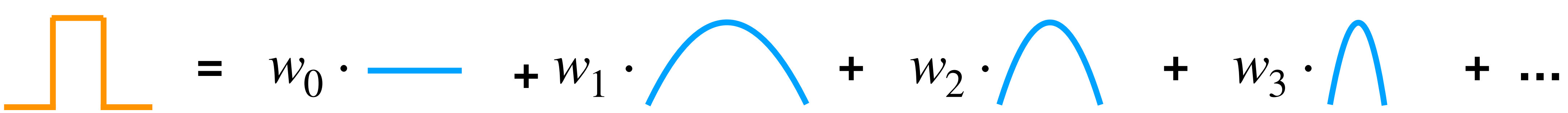
What is the Fourier Transform on Graphs?

What is the Inverse Fourier Transform on Graphs?

Spectral Analysis



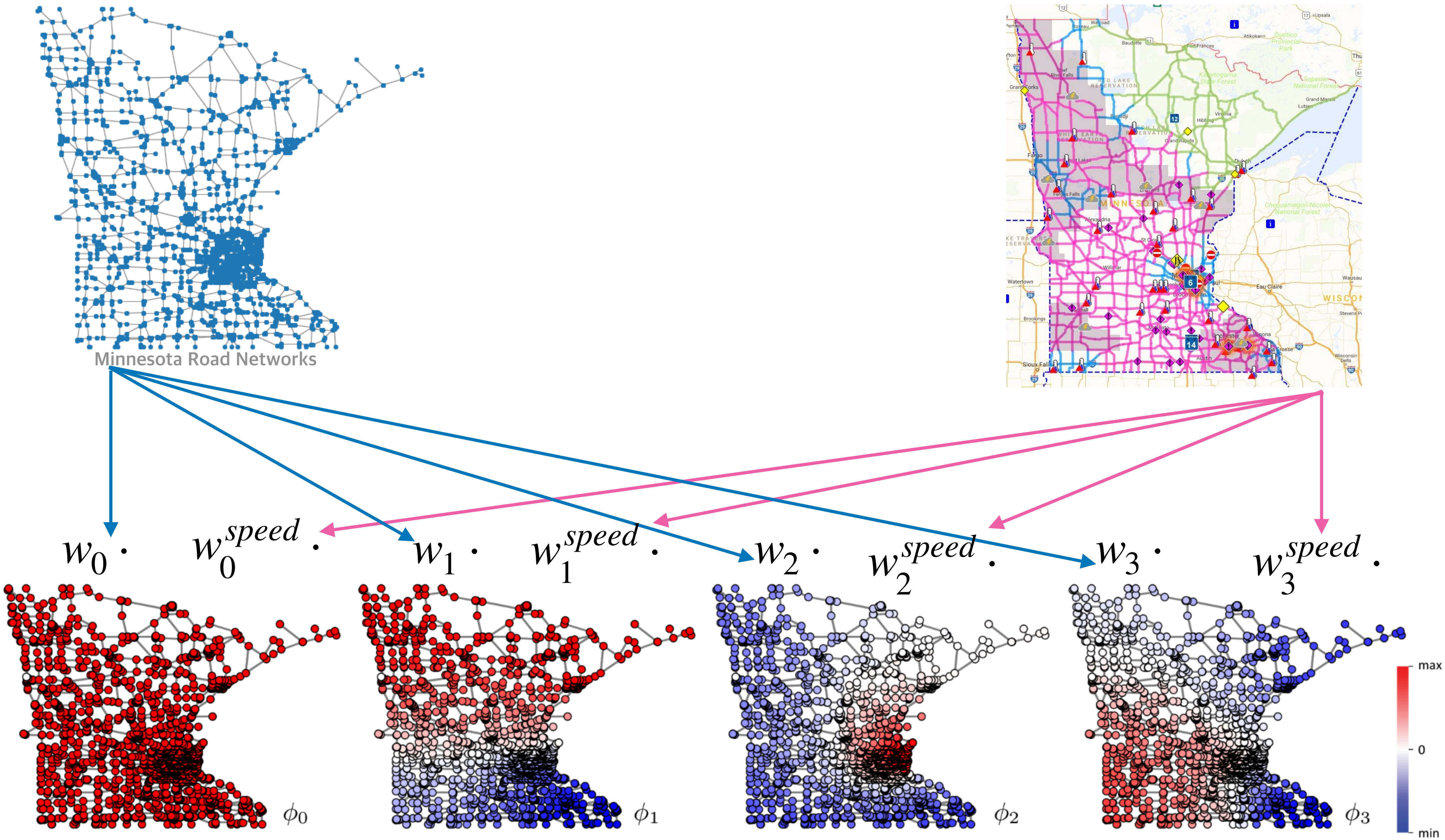
credit: giphy



Spectral Analysis for Graph

Graph Structure

Graph Signal (e.g.,Traffic Speed)



eigen-vector 0 eigen-vector 1 eigen-vector 2 eigen-vector 3

Graph Fourier Transform (Spectral Decomposition)

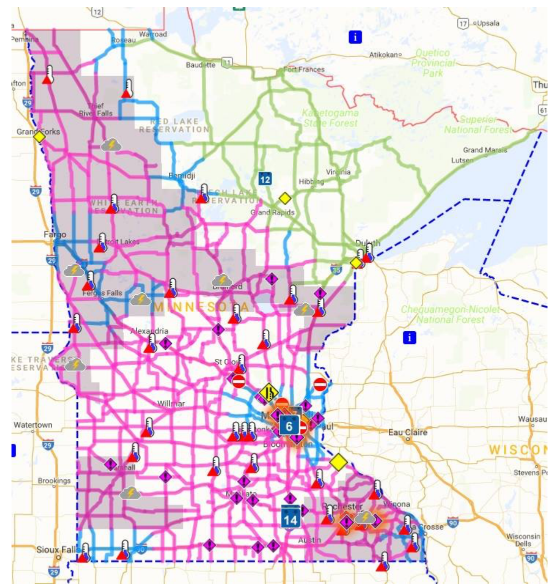
Convolution on Graph Data

- Convolution theorem: $f * g = \mathscr{F}^{-1}\{\mathscr{F}\{f\} \cdot \mathscr{F}\{g\}\}$
- What is each of the components **on a graph**?
- Fourier transform of f: $U^T f$
- Inverse Fourier transform of f: Uf
- Now, what is U, and U^T ?
- $L = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U \Lambda U^T$
- Finally, $g * X = U g(\Lambda) U^T X$

Convolution on Graph Data

Graph Structure

Graph Signal (e.g.,Traffic Speed)



$$\boxed{g_\theta} * \boxed{x} = \boxed{U \boxed{g_\theta(\Lambda) \boxed{U^\top x}}}$$

1 **graph Fourier transform**

Get base by $L = U \Lambda U^\top$

L is graph Laplacian matrix

2 **convolution (theorem)**

3 **Inverse graph Fourier transform**

*Chung, Fan RK. **Spectral graph theory**. Vol. 92. American Mathematical Soc., 1997.*

Convolution on Graph Data

$$g_\theta * x = U g_\theta(\Lambda) U^\top x$$

$$L = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U \Lambda U^T$$

How to design g_θ ?

$$g_\theta(\Lambda) = \begin{pmatrix} \theta_1 & & \\ & \ddots & \\ & & \theta_n \end{pmatrix}$$

This is the weight matrix/ convolution kernel / mask in CNN

Convolution on Graph Data

$$g_\theta * x = U \begin{pmatrix} \theta_1 & & \\ & \ddots & \\ & & \theta_n \end{pmatrix} (\Lambda) U^\top x$$

It works, but it's expensive to calculate.
We can approximate it with the polynomial of Λ

Convolution on Graph Data

If constraint g_θ is polynomial

$$g_\theta * f = U g_\theta U^\top f \quad = g_\theta(L) \cdot f$$

$$g_\theta = g(\theta) = 2 - \theta$$

$$= g_\theta(L) \cdot f$$

$$= (2 \cdot I - L) \cdot f$$

1-order polynomial without weights

$$= (2 \cdot I - (I - A)) \cdot f$$

A and L are normalized

$$= (I + A) \cdot f$$

$$= f + A \cdot f$$

Now we have GCN

Kipf, T. N., & Welling, M. (2017). ***Semi-supervised classification with graph convolutional networks***. ICLR,

Convolution on Graph Data

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1-order polynomial without weights

$$= (2 \cdot I - (I - A)) \cdot f$$

A and L are normalized

$$= (I + A) \cdot f$$

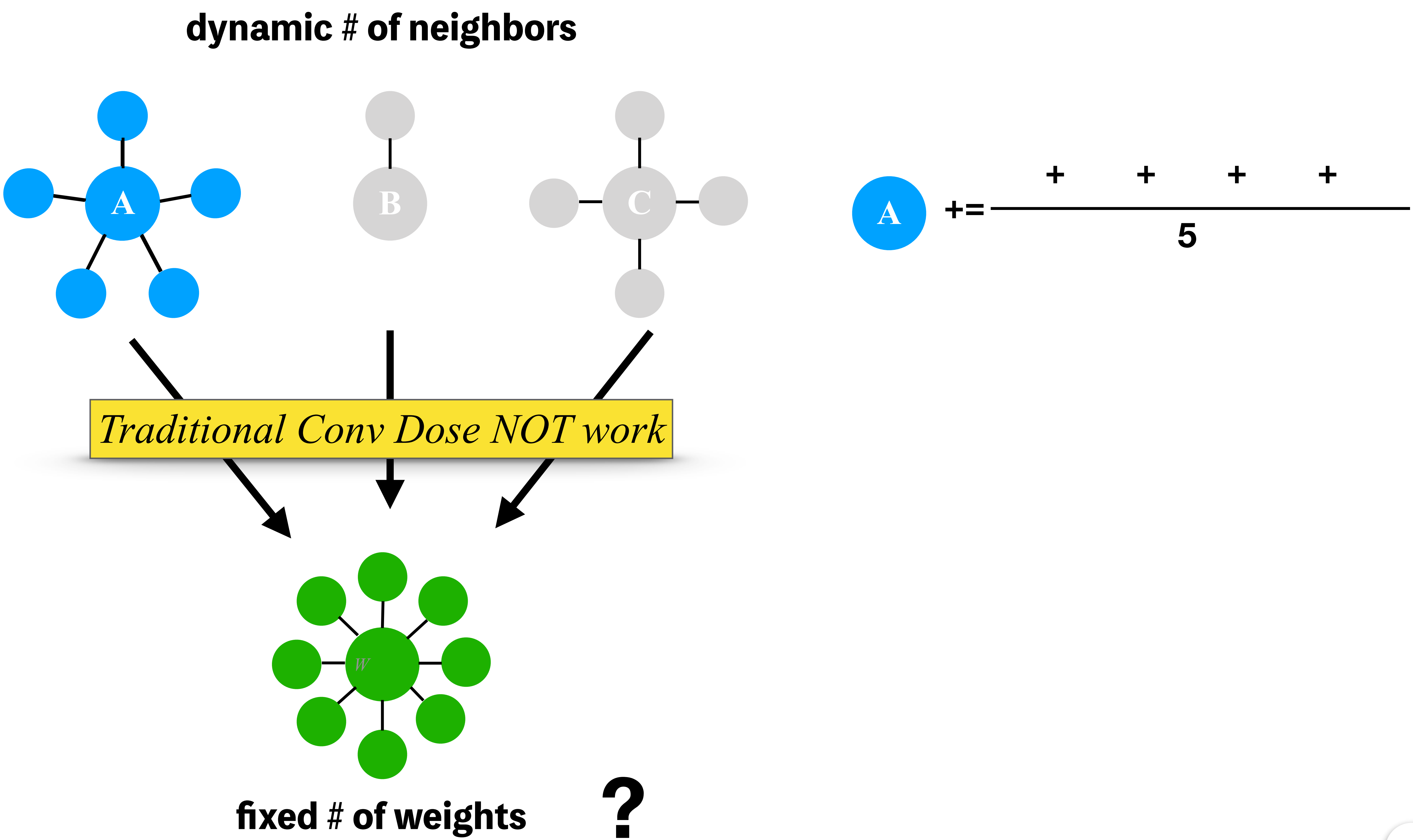
$$= \boxed{f} + \boxed{A \cdot f}$$

Self   Average of neighbors

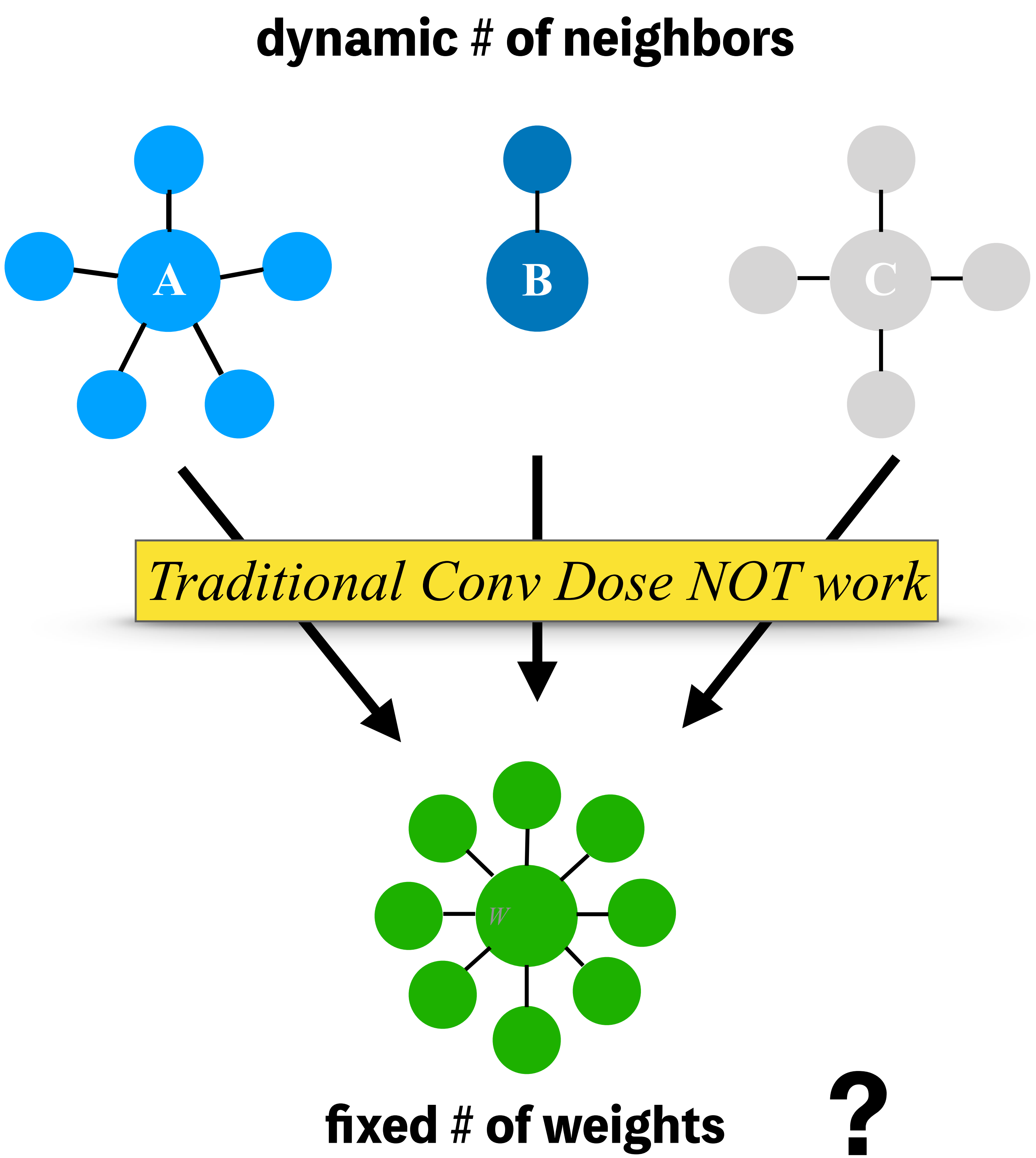
We reach here with the spectral method, but it also makes sense in spatial domain

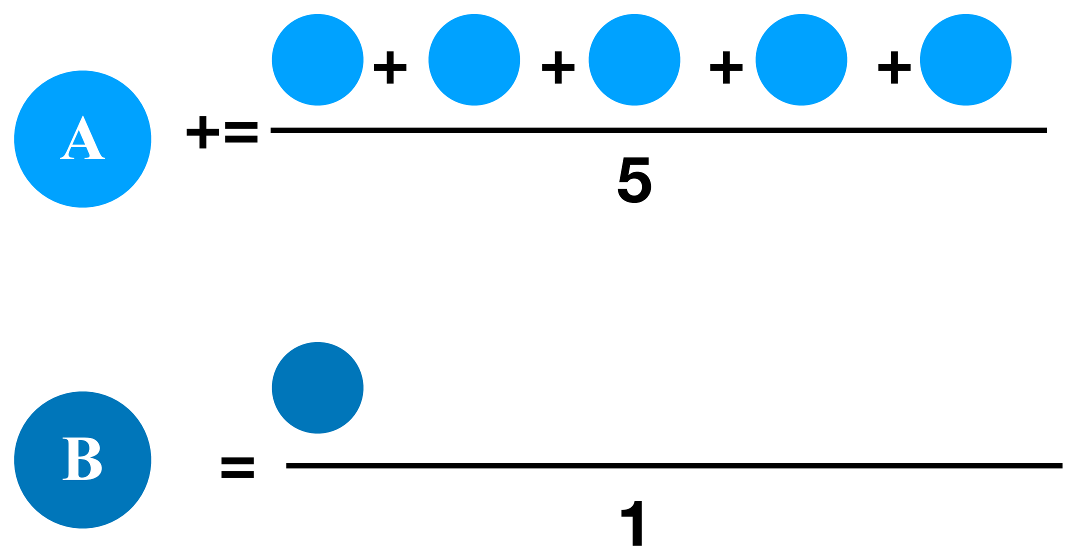
Kipf, T. N., & Welling, M. (2017). ***Semi-supervised classification with graph convolutional networks***. ICLR,

