Approximation Theory for Graph Machine Learning

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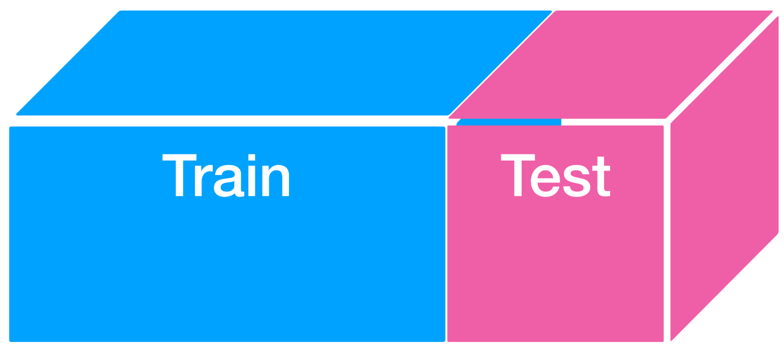
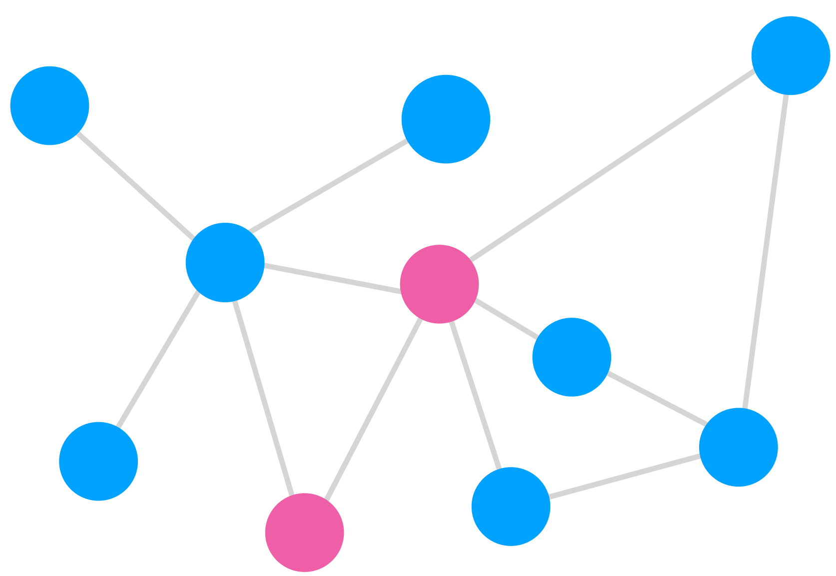
Graph Machine Learning