Convolution on Graph Data

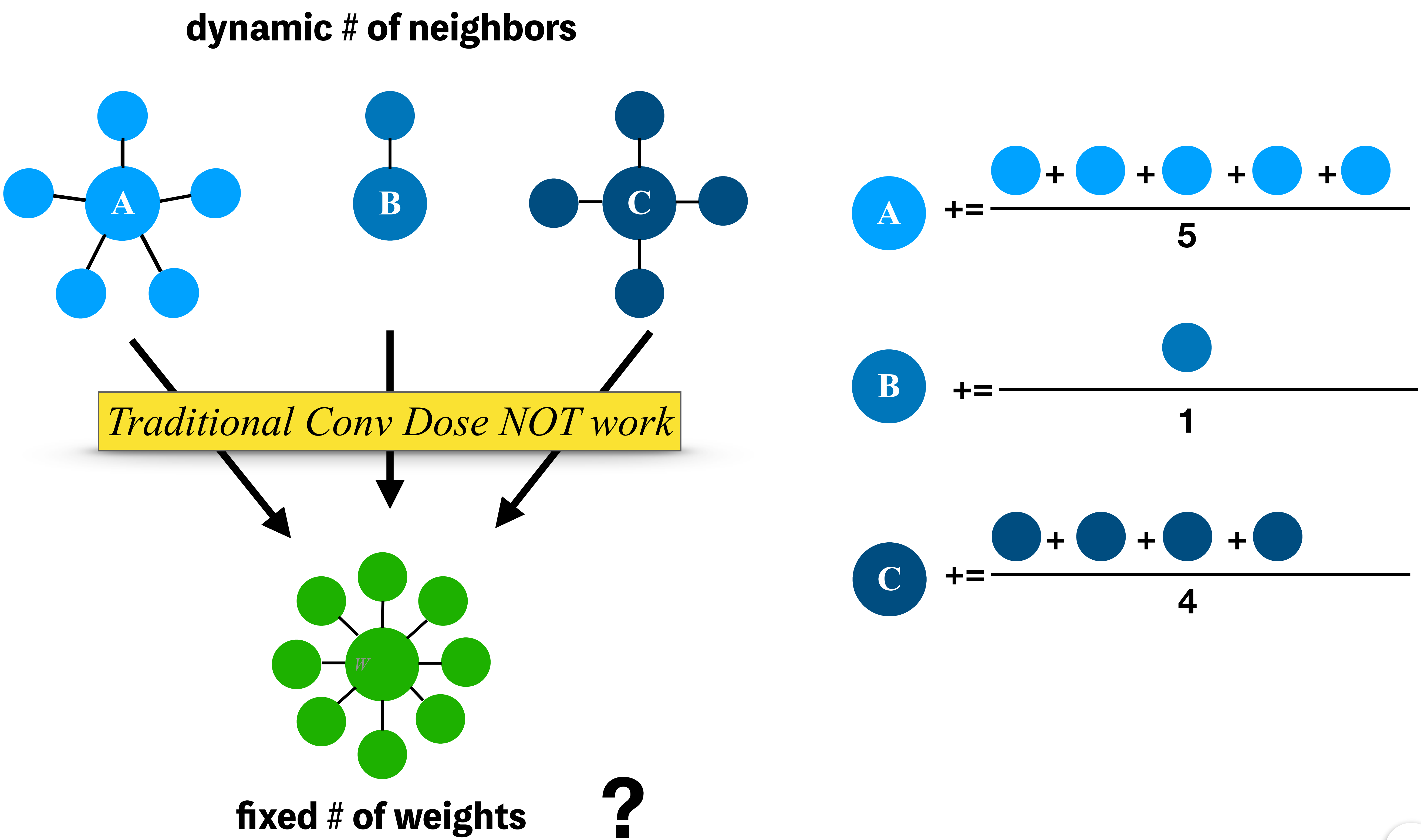


Convolution on Graph Data



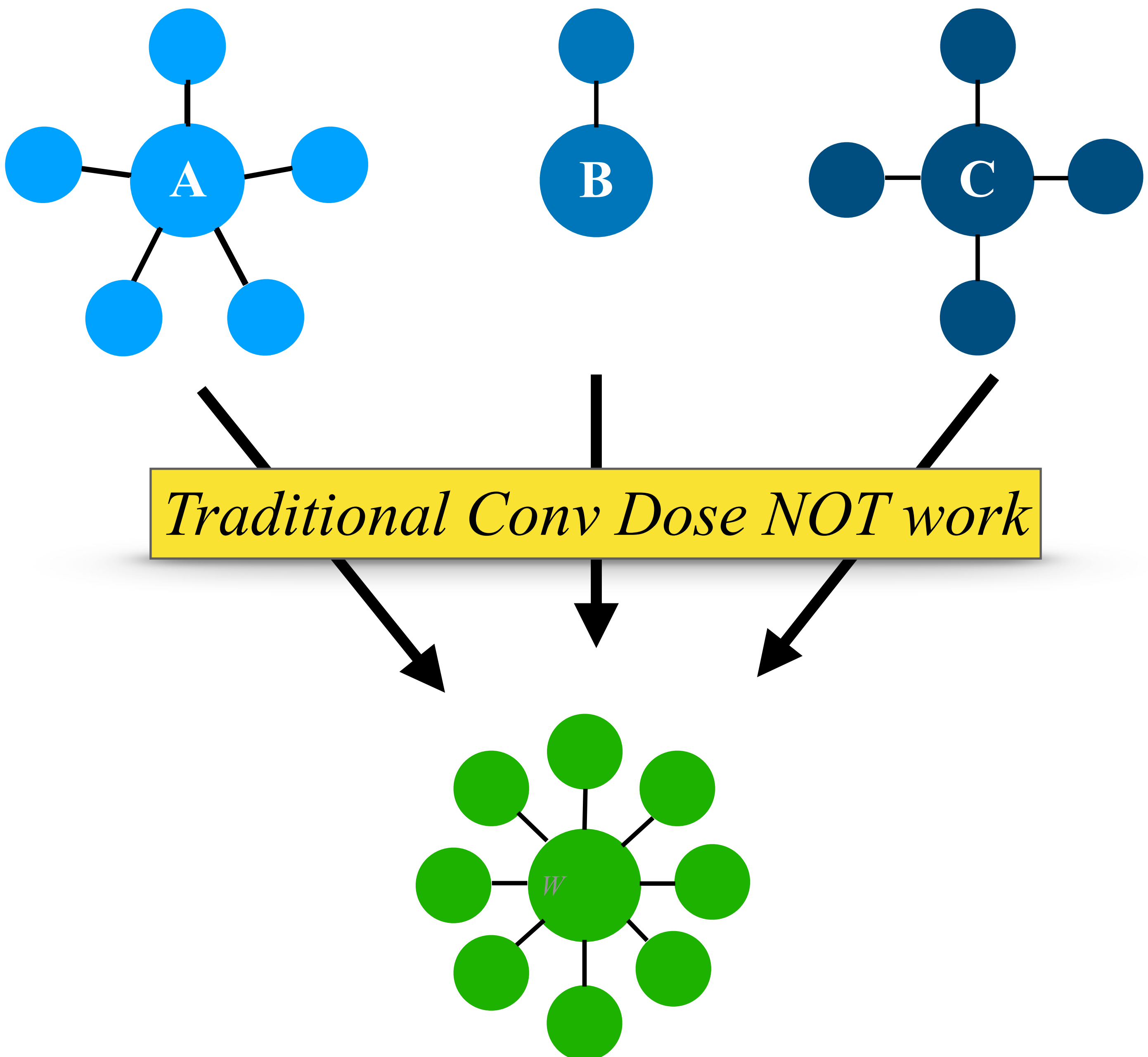


Convolution on Graph Data



Convolution on Graph Data

dynamic # of neighbors



fixed # of weights **?**

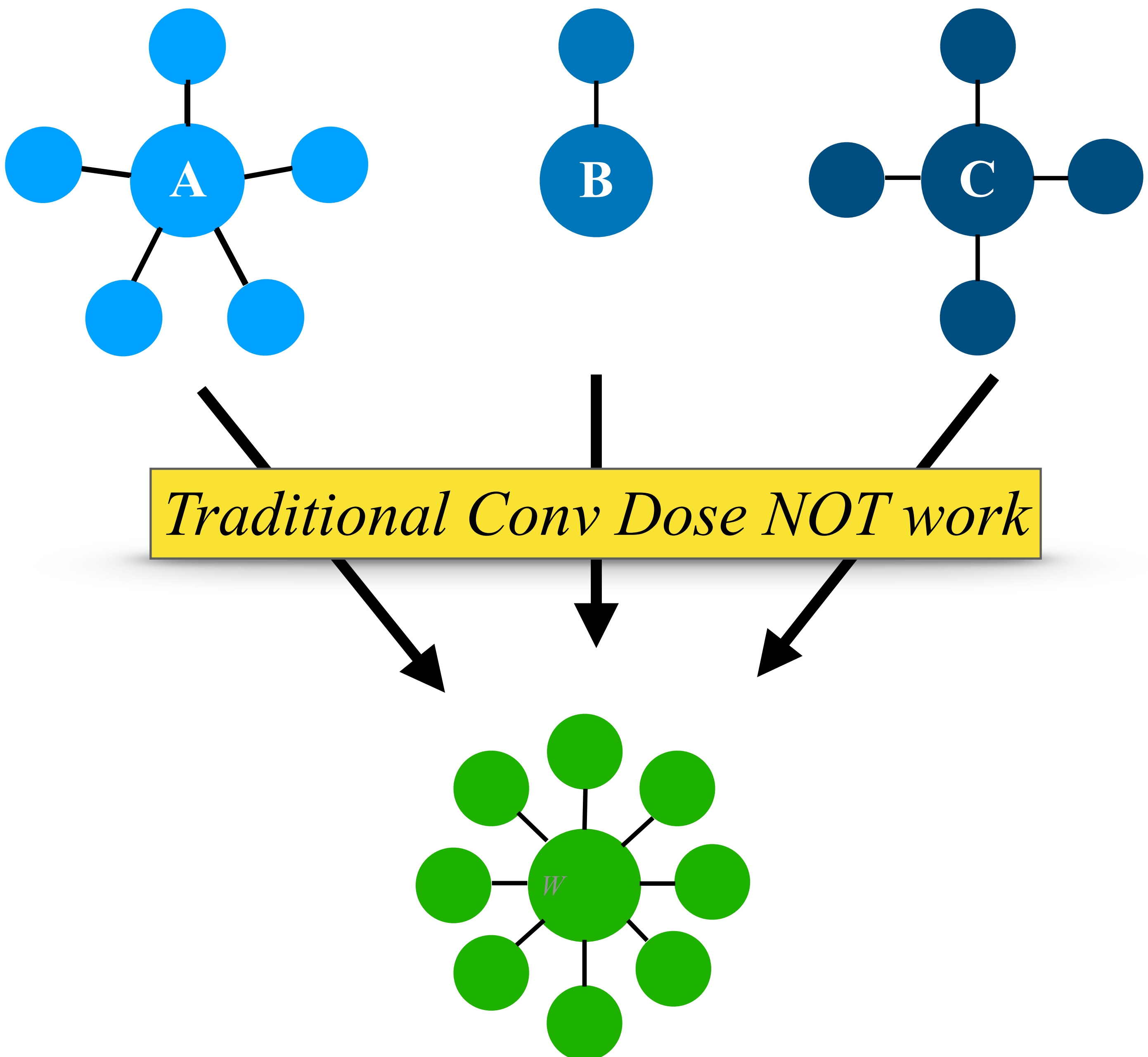
$A \in \mathbb{R}^{node}$

$B \in \mathbb{R}^{node}$

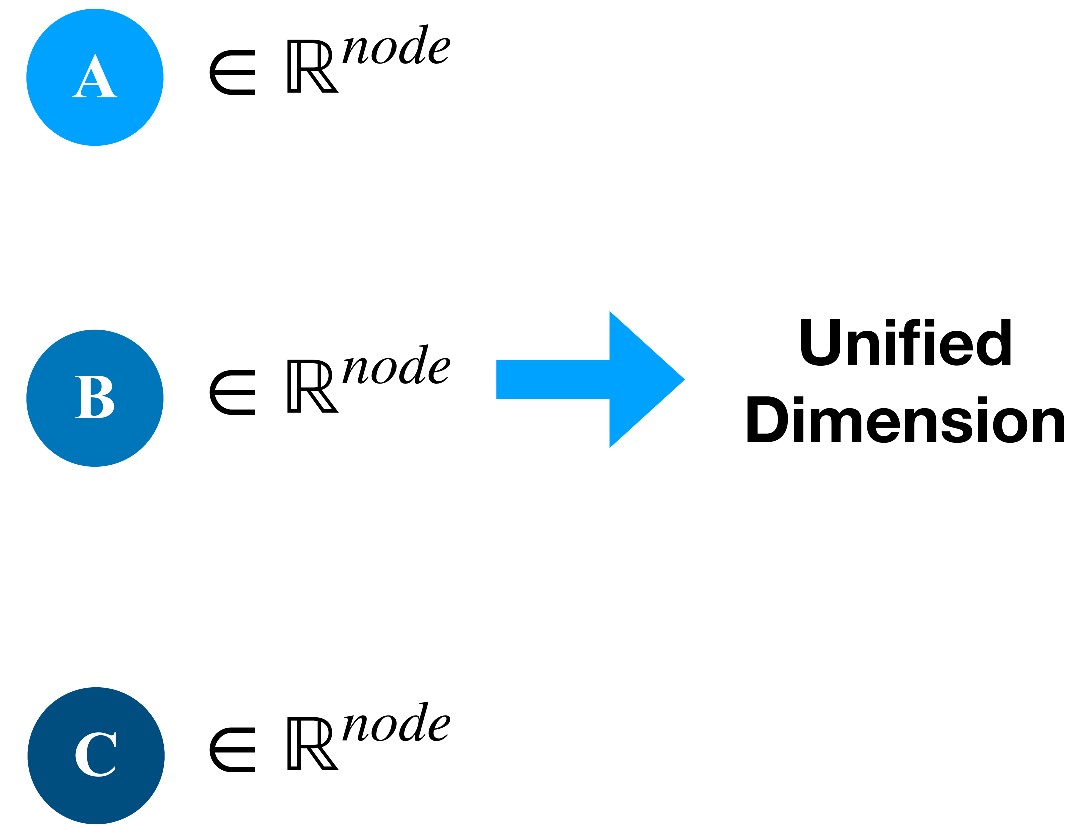
$C \in \mathbb{R}^{node}$

Convolution on Graph Data

dynamic # of neighbors



fixed # of weights **?**

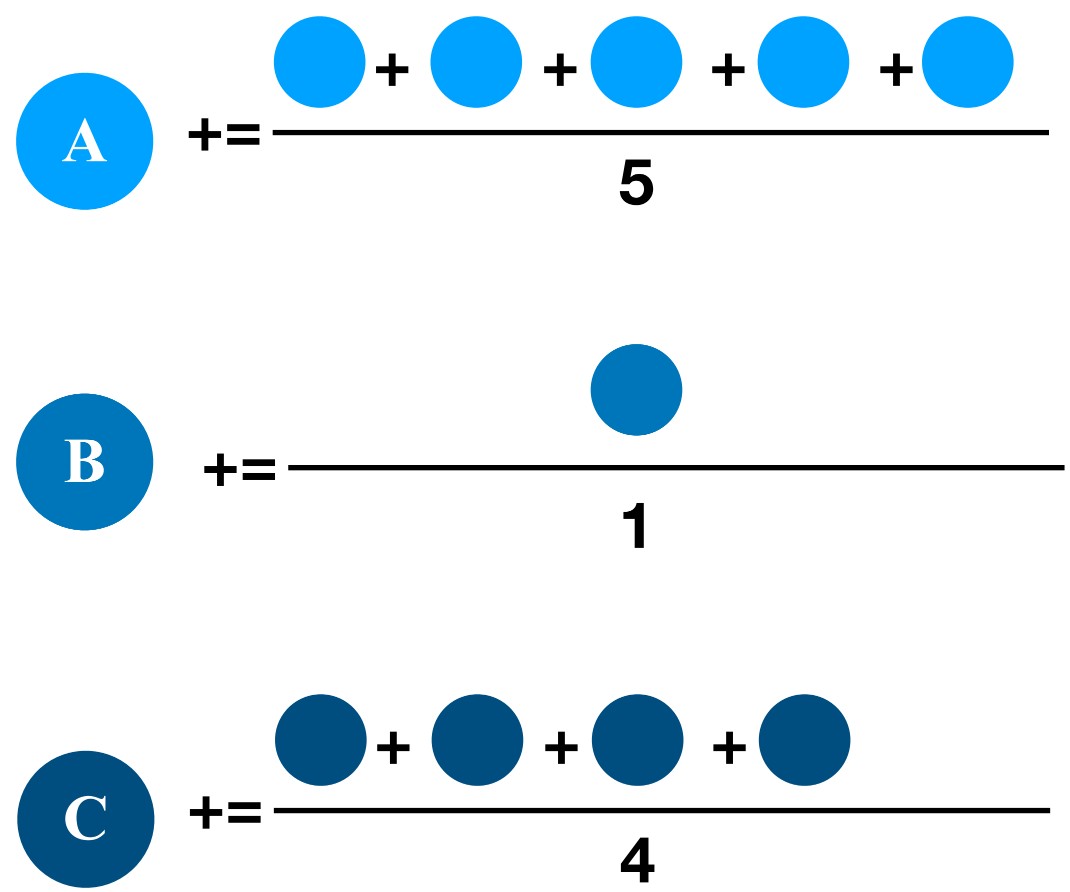


GCN works!

Convolution on Graph Data

If constraint g_θ is polynomial, rational or exp function

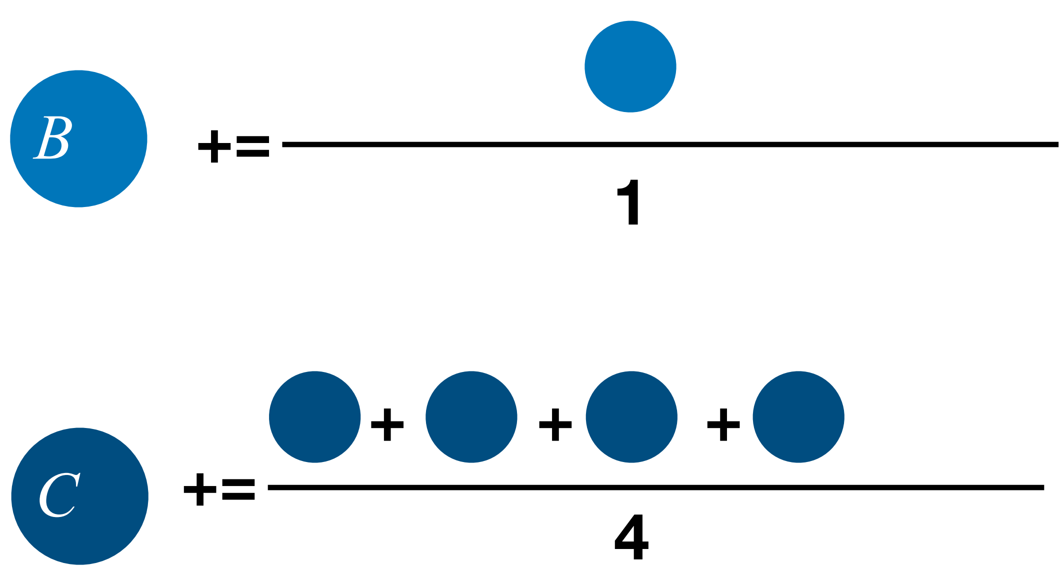
$$g_\theta * f = U g_\theta U^\top f \quad = \overset{\text{Self}}{\boxed{f}} + \overset{\text{Average of neighbors}}{\boxed{A \cdot f}}$$



*Kipf, T. N., & Welling, M. (2017). **Semi-supervised classification with graph convolutional networks**. ICLR,*

Convolution on Graph Data

How about g_θ in other GNNs?



Convolution on Graph Data

How about g_θ in other GNNs?

What does the space and frequency look like in graph domain?

Convolution theorem

$$f(x,y) * h(x,y) \quad \Leftrightarrow \quad F(u,v)H(u,v)$$

Space convolution = frequency multiplication

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Spatial & Spectral Methods

- **Spatial** Methods $g(A, X) = g_\theta(A)X$

  Function of ***graph*** *(matrix)*

- **Spectral** Methods $g(\Lambda, X) = Ug_\theta(\Lambda)U^T X$

  Function of ***eigenvalue*** *of (graph matrix)*

Normalization

Normalized vs Unnormalized

"Mean" *"Sum"*

Notations	Descriptions
$\mathbf{A}$	Adjacency matrix
$\mathbf{L}$	Graph Laplacian
$\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$	Adjacency with self loop
$\mathbf{D}^{-1}\mathbf{A}$	Random walk row normalized adjacency
$\mathbf{A}\mathbf{D}^{-1}$	Random walk column normalized adjacency
$\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$	Symmetric normalized adjacency
$\tilde{\mathbf{D}}^{-1}\tilde{\mathbf{A}}$	Left renormalized adjacency, $\tilde{\mathbf{D}}_{ii} = \sum_j \tilde{\mathbf{A}}_{ij}$
$\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-1}$	Right renormalized
$\tilde{\mathbf{D}}^{-1/2}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-1/2}$	Symmetric renormalized

Normalization

- Spatial reason
  - Suppose a two-cluster partitioning for A and B

- **Ratio Cut**: $cut(A,B)(\frac{1}{|A|}+\frac{1}{|B|})$
  - Use # **node** to cluster graph

Unnormalized

- **Normalized Cut**: $cut(A,B)(\frac{1}{Vol(A)}+\frac{1}{Vol(B)})$
  - Use # **link** to cluster graph

Normalized

Von Luxburg, Ulrike. "**A tutorial on spectral clustering.**" Statistics and computing 17 (2007): 395-416.

Normalization

- Spectral reason

- Eigenvalue $\in [0, \lambda_{max}]$

- $\lambda_{max} <$ max degree of the graph

Unnormalized

- Eigenvalue $\in [0,2]$

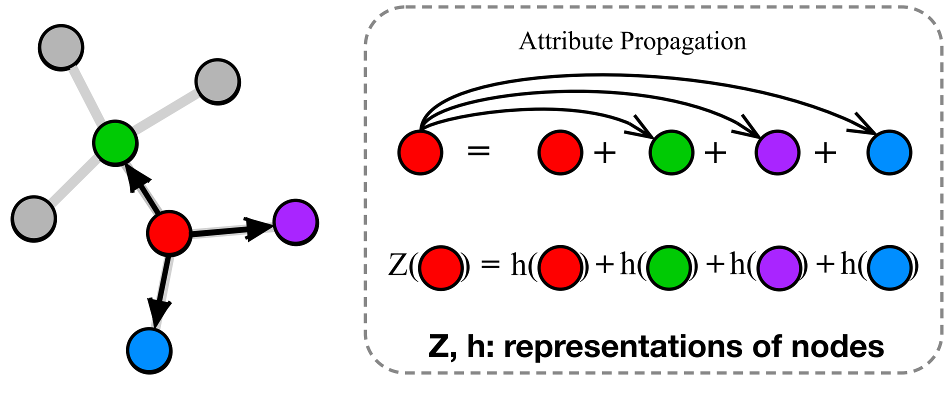
- random walk or symmetric normalization

Normalized

*Von Luxburg, Ulrike. "**A tutorial on spectral clustering.**" Statistics and computing 17 (2007): 395-416.*

Case Study 1: GCN

GCN *Thomas N. Kipf et al. (2017)*



$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}\hat{\mathbf{A}}\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I} + \mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I} + \tilde{\mathbf{A}})\mathbf{X}$$

In form of $g_\theta(A)X$

Kipf, T. N., & Welling, M. (2017). Semi-supervised classification with graph convolutional networks. ICLR,

Case Study 1: GCN

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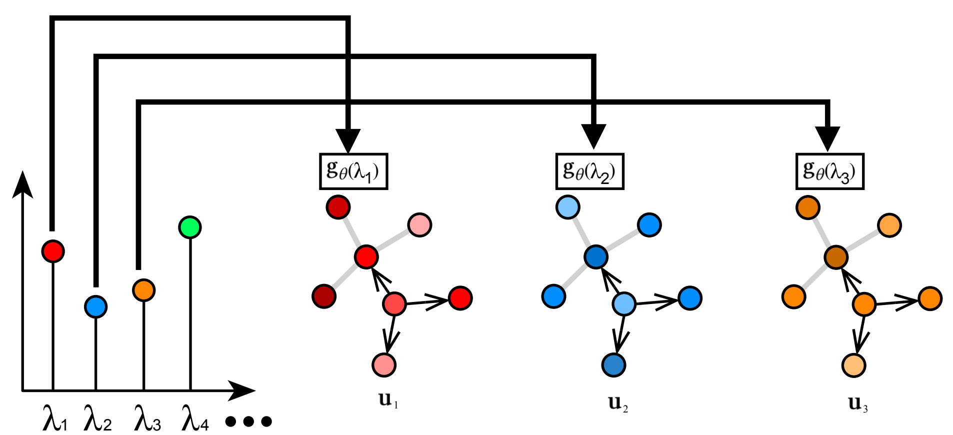


$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{A} + \mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{D} - \mathbf{L} + \mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{U}(2 - \Lambda)\mathbf{U}^{\top}\mathbf{X}$$

In form of $U g_\theta(\Lambda) U^T X$

Case Study 1: GCN

GCN *Thomas N. Kipf et al. (2016)*

Spatial

Average neighbors

$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I} + \mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I} + \tilde{\mathbf{A}})\mathbf{X}$$

$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I} + \mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{U}(2 - \Lambda)\mathbf{U}^{\top}\mathbf{X}$$

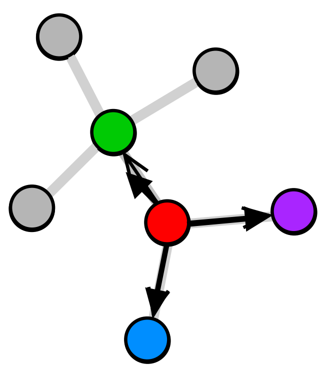
Spectral

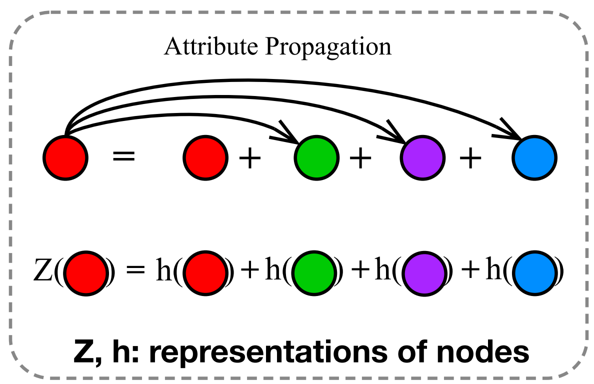
Linear function

Spatial-based GNN: Linear

Function of **graph matrix** $g(A)X$

Linear





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GraphSAGE

$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I}+\mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}+\tilde{\mathbf{A}})\mathbf{X}$$

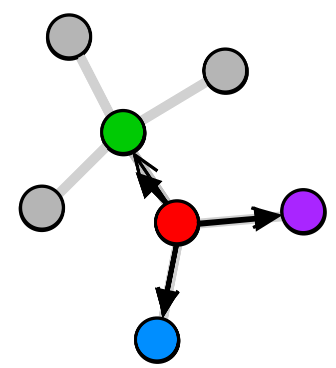
w/ mean aggregator

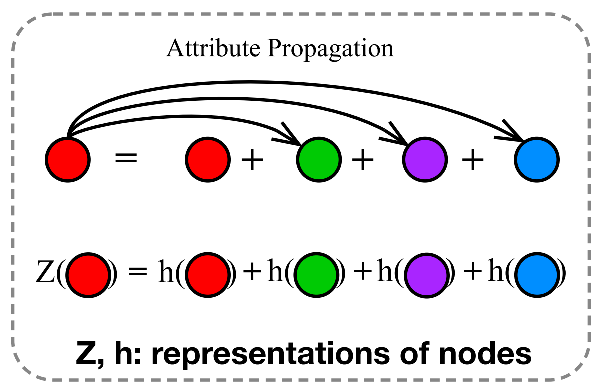
Hamilton, Will, Zhitao Ying, and Jure Leskovec. "Inductive representation learning on large graphs." Advances in neural information processing systems 30 (2017).

Spatial-based GNN: Linear

Function of **graph matrix** $g(A)X$

Linear





GCN *Thomas N. Kipf et al. (2016)*

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GraphSAGE *Will Hamilton et al. (2017)*

$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I}+\mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}+\tilde{\mathbf{A}})\mathbf{X}$$

GIN

$$\mathbf{Z} = (1+\epsilon)\cdot\mathbf{h}(v) + \sum_{u_j\in\mathcal{N}(v_i)}\mathbf{h}_{(u_j)} = [(1+\epsilon)\mathbf{I} + \mathbf{A}]\mathbf{X}$$

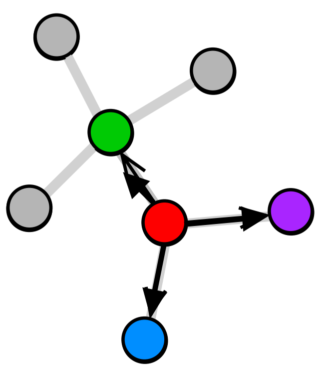
Control hyperparameter

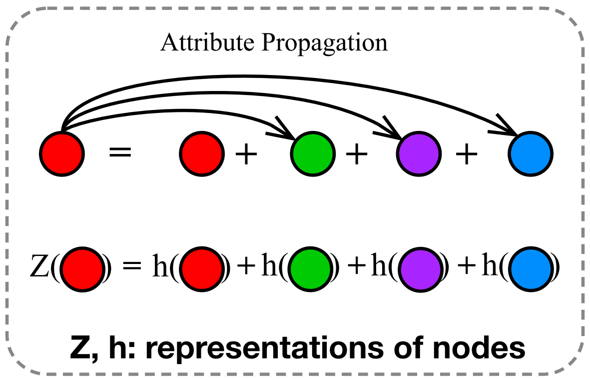
Xu, Keyulu, et al. "How Powerful are Graph Neural Networks?." International Conference on Learning Representations. 2018.

Spatial-based GNN: Linear

Function of **graph matrix** $g(A)X$

Linear





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GraphSAGE *Will Hamilton et al. (2017)*

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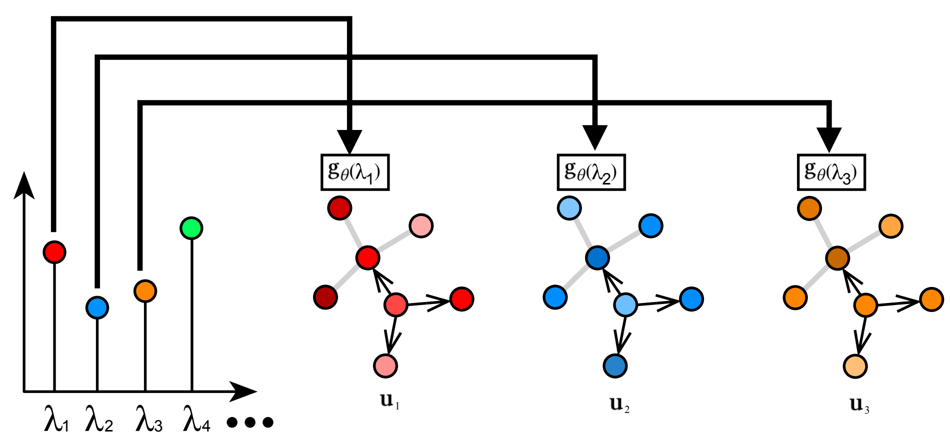
GIN

$$\mathbf{Z} = (1+\epsilon)\cdot\mathbf{h}(v) + \sum_{u_j \in \mathcal{N}(v_i)} \mathbf{h}(u_j) = [(1+\epsilon)\mathbf{I}+\mathbf{A}]\mathbf{X}$$

Function of **eigenvalue** $Ug_\theta(\Lambda)U^TX$

Linear



GCN *Thomas N. Kipf et al. (2016)*

$$\mathbf{Z} = \tilde{\mathbf{A}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{D}-\mathbf{L}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}-\mathbf{L}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{U}(2-\Lambda)\mathbf{U}^\top\mathbf{X}$$

GraphSAGE *Will Hamilton et al. (2017)*

$$Z = D^{-\frac{1}{2}}(I+A)D^{-\frac{1}{2}}X = (I+\tilde{A})X = (2I-\tilde{L})X = U(2-\Lambda)U^\top X$$

GIN *Xukeyu Lu et al. (2019)*

$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}[(1+\epsilon)\mathbf{I}+\mathbf{A}]\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}[(2+\epsilon)\mathbf{I}-\tilde{\mathbf{L}}]\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{U}(2+\epsilon-\Lambda)\mathbf{U}^\top\mathbf{X}$$