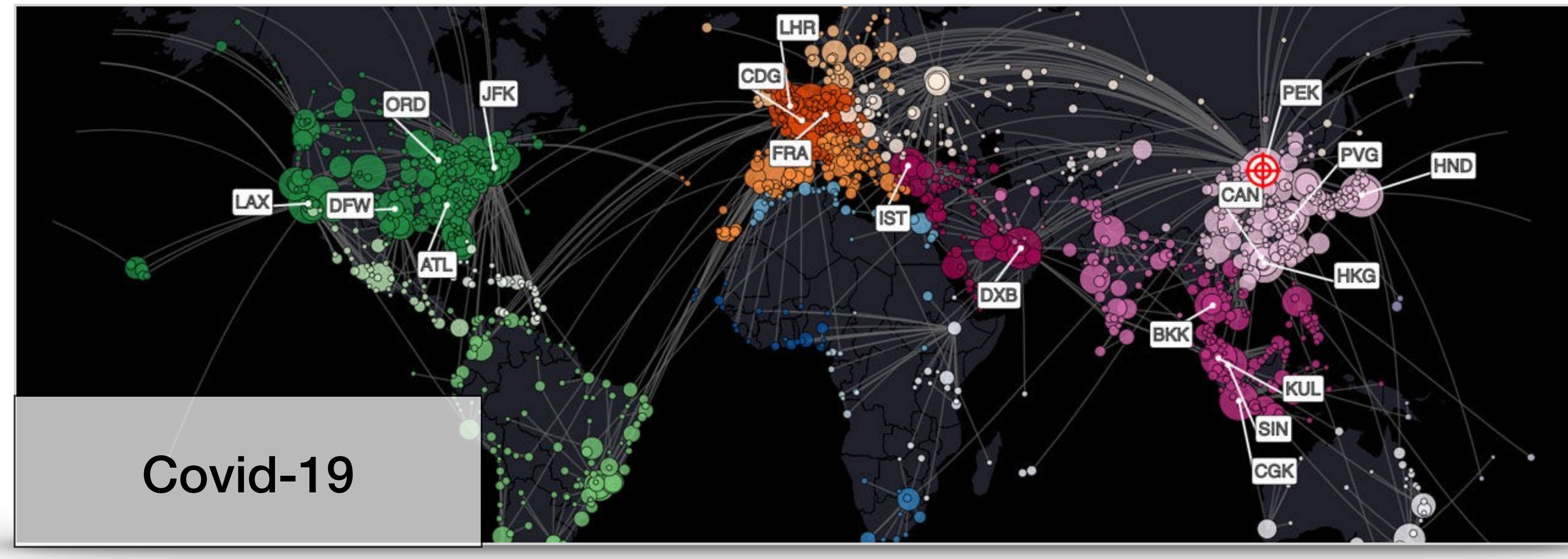


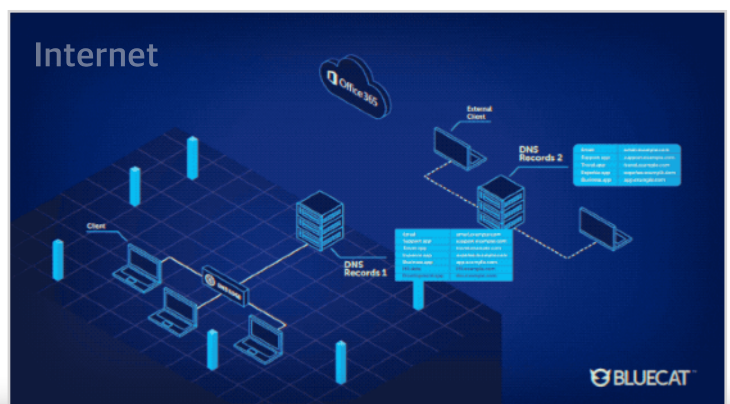
Machine Learning
Block Split

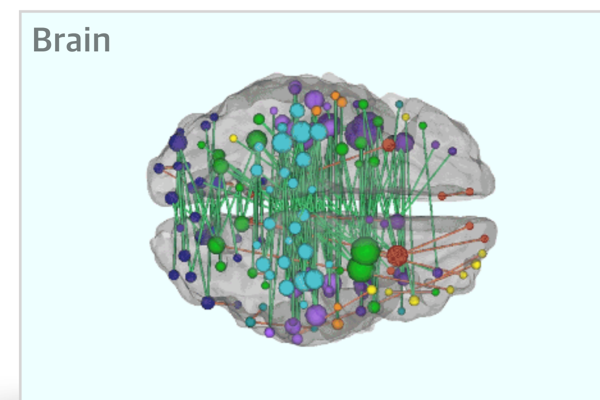