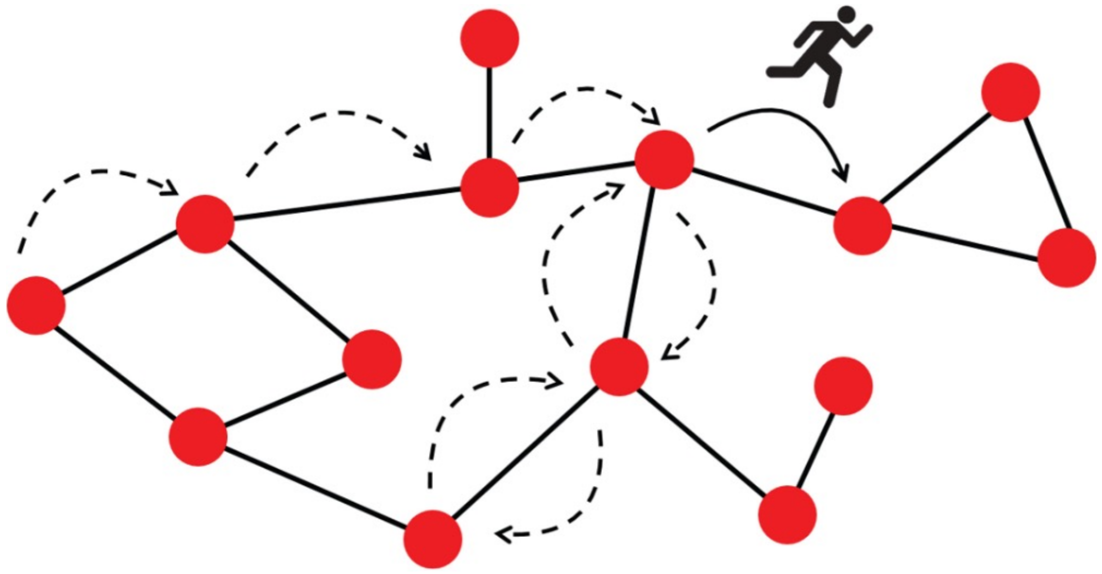
Case Study 2: DeepWalk

- Draw a group of random paths from a graph

$$\tilde{\mathbf{A}} = \mathbf{D}^{-1}\mathbf{A}$$

- Let the window size (path length) of skip-gram be $2t$+1and the current node is the (t+1)-th

$$\mathbf{Z} = \frac{1}{t+1}(\mathbf{I} + \tilde{\mathbf{A}} + \tilde{\mathbf{A}}^2 + \ldots + \tilde{\mathbf{A}}^t)\,\mathbf{X}$$

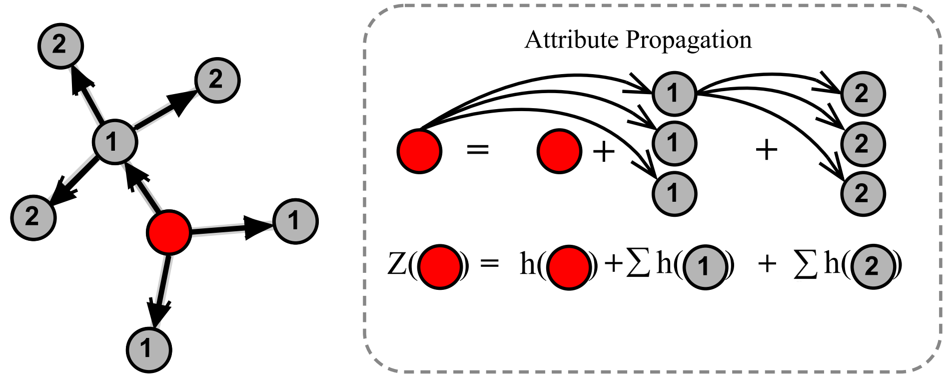


Img credit: DOI: (10.1002/sim.9346)

Spectral-based GNN: Polynomial

Function of **graph matrix** $g(A)X$

Polynomial



DeepWalk *Bryan Perozzi et al. (2014)*

$$\mathbf{Z} = \frac{1}{t+1}\left(\mathbf{I} + \tilde{\mathbf{A}} + \tilde{\mathbf{A}}^2 + \ldots + \tilde{\mathbf{A}}^t\right)\mathbf{X} = \frac{1}{t+1}\mathbf{P}(\tilde{\mathbf{A}})\mathbf{X}$$

ChebyNet *Defferrard, Michael et al. (2016)*

$$\mathbf{Z} = \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\mathbf{L}})\mathbf{X} = \left[\tilde{\theta}_0\mathbf{I} + \tilde{\theta}_1(\mathbf{I} - \tilde{\mathbf{A}}) + \tilde{\theta}_2(\mathbf{I} - \tilde{\mathbf{A}})^2 + \ldots\right]\mathbf{X} = \left(\phi\mathbf{I} + \sum_{i=1}^{k} \psi_i \tilde{\mathbf{A}}^i\right)\mathbf{X} = \mathbf{P}(\tilde{\mathbf{A}})\mathbf{X}$$

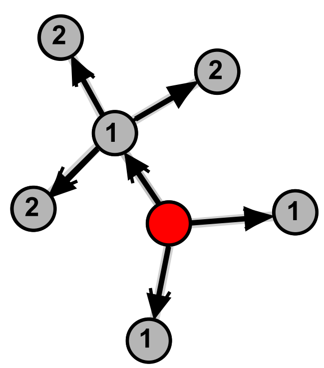
Chebyshev polynomial (1st kind) of L

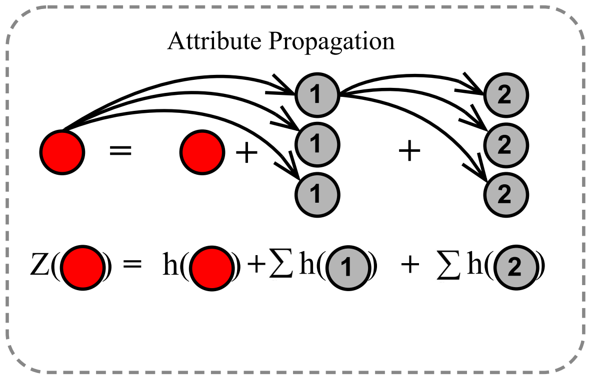
*Defferrard, et al., "**Convolutional neural networks on graphs with fast localized spectral filtering.**" Advances in neural information processing systems 29 (2016).*

Spectral-based GNN: Polynomial

Function of **graph matrix** $g(A)X$

Polynomial





DeepWalk *Bryan Perozzi et al. (2014)*

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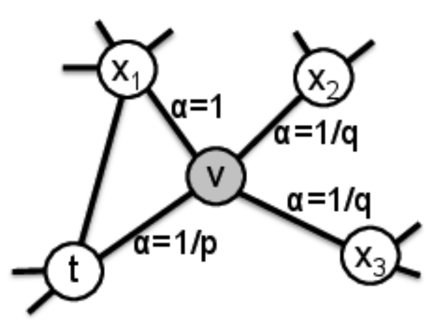
Node2Vec *Aditya Grover et al. (2016)*

$$\mathbf{Z} = \left(\frac{1}{p}\cdot\overbrace{\mathbf{I}}^{\text{source}} + \overbrace{\tilde{\mathbf{A}}}^{\text{BFS}} + \frac{1}{q}\overbrace{(\tilde{\mathbf{A}}^2 - \tilde{\mathbf{A}})}^{\text{DFS}}\right)\mathbf{X}$$

$$P(t \to x) = \begin{cases} \frac{1}{p} & \text{if } d(t,x) = 0, \text{ return to the source} \\ 1 & \text{if } d(t,x) = 1, \text{ BSF} \\ \frac{1}{q} & \text{if } d(t,x) = 2, \text{ DFS} \end{cases}$$



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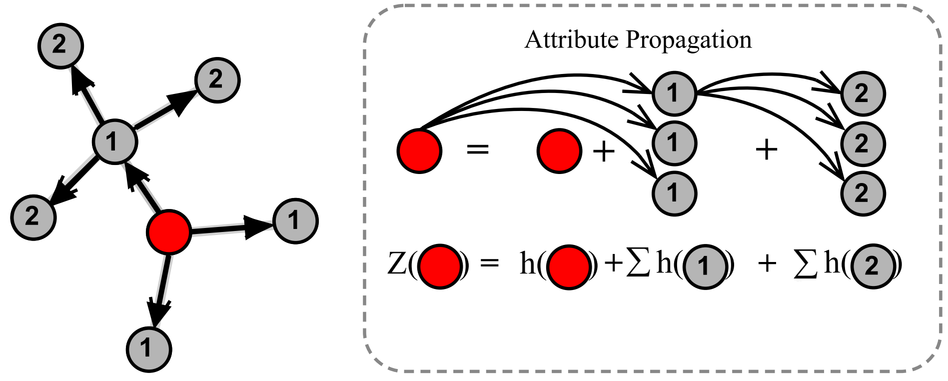
Spectral-based GNN: Polynomial

Function of **graph matrix** $g(A)X$

Polynomial



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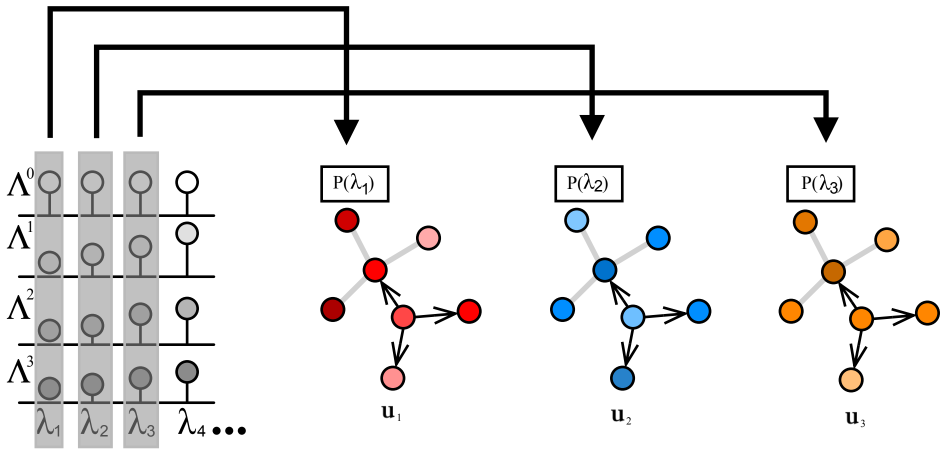
Function of **eigenvalue** $Ug_\theta(\Lambda)U^TX$

Polynomial



DeepWalk *Bryan Perozzi et al. (2014)*

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ChebyNet *Defferrard, Michael et al. (2016)*

$$\mathbf{Z} = \sum_{k=0}^{K-1}\theta_k T_k(\tilde{\mathbf{L}})\mathbf{X} = \mathbf{U}\left(\tilde{\theta}_0\cdot 1 + \tilde{\theta}_1\Lambda + \tilde{\theta}_2\Lambda^2 + \ldots\right)\mathbf{U}^\top\mathbf{X}$$

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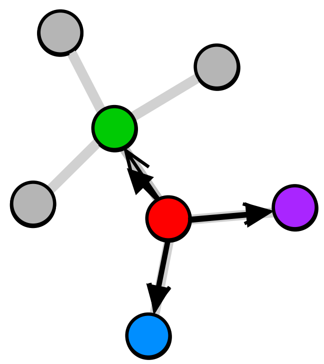
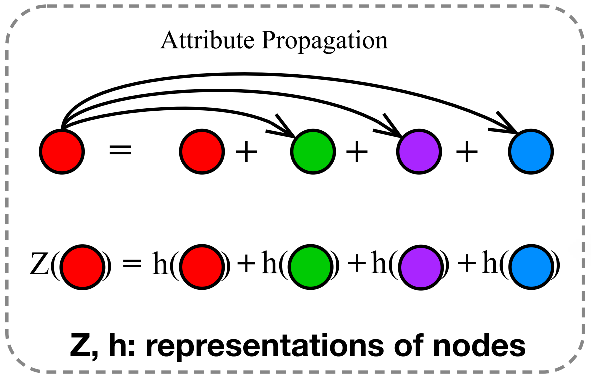
$$\mathbf{Z} = \left[\left(1+\frac{1}{p}\right)\mathbf{I} - \left(1+\frac{1}{q}\right)\tilde{\mathbf{L}} + \frac{1}{q}\tilde{\mathbf{L}}^2\right]\mathbf{X} = \mathbf{U}\left[\left(1+\frac{1}{p}\right) - \left(1+\frac{1}{q}\right)\tilde{\Lambda} + \frac{1}{q}\tilde{\Lambda}^2\right]\mathbf{U}^\top\mathbf{X}$$

Linear v.s. Polynomial

Function of **graph matrix** $g(A)X$

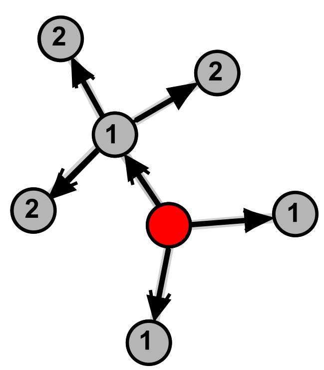
Linear

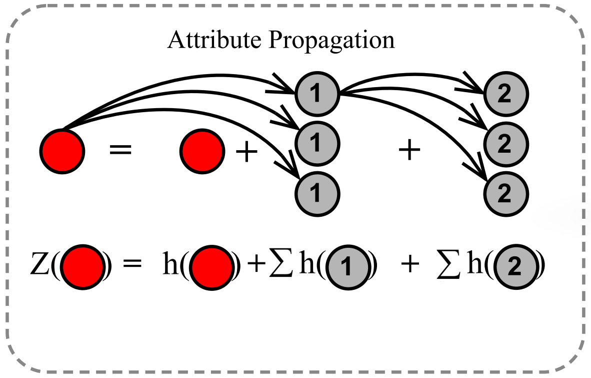




*only consider the **direct** neighbors*

Polynomial





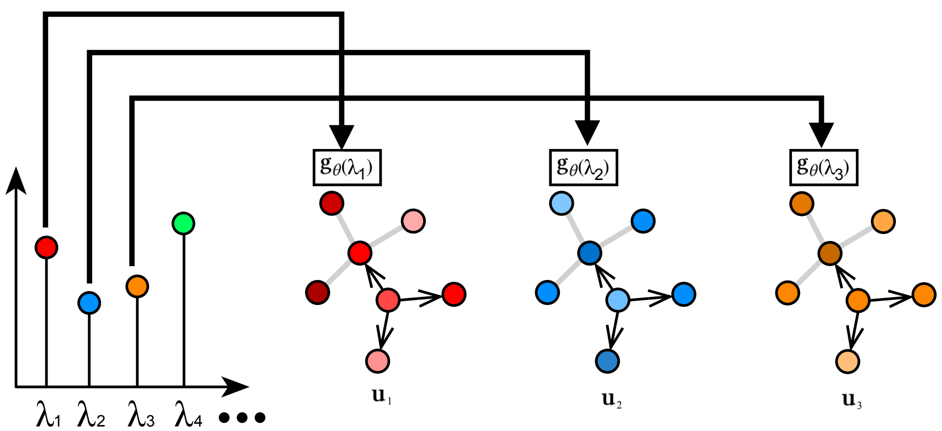
*consider the **higher-order** neighbors*

Linear v.s. Polynomial

"spectral response functions"

Function of **eigenvalue** $\quad U g_\theta(\Lambda) U^T X$

Linear



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GraphSAGE *Will Hamilton et al. (2017)*

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GIN *Xukeyu Lu et al. (2019)*

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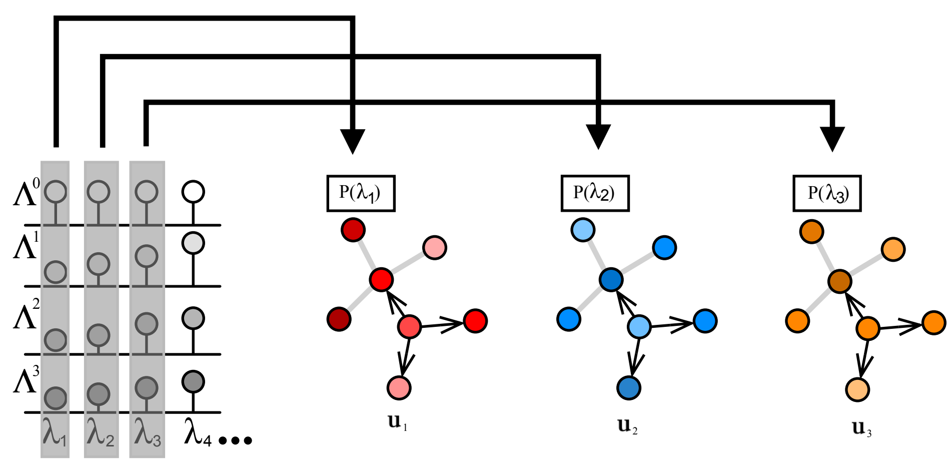
Polynomial



DeepWalk *Bryan Perozzi et al. (2014)*

$$\mathbf{Z} = \frac{1}{t+1}\left(\mathbf{I}+(\mathbf{I}-\tilde{\mathbf{L}})+(\mathbf{I}-\tilde{\mathbf{L}})^2+\ldots+(\mathbf{I}-\tilde{\mathbf{L}})^t\right)\mathbf{X} = \mathbf{U}\left(\theta_0+\theta_1\mathbf{\Lambda}+\theta_2\mathbf{\Lambda}^2+\ldots+\theta_t\mathbf{\Lambda}^t\right)\mathbf{U}^\top\mathbf{X}$$