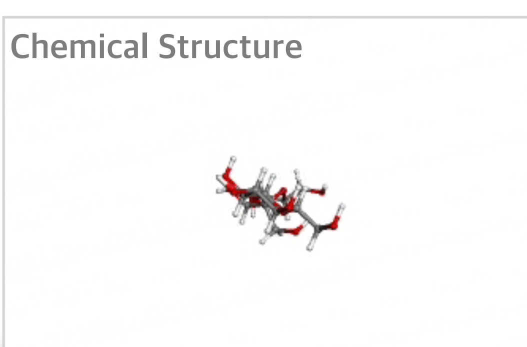
Graph Machine Learning
Geometric Split

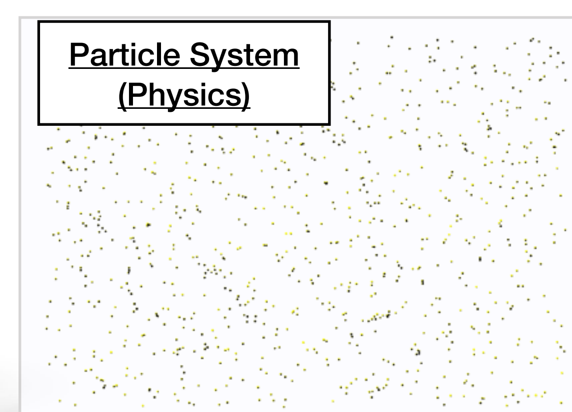