ChebyNet *Defferrard, Michael et al. (2016)*

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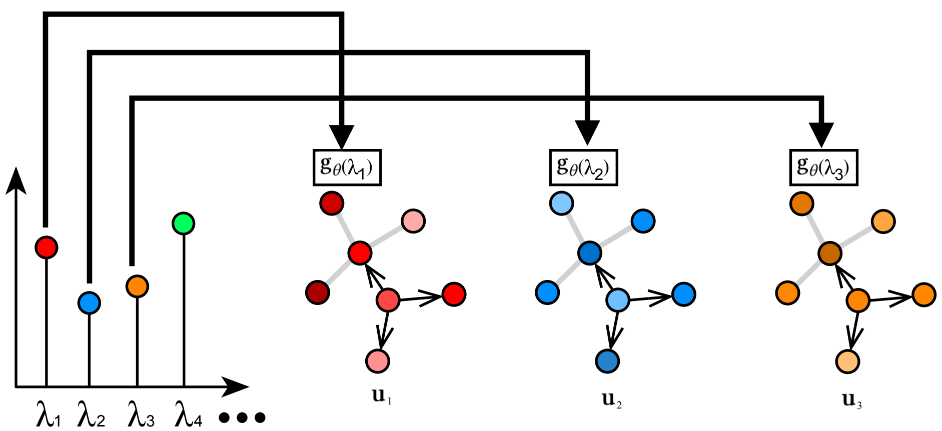
Linear v.s. Polynomial

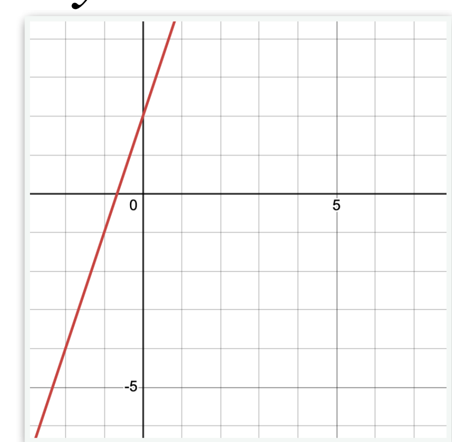
"spectral response functions"

Function of **eigenvalue** $\quad Ug_\theta(\Lambda)U^TX$

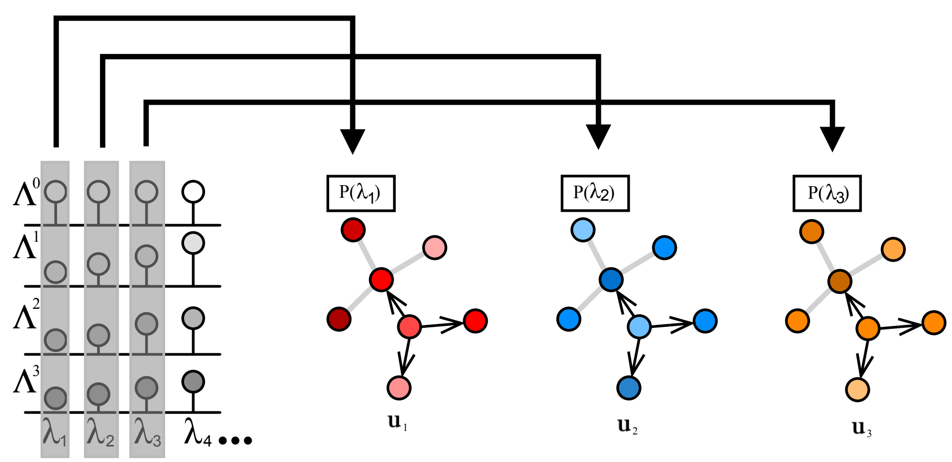
Linear



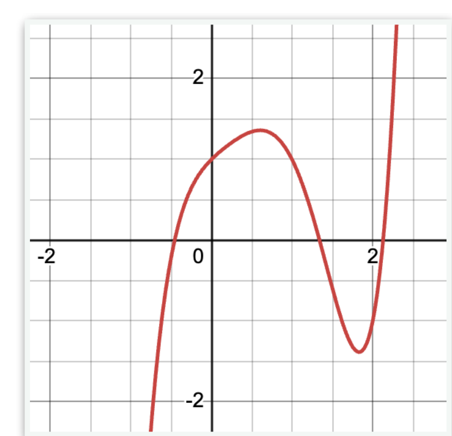
$y = 3x + 2$



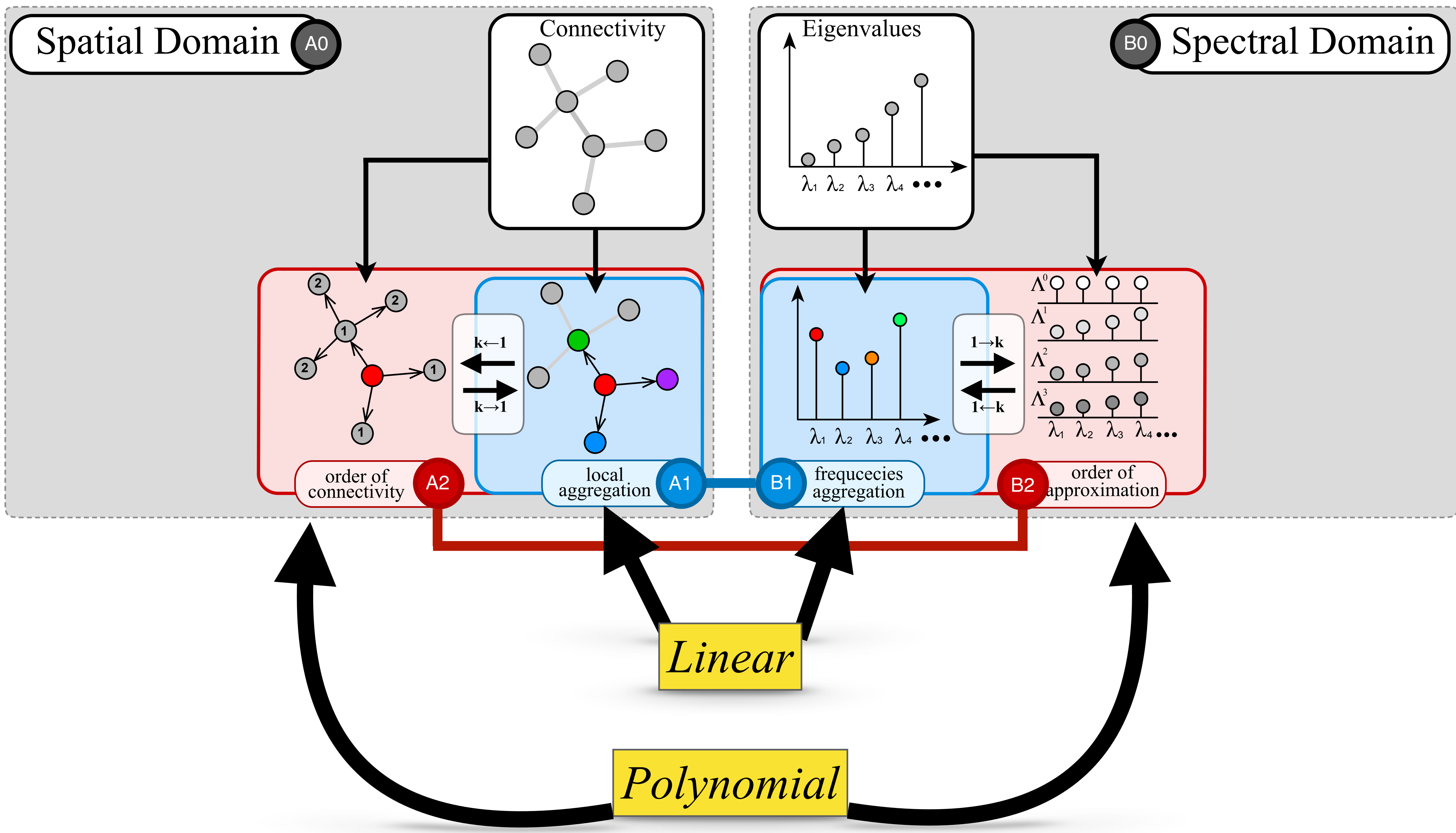
Polynomial



$y = x^5 - 3x^4 + 2x^3 - 0.3x^2 + x + 1$



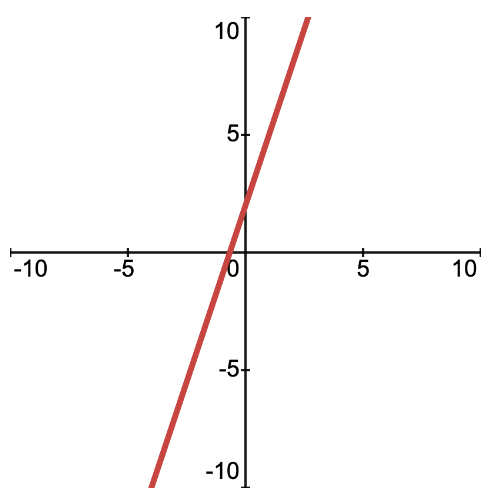
Linear v.s. Polynomial



Beyond Polynomial: Rational Model

GCN

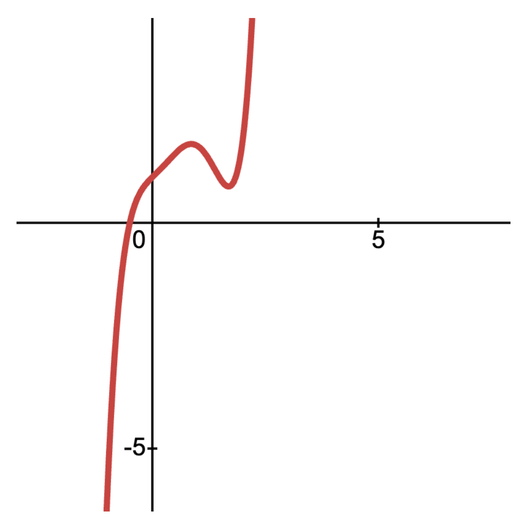
$$y = 3x + 2$$



Linear

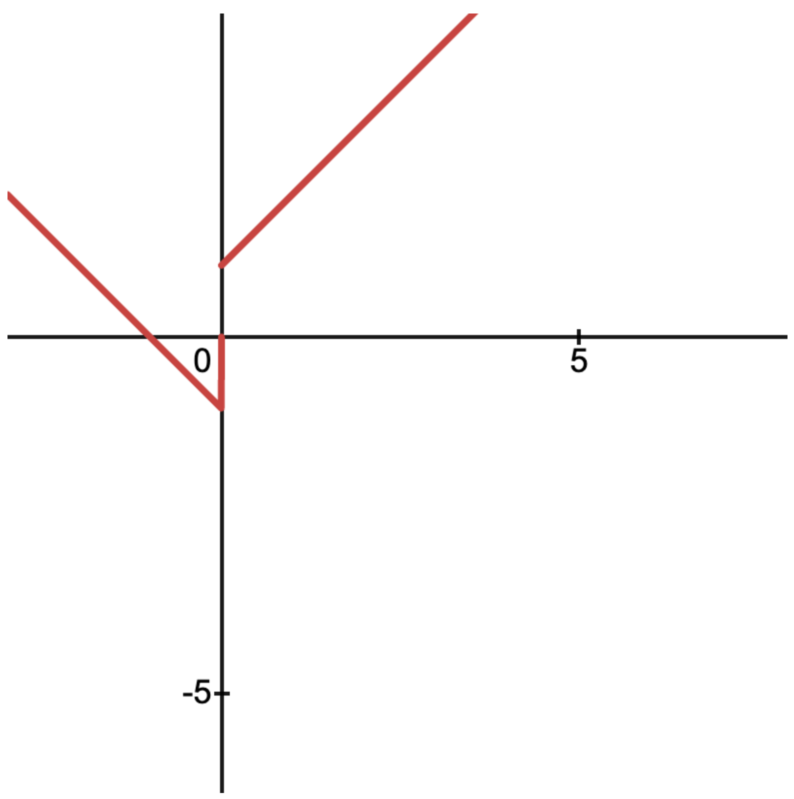
ChebNet

$$y = x^5 - 3x^4 + 2x^3 - 0.3x^2 + x + 1$$



Polynomial

What if non-smooth function



*Defferrard, et al., "**Convolutional neural networks on graphs with fast localized spectral filtering.**" Advances in neural information processing systems 29 (2016).*

Beyond Polynomial: Rational Model

Polynomial approximation

$$f(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_2 x^2 + a_1 x + a_0$$

Cheaper
Less accurate

- **simple** form, well known properties
- computationally **easy** to use

- **notorious** for oscillations between exact-fit value
- only high degree can model **complicated** structure
- **poor** interpolatory/extrapolatory/asymptotic properties

Rational approximation

$$f(x) = \frac{p(x)}{q(x)}$$

More expensive
More accurate

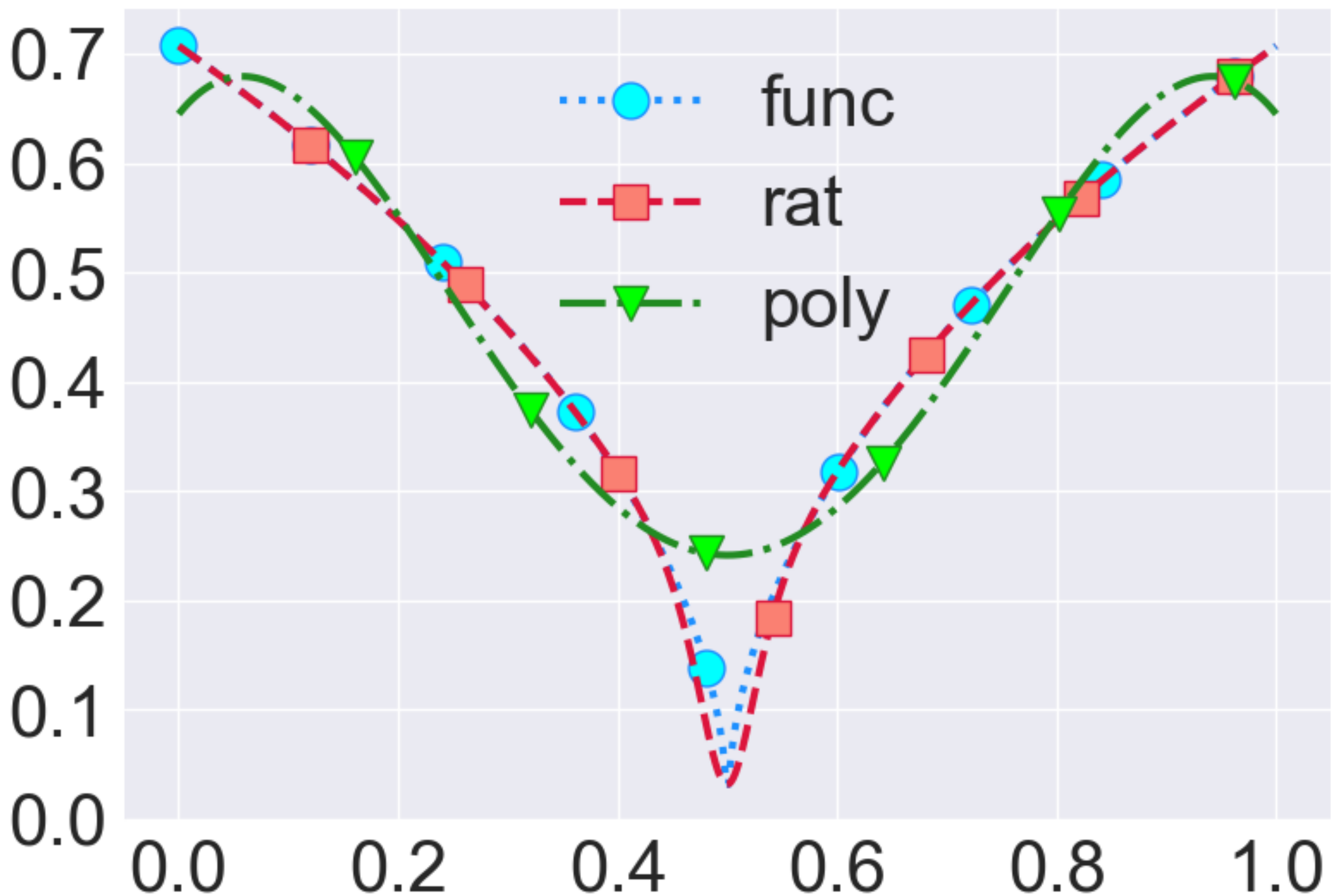
- moderately **simple** form, not well-known properties
- moderately **easy** to handle computationally

- **excellent** for oscillations between exact-fit value
- model **complicated** structure with a fairly low degree
- **excellent** interpolatory/extrapolatory/asymptotic properties

Trefethen, Lloyd N. ***Approximation theory and approximation practice***, *extended edition*. Society for Industrial and Applied Mathematics, 2019.

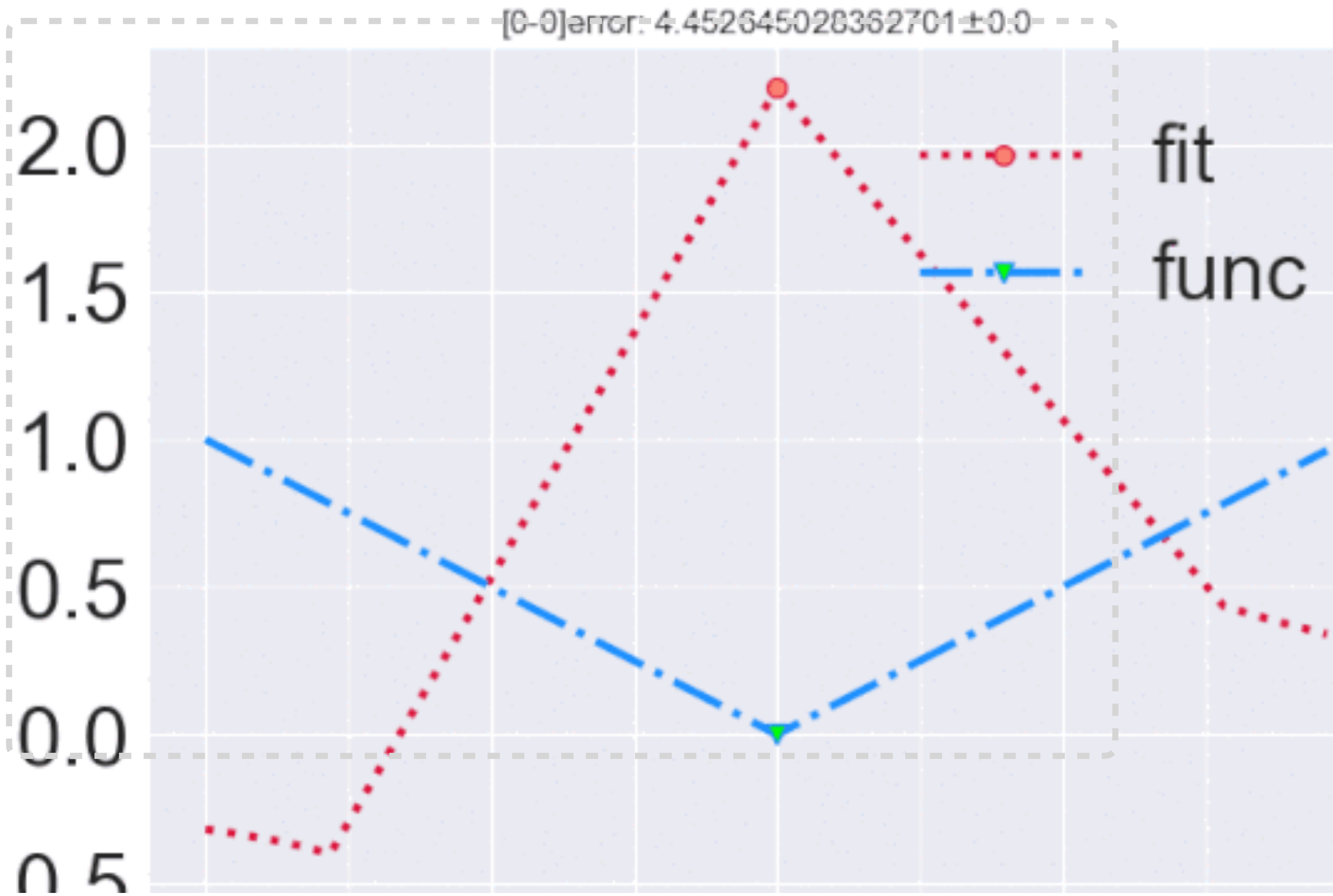
Beyond Polynomial: Rational Model

func: target function;
poly: polynomial approximation
rat: rational approximation



Telgarsky, M. (2017, July). ***Neural networks and rational functions***. *In International Conference on Machine Learning*

Beyond Polynomial: Rational Model



[Screenshots in every 100 epochs]

Rational Neural Network: iteratively close to the target

*Boullé, N., Nakatsukasa, Y., & Townsend, A. (2020). **Rational neural networks**. Advances in neural information processing systems*

*Zhiqian Chen, et al. **Rational Neural Networks for Approximating Graph Convolution Operator on Jump Discontinuities**, ICDM 2018*

Polynomial v.s. Rational

Polynomial

Thomas N. Kipf et al. (2016)

$$\mathbf{g} * x = \mathbf{U}\,\mathbf{g}(\mathbf{\Lambda})\,\mathbf{U}^\intercal x$$

$$\approx \mathbf{U}\sum_k \theta_k T_k(\tilde{\mathbf{\Lambda}})\,\mathbf{U}^\intercal x \qquad (\tilde{\mathbf{\Lambda}} = \frac{2}{\lambda_{max}}\mathbf{\Lambda} - \mathbf{I_N})$$

$$= \sum_k \theta_k T_k(\tilde{\mathbf{L}})x \qquad (\mathbf{U}\,\mathbf{\Lambda}^k\,\mathbf{U}^\intercal = (\mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^\intercal)^k)$$

$$= \mathbf{P}(\mathbf{L})\,x$$

$$= \boxed{\mathbf{P}(\mathbf{L})}\,\boxed{x}$$

$\mathbf{L}$ graph Laplacian

x node attributes

Rational

Z. Chen et al. (2018)

$$\mathrm{g}_\theta * x = \mathbf{U}\,\mathrm{g}_\theta\,\mathbf{U}^\intercal x \qquad \text{(convolution theorem)}$$

$$\approx \mathbf{U}\,\frac{\sum_{i=0}^{m}\psi_i\tilde{\mathbf{\Lambda}}^i}{1+\sum_{j=1}^{n}\phi_j\tilde{\mathbf{\Lambda}}^j}\,\mathbf{U}^\intercal x \qquad (\tilde{\mathbf{\Lambda}} = \frac{\mathbf{\Lambda}}{\lambda_{max}})$$

$$= \mathbf{U}\,\frac{\mathbf{P}(\mathbf{\Lambda})}{\mathbf{Q}(\mathbf{\Lambda})}\,\mathbf{U}^\intercal x, \qquad \text{(define P and Q)}$$

$$= \mathbf{P}(\mathbf{L})\,\mathbf{Q}(\mathbf{L})^{-1}x,$$

$$= \boxed{\mathbf{P}(\mathbf{L})}\,\boxed{\mathbf{Q}(\mathbf{L})^{-1}}\,\boxed{x}$$

Polynomial v.s. Rational

Polynomial

$\mathbf{P}(\mathbf{L})\ x$

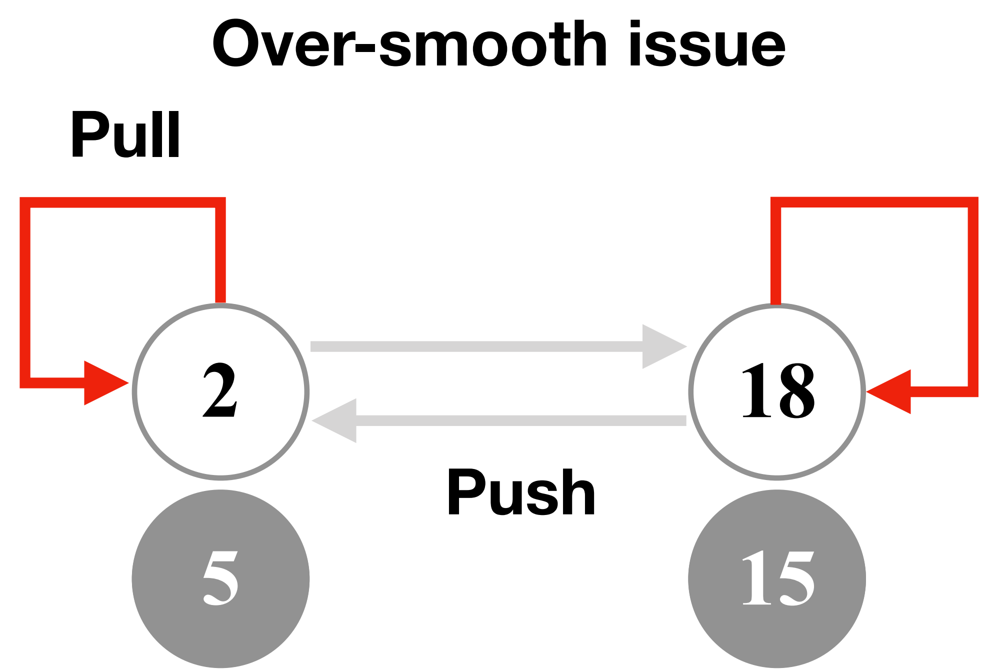
Label propagation

Rational

$\mathbf{P}(\mathbf{L})\,\mathbf{Q}(\mathbf{L})^{-1}\ x$

Label propagation

Reverse Label propagation



Polynomial v.s. Rational

Polynomial

$$\boxed{\mathbf{P}(\mathbf{L})}\ x$$

Label propagation

Rational

$$\boxed{\mathbf{P}(\mathbf{L})}\boxed{\mathbf{Q}(\mathbf{L})^{-1}}\ x$$

Reverse Label propagation

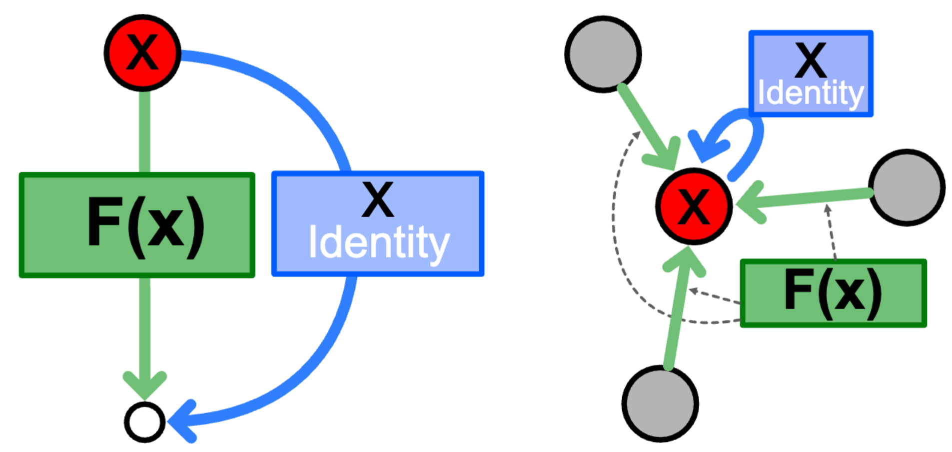


FIG. 6. Left: Residual Learning $x' = F(x) + x$; Right: Rational Aggregation: $x' = F(x) + x$

Polynomial v.s. Rational

Polynomial

$\boxed{\mathbf{P}(\mathbf{L})}\ x$

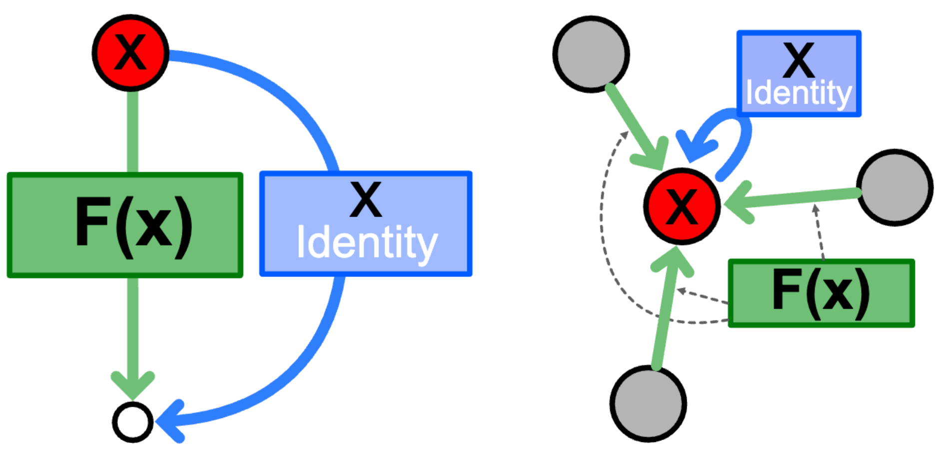
Label propagation

Rational

$\boxed{\mathbf{P}(\mathbf{L})}\boxed{\mathbf{Q}(\mathbf{L})^{-1}}\ x$

Reverse Label propagation

Polynomial



$$f + A \cdot f$$

Rational

Self Average of neighbors

$$g_\theta * f = U g_\theta U^\top f \quad = \underbrace{\boxed{f}}_{\text{Self}} + \underbrace{\boxed{A \cdot f}}_{\text{Average of neighbors}}$$

Polynomial v.s. Rational

Polynomial

$\mathbf{P}(\mathbf{L})\ x$

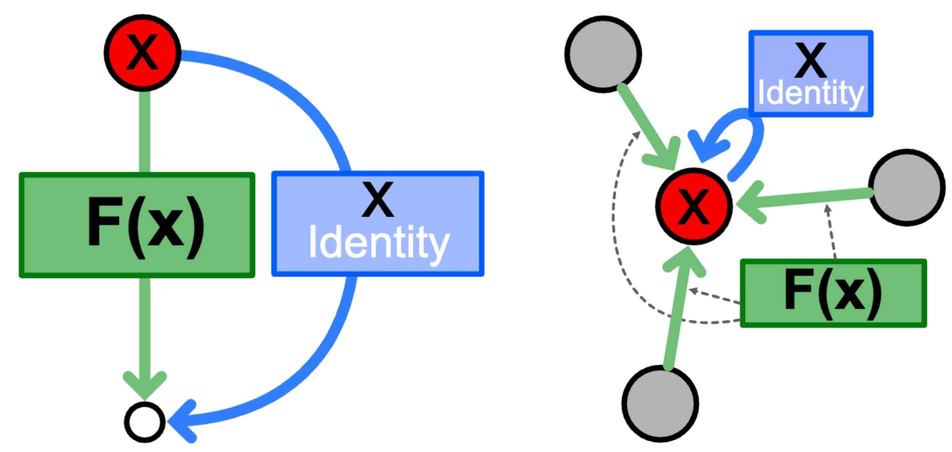
Label propagation

Rational

$\mathbf{P}(\mathbf{L})\,\mathbf{Q}(\mathbf{L})^{-1}\ x$

Reverse Label propagation

Polynomial



$f + A \cdot f$

*Add the **<u>original</u>** f at each iteration*

Rational

Self   Average of neighbors

$$g_\theta * f = U g_\theta U^\top f \ = \boxed{f} + \boxed{A \cdot f}$$

*Add the **<u>last</u>** f at each iteration*

Beyond Polynomial: Rational Model

Johannes Klicpera et al. (2018)

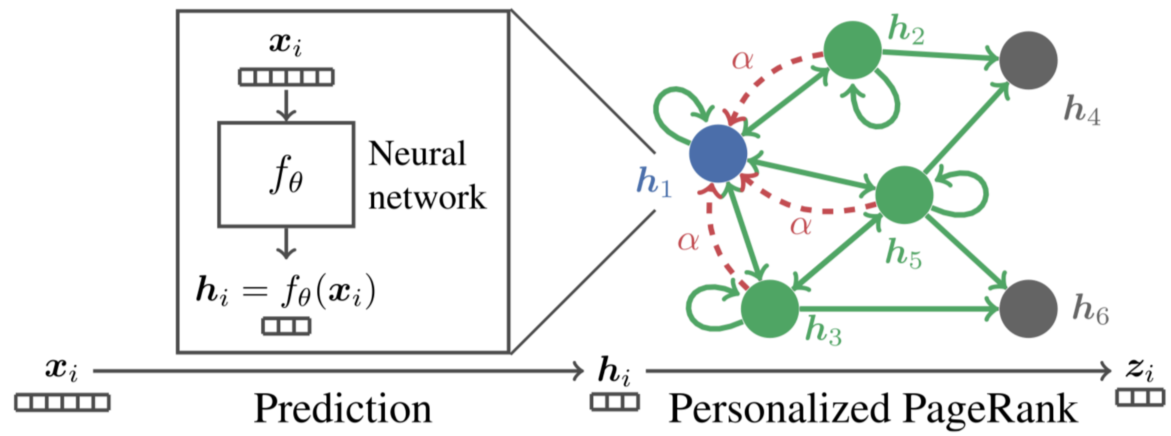
Personalized Page Rank (information retrieval)

$$\boldsymbol{\pi}_{\mathrm{ppr}}\left(\boldsymbol{i}_x\right) = (1-\alpha)\hat{\tilde{\boldsymbol{A}}}\boldsymbol{\pi}_{\mathrm{ppr}}\left(\boldsymbol{i}_x\right) + \alpha \boldsymbol{i}_x$$

$(1-\alpha)$ $\qquad$ α

PPNP

Personalized Propagation of Neural Predictions



Use personalized PageRank matrix $\boldsymbol{\Pi}_{\mathrm{ppr}}$ to propagate further while retaining information about root node, adjust via teleport probability α:

$$\boldsymbol{\Pi}_{\mathrm{ppr}} = \alpha\left(\boldsymbol{I}_n - (1-\alpha)\hat{\tilde{\boldsymbol{A}}}\right)^{-1}$$

$$\boxed{\frac{\alpha}{1-(1-\alpha)\lambda}}$$

Beyond Polynomial: Rational Model

Johannes Klicpera et al. (2018)

Personalized Page Rank (information retrieval)

Filippo Maria Bianchi et al. (2018)

ARMA (time series)

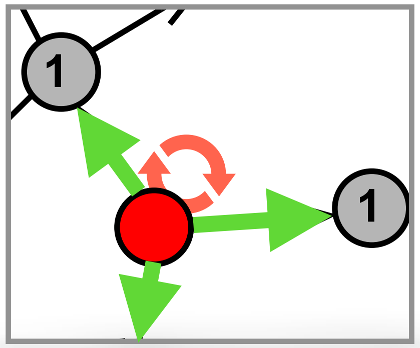
$$\boldsymbol{\pi}_{\text{ppr}}(\boldsymbol{i}_x) = (1-\alpha)\hat{\tilde{\mathbf{A}}}\boldsymbol{\pi}_{\text{ppr}}(\boldsymbol{i}_x) + \alpha\boldsymbol{i}_x$$

$(1-\alpha)$ $\qquad$ α

$$\bar{\mathbf{X}}^{(t+1)} = a\mathbf{M}\bar{\mathbf{X}}^{(t)} + b\mathbf{X}$$

a $\qquad$ b

$$\textit{next} = \alpha\ \textit{Push} + \beta\ \textit{Pull}$$



One iteration

K iterations →K-order rational function

Bianchi, Filippo Maria, et al. "Graph neural networks with convolutional arma filters." IEEE transactions on pattern analysis and machine intelligence 44.7 (2021): 3496-3507.

Why Rational, and Why Not?

- **Yes**
  - Non-smooth functions (Spectral) Physical meaning of non-smooth func in spatial?
  - Avoid over-smoothing (Spatial)
  - Approximation theory
    - rational is better than polynomial when order ≥ 5

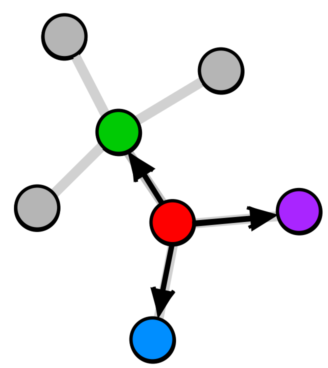
      Imply 5 iterations/layers
- **No**
  - Computational Complexity: Matrix Inversion

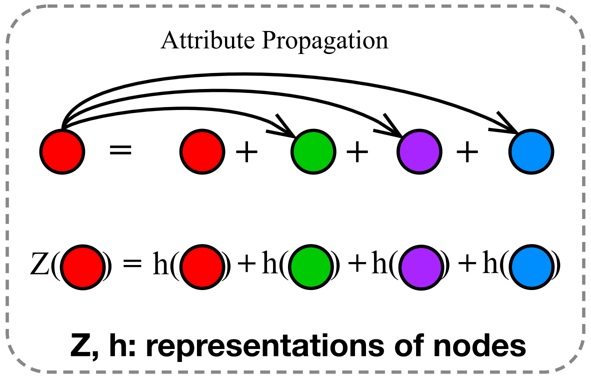
    $\mathcal{O}(n^3)$

Spatial-based GNN

Function of **graph matrix** $g(A)X$

Linear





GCN *Thomas N. Kipf et al. (2016)*

$$\mathbf{Z} = \hat{\mathbf{D}}^{-\frac{1}{2}}\hat{\mathbf{A}}\hat{\mathbf{D}}^{-\frac{1}{2}}\mathbf{X} = \hat{\mathbf{D}}^{-\frac{1}{2}}(\mathbf{I}+\mathbf{A})\hat{\mathbf{D}}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}+\tilde{\mathbf{A}})\mathbf{X}$$

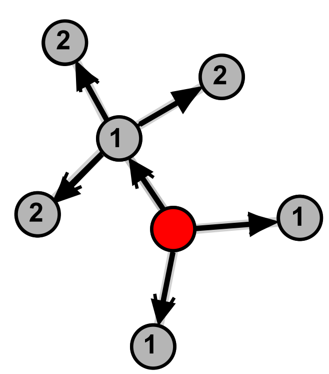
GraphSAGE *Will Hamilton et al. (2017)*

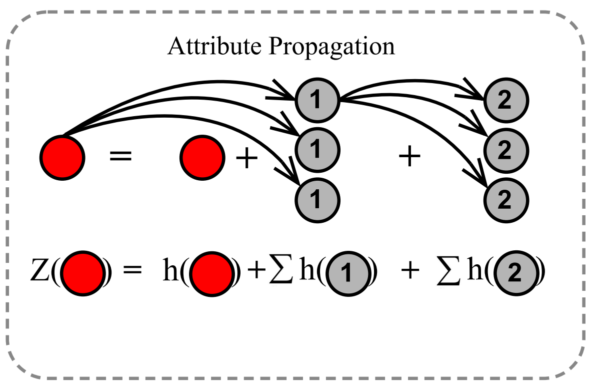
$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I}+\mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}+\tilde{\mathbf{A}})\mathbf{X}$$

GIN *Xukeyu Lu et al. (2019)*

$$\mathbf{Z} = (1+\epsilon)\cdot\mathbf{h}(v) + \sum\nolimits_{u_j\in\mathcal{N}(v_i)}\mathbf{h}\left(u_j\right) = [(1+\epsilon)\mathbf{I}+\mathbf{A}]\mathbf{X}$$

Polynomial





DeepWalk *Bryan Perozzi et al. (2014)*

$$\mathbf{Z} = \frac{1}{t+1}\left(\mathbf{I}+\tilde{\mathbf{A}}+\tilde{\mathbf{A}}^2+\ldots+\tilde{\mathbf{A}}^t\right)\mathbf{X} = \frac{1}{t+1}\mathbf{P}(\tilde{\mathbf{A}})\mathbf{X}$$

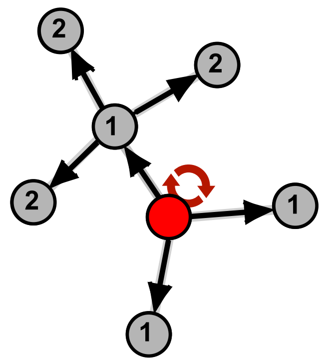
ChebyNet *Defferrard, Michael et al. (2016)*

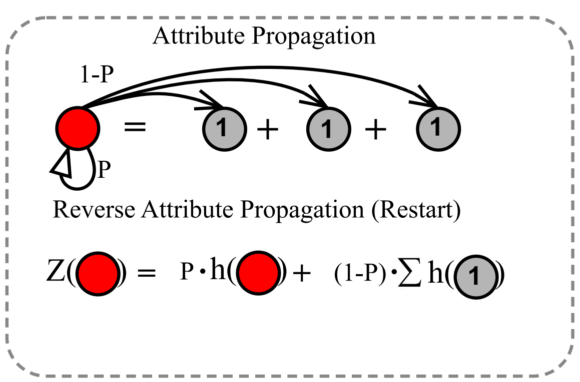
$$\mathbf{Z} = \sum\nolimits_{k=0}^{K-1}\theta_k T_k(\tilde{\mathbf{L}})\mathbf{X} = \left[\tilde{\theta}_0\mathbf{I}+\tilde{\theta}_1(\mathbf{I}-\tilde{\mathbf{A}})+\tilde{\theta}_2(\mathbf{I}-\tilde{\mathbf{A}})^2+\ldots\right]\mathbf{X} = \left(\phi\mathbf{I}+\sum\nolimits_{i=1}^{k}\psi_i\tilde{\mathbf{A}}^i\right)\mathbf{X} = \mathbf{P}(\tilde{\mathbf{A}})\mathbf{X}$$

Node2Vec *Aditya Grover et al. (2016)*

$$\mathbf{Z} = \left(\frac{1}{p}\cdot\mathbf{I}+\tilde{\mathbf{A}}+\frac{1}{q}\left(\tilde{\mathbf{A}}^2-\tilde{\mathbf{A}}\right)\right)\mathbf{X} = \left[\frac{1}{p}\mathbf{I}+\left(1-\frac{1}{q}\right)\tilde{\mathbf{A}}+\frac{1}{q}\tilde{\mathbf{A}}^2\right]\mathbf{X} = \mathbf{P}(\tilde{\mathbf{A}})\mathbf{X}$$

Rational





Personalized PageRank *Johannes Klicpera et al. (2018)*

$$\mathbf{Z} = \frac{\alpha}{\mathbf{I}-(1-\alpha)\tilde{\mathbf{A}}}\mathbf{X}$$

ARMA Filter *Filippo Maria Bianchi et al. (2018)*

$$\mathbf{Z} = \frac{b}{\mathbf{I}-a\tilde{\mathbf{A}}}\mathbf{X}$$

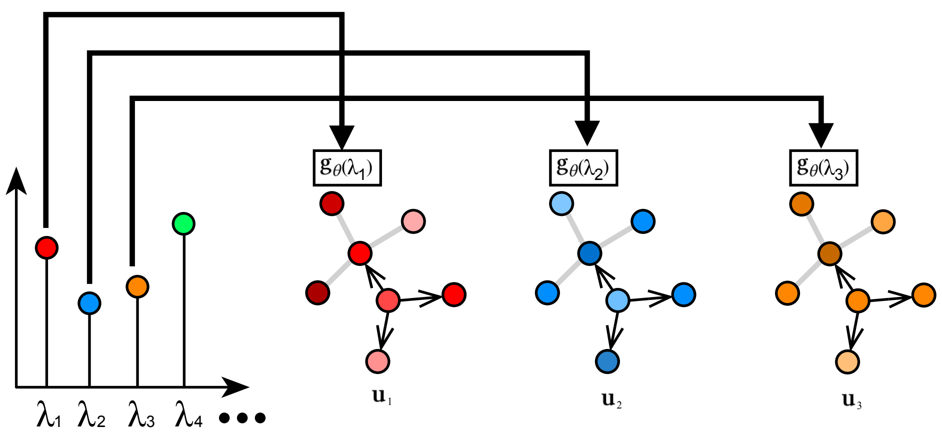
Auto Regressive Filter *Qimai Li et al. (2019)*

$$\mathbf{Z} = (\mathbf{I}+\alpha\tilde{\mathbf{L}})^{-1}\mathbf{X} = \frac{\mathbf{I}}{\mathbf{I}+\alpha(\mathbf{I}-\tilde{\mathbf{A}})}\mathbf{X}$$

Spectral-based GNN

Function of **eigenvalue** $Ug_{\theta}(\Lambda)U^{T}X$

Linear



GCN *Thomas N. Kipf et al. (2016)*

$$\mathbf{Z} = \tilde{\mathbf{A}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{D}-\mathbf{L}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}-\mathbf{L}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{U}(2-\Lambda)\mathbf{U}^{\top}\mathbf{X}$$

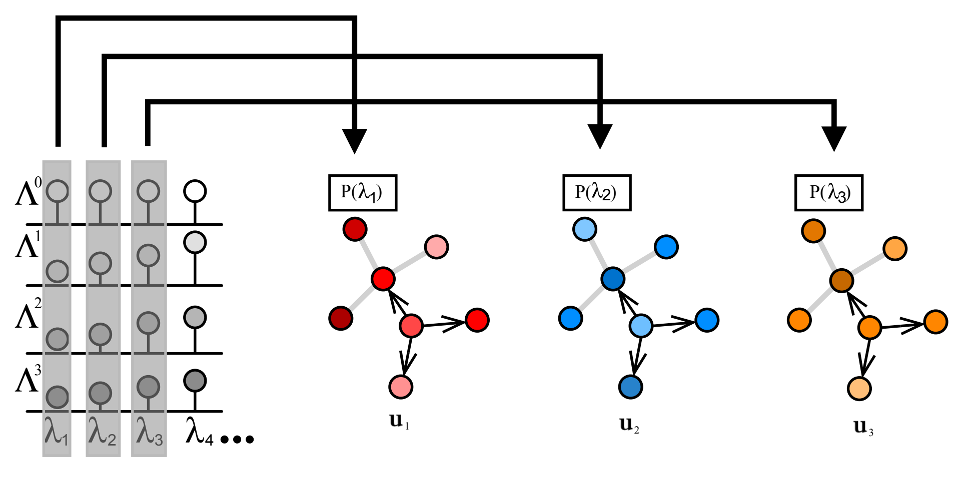
GraphSAGE *Will Hamilton et al. (2017)*

$$\mathrm{Z} = \mathrm{D}^{-\frac{1}{2}}(\mathrm{I}+\mathrm{A})\mathrm{D}^{-\frac{1}{2}}\mathrm{X} = (\mathrm{I}+\tilde{\mathrm{A}})\mathrm{X} = (2\mathrm{I}-\tilde{\mathrm{L}})\mathrm{X} = \mathrm{U}(2-\Lambda)\mathrm{U}^{\top}\mathrm{X}$$

GIN *Xukeyu Lu et al. (2019)*

$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}[(1+\epsilon)\mathbf{I}+\mathbf{A}]\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{D}^{-\frac{1}{2}}[(2+\epsilon)\mathbf{I}-\tilde{\mathbf{L}}]\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = \mathbf{U}(2+\epsilon-\Lambda)\mathbf{U}^{\top}\mathbf{X}$$

Polynomial



DeepWalk *Bryan Perozzi et al. (2014)*

$$\mathbf{Z} = \frac{1}{t+1}\left(\mathbf{I}+(\mathbf{I}-\tilde{\mathbf{L}})+(\mathbf{I}-\tilde{\mathbf{L}})^2+\ldots+(\mathbf{I}-\tilde{\mathbf{L}})^t\right)\mathbf{X} = \mathbf{U}\left(\theta_0+\theta_1\boldsymbol{\Lambda}+\theta_2\boldsymbol{\Lambda}^2+\ldots+\theta_t\boldsymbol{\Lambda}^t\right)\mathbf{U}^{\top}\mathbf{X}$$

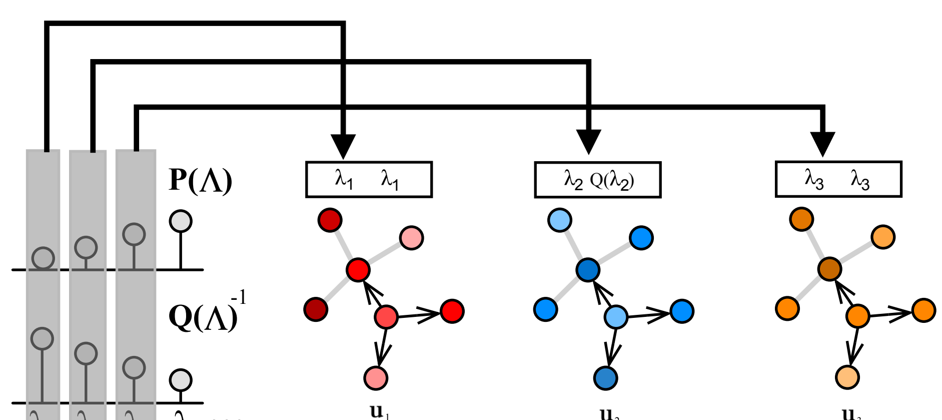
ChebyNet *Defferrard, Michael et al. (2016)*

$$\mathbf{Z} = \sum_{k=0}^{K-1}\theta_k T_k(\tilde{\mathbf{L}})\mathbf{X} = \mathbf{U}\left(\tilde{\theta}_0\cdot 1+\tilde{\theta}_1\Lambda+\tilde{\theta}_2\Lambda^2+\ldots\right)\mathbf{U}^{\top}\mathbf{X}$$

Node2Vec *Aditya Grover et al. (2016)*

$$\mathbf{Z} = \left[\left(1+\frac{1}{p}\right)\mathbf{I}-\left(1+\frac{1}{q}\right)\tilde{\mathbf{L}}+\frac{1}{q}\tilde{\mathbf{L}}^2\right]\mathbf{X} = \mathbf{U}\left[\left(1+\frac{1}{p}\right)-\left(1+\frac{1}{q}\right)\tilde{\Lambda}+\frac{1}{q}\tilde{\Lambda}^2\right]\mathbf{U}^{\top}\mathbf{X}$$

Rational



Personalized PageRank *Johannes Klicpera et al. (2018)*

$$\mathbf{Z} = \frac{\alpha}{\mathbf{I}-(1-\alpha)(\mathbf{I}-\tilde{\mathbf{L}})}\mathbf{X} = \mathbf{U}\frac{\alpha}{\alpha\mathbf{I}+(1-\alpha)\Lambda}\mathbf{U}^{\top}\mathbf{X}$$

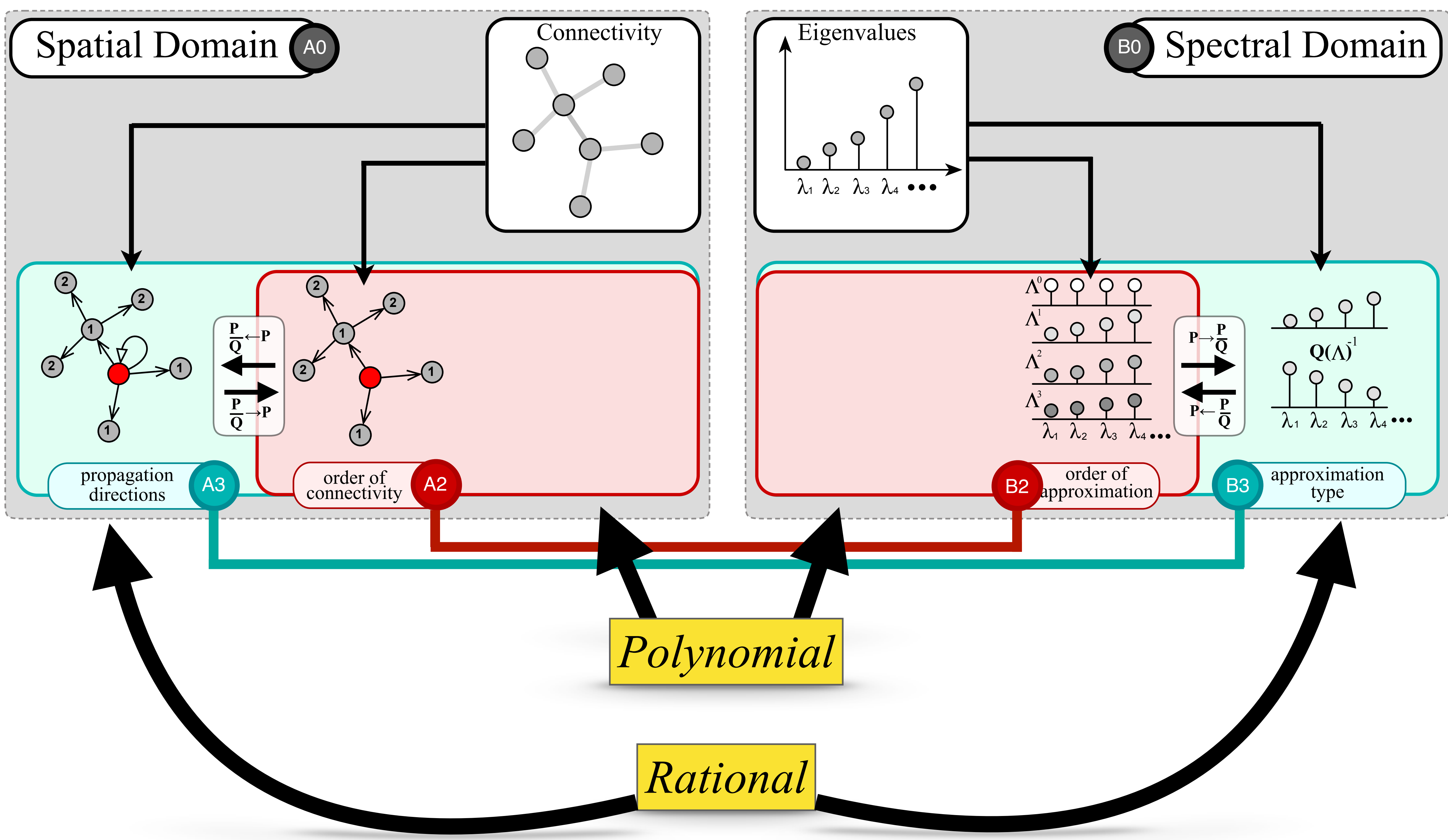
ARMA Filter *Filippo Maria Bianchi et al. (2018)*

$$\mathbf{Z} = \frac{b}{1-a(\mathbf{I}-\tilde{\mathbf{L}})}\mathbf{X} = \mathbf{U}\frac{b}{(1-a)\mathbf{I}+a\Lambda}\mathbf{U}^{\top}\mathbf{X}$$

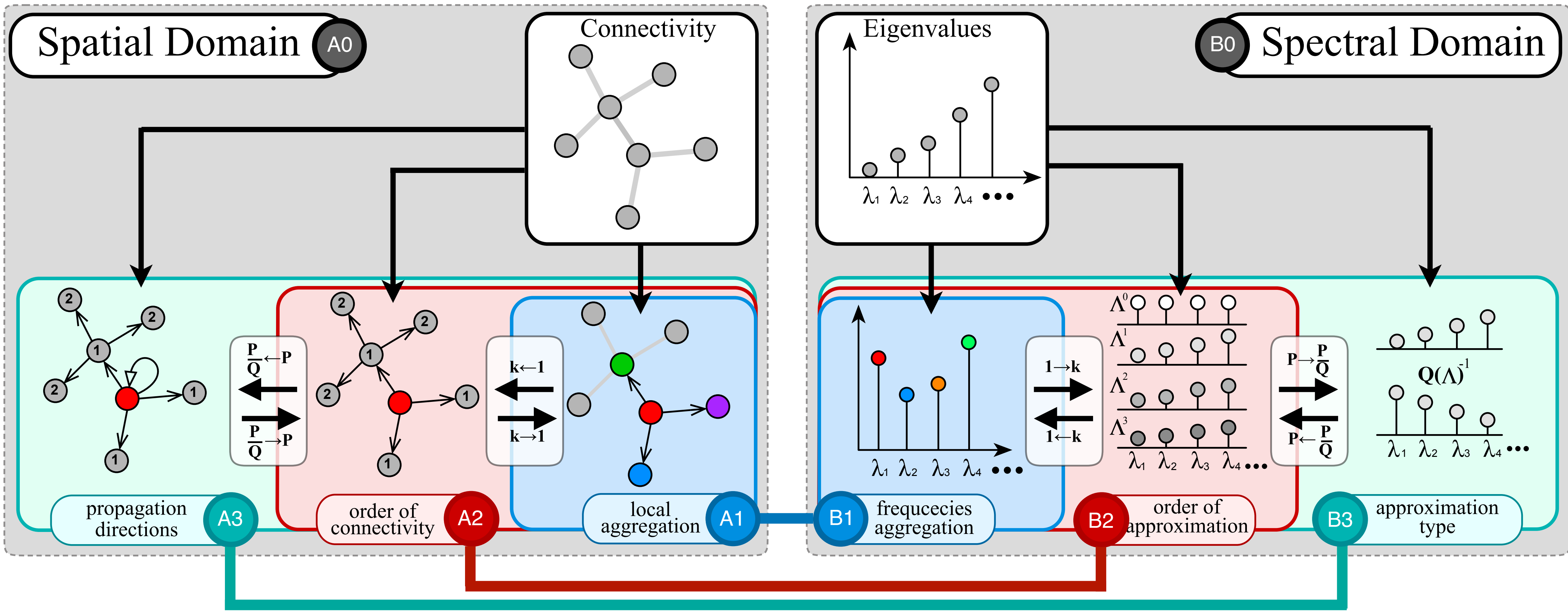
Auto Regressive Filter *Qimai Li et al. (2019)*

$$\mathbf{Z} = (\mathbf{I}+\alpha\tilde{\mathbf{L}})^{-1}\mathbf{X} = \mathbf{U}\frac{1}{1+\alpha(1-\Lambda)}\mathbf{U}^{\top}\mathbf{X}$$

Rational v.s. Polynomial



The Unified Framework



	Linear	Polynomial	Rational
Spatial			
Spectral			

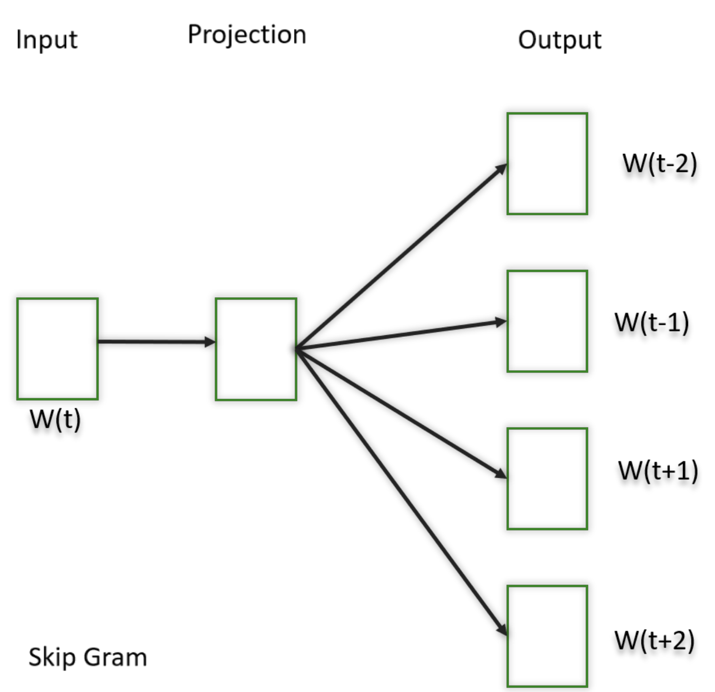
Complex, Powerful

Spatial v.s. Spectral

Spatial, local ⟷ **Spectral, global**

Word2Vec

Tomas Mikolvet et al. (2013)



W2V as Implicit MF

Omer Levy et al. (2014)

$$WC^T = M$$

↑

Shifted PMI (co-occurrence matrix)

Matrix Factorization, O(n^3)

I am similar to neighbors

Co-Occurrence matrix decomposition

Levy, Omer, and Yoav Goldberg. "**Neural word embedding as implicit matrix factorization.**" Advances in neural information processing systems 27 (2014).

Spatial v.s. Spectral

Spatial, local ⟷ **Spectral, global**

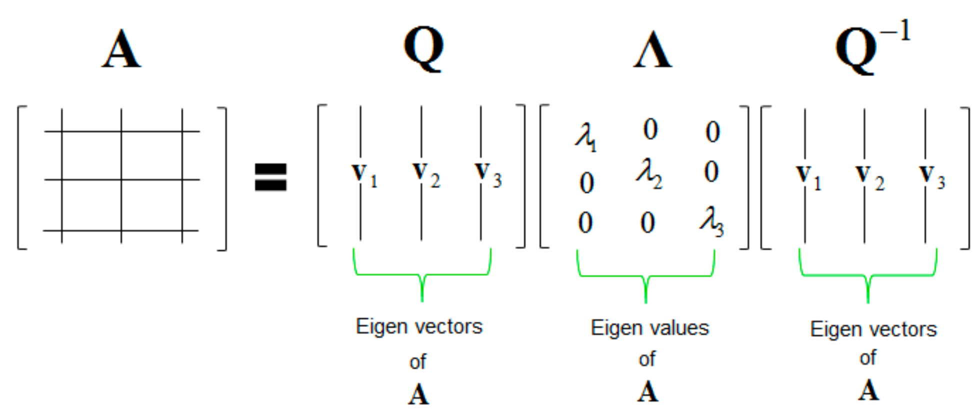
SpectralNet

Uri Shaham et al. (2018)

$$L_{\text{SpectralNet}}(\theta) = \frac{1}{m^2} \sum_{i,j=1}^{m} W_{i,j} \|y_i - y_j\|^2,$$

$$\mathbb{E}\left[yy^T\right] = I_{k \times k}$$

Spectral Clustering



Spectral Decomposition

Complexity	Spatial	Spectral
Space	Only involves local neighbors each time	Matrix factorization takes more
Time	Many iterations, trade-off between #iteration vs convergence	One-time expensive matrix factorization

Shaham, Uri, et al. "**Spectralnet: Spectral clustering using deep neural networks.**" ICLR (2018).

Spatial v.s. Spectral

	Methodology	Computation	Space Complexity	Stability
Spectral	Global	One-step	High	Exact
Spatial	Local	Iterative	Low	Approximate

Agenda

- **First Half (1 hour 15 min)**
  - *Background*: **unified frameworks for GNN** (35 min)
  - *Preliminary*: **graph convolutions** (40 min)
  - BREAK (15min)
- **Second Half (1 hour)**
  - *Introduction*: **a new unified framework** (40 min)
  - *Future directions* (20min)
  - Q&A (15min)

Future Directions

- PDE
  - Waves v.s. Diffusions is similar to Rational v.s. Polynomial

2.5 COMPARISON OF WAVES AND DIFFUSIONS

Property		Waves	Diffusions
(i)	Speed of propagation?	Finite ($\leq c$)	Infinite
(ii)	Singularities for $t > 0$?	Transported along characteristics (speed $= c$)	Lost immediately
(iii)	Well-posed for $t > 0$?	Yes	Yes (at least for bounded solutions)
(iv)	Well-posed for $t < 0$?	Yes	No
(v)	Maximum principle	No	Yes
(vi)	Behavior as $t \to +\infty$?	Energy is constant so does not decay	Decays to zero (if ϕ integrable)
(vii)	Information	Transported	Lost gradually

Rational Polynomial

Strauss, W. A. (2007). ***Partial differential equations: An introduction***. John Wiley & Sons.

Future Directions

- Spectral graph beyond simple graph
  - Signed
  - **Directed**
  - Higher-order (hypergraph, simplicial complex)
  - etc

*Levie, Ron, et al. "**Transferability of spectral graph convolutional neural networks.**" Journal of Machine Learning Research 22.272 (2021): 1-59.*

Future Directions

- Hodge Laplacian

$$L_k := L_k^{\text{down}} + L_k^{\text{up}}$$

$$L_k^{\text{down}} := B_k^\top B_k$$

$$L_k^{\text{up}} := B_{k+1} B_{k+1}^\top$$

L_1 is normal graph Laplacian

- GCN: 0**st-order** information propagate over 1**nd-order** connectivity

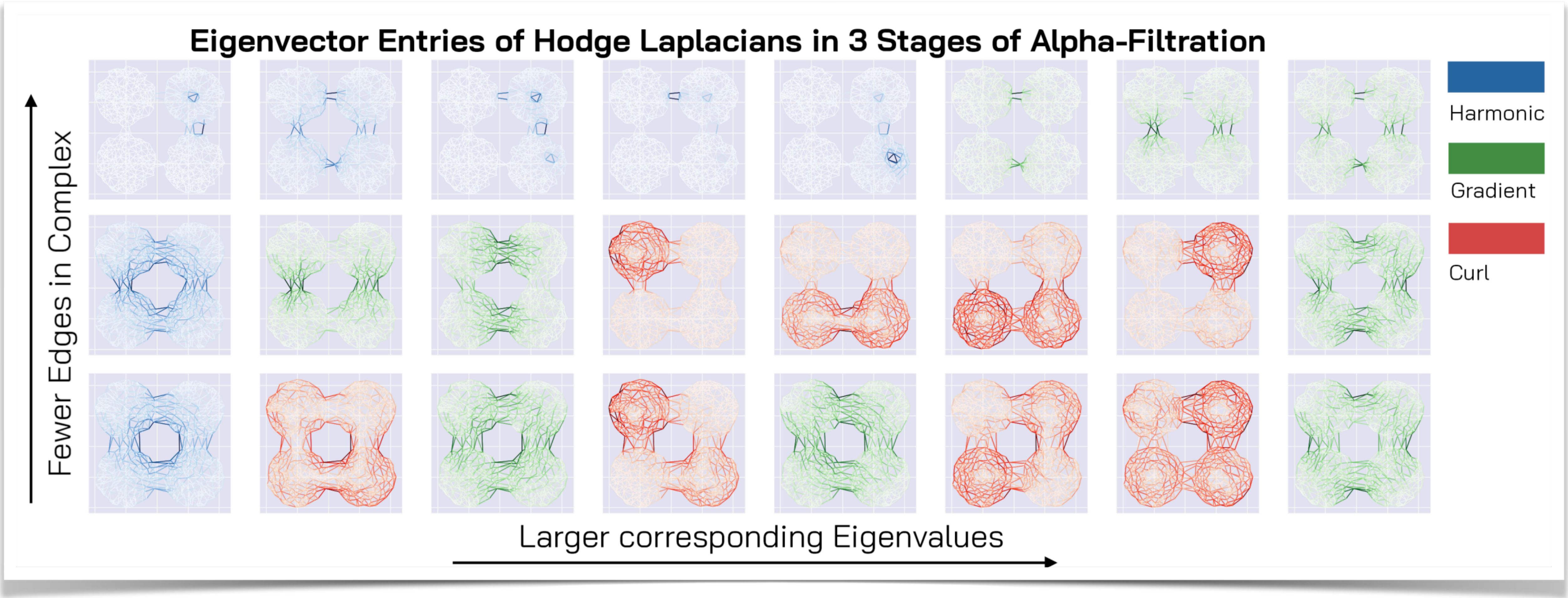
Function of **graph matrix** $g(A)X$

- xGCN: (x)**st-order** information propagate over (x+1)**nd-order** connectivity

Grande, Vincent P., and Michael T. Schaub. "Disentangling the Spectral Properties of the Hodge Laplacian: not all small Eigenvalues are Equal." ICASSP 2024. IEEE, 2024.

Future Directions

- Hodge decomposition
  - Decompose dynamics into 3 categories



Grande, Vincent P., and Michael T. Schaub. "Disentangling the Spectral Properties of the Hodge Laplacian: not all small Eigenvalues are Equal." ICASSP 2024. IEEE, 2024.

Future Directions

- Quantum Computing for Spectral Method
  - Quantum algorithms such as the Quantum Phase Estimation (QPE) algorithm can be used to find the eigenvalues and eigenvectors of a matrix more efficiently than classical algorithms

- *Classical Algorithm:* $\mathcal{O}(n^3)$
- *QPE:* $\mathcal{O}((log(n))^2/\epsilon)$ *with precision* ϵ

Conclusion

- Connection between spectral and spatial domain
  - Spatial: function of adjacency matrix
  - Spectral: function of eigenvalues
- Linear, polynomial and rational function
  - more power, more computation
- Computation
  - Spatial method: iterative and cheap approximation
  - Spectral method: one-step, expensive and exact

Thank You & Q/A

Awesome Spectral Graph Neural Networks

PRs Welcome awesome

Contents

- Survey Papers
- Milestone Papers
- Spatial and Spectral Views
- Twin Papers
- Applications
- Code
- Citation

https://github.com/XGraph-Team/Spectral-Graph-Survey