Graph is Pervasive



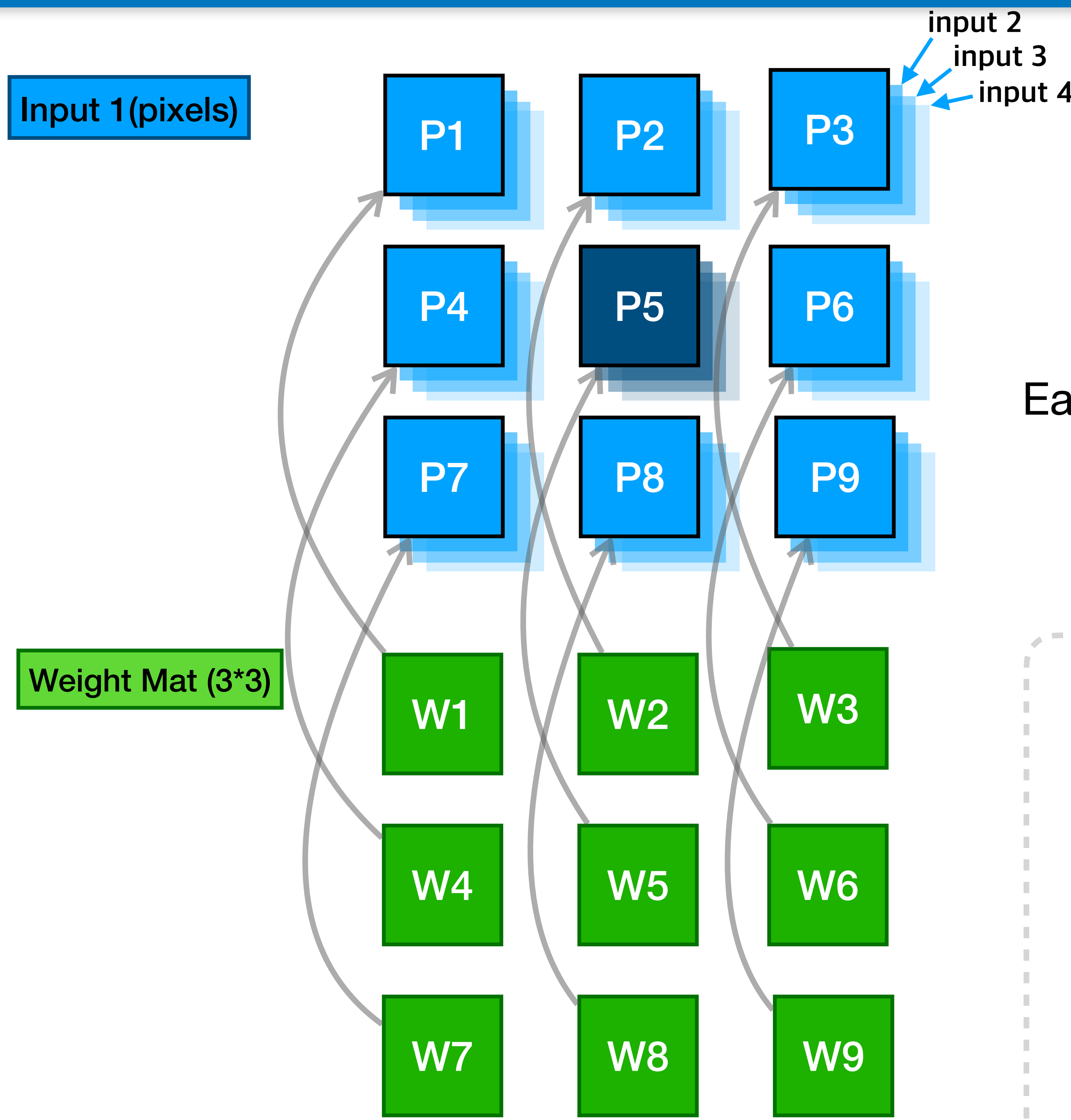








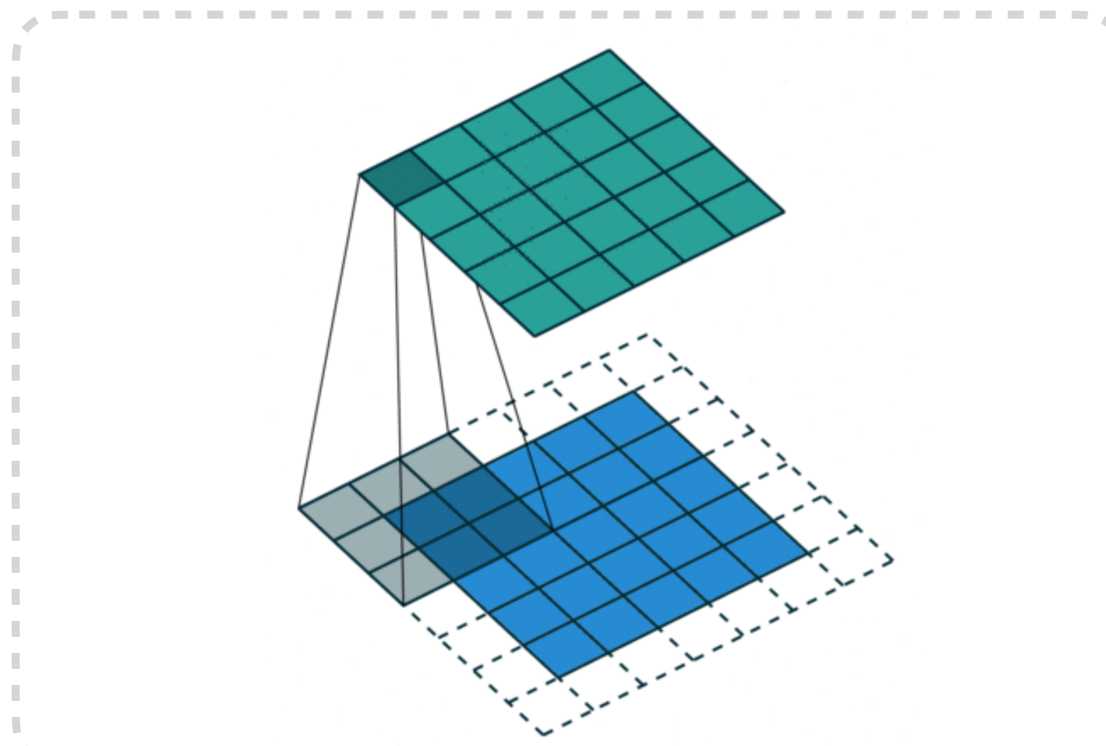
Convolutional Neural Networks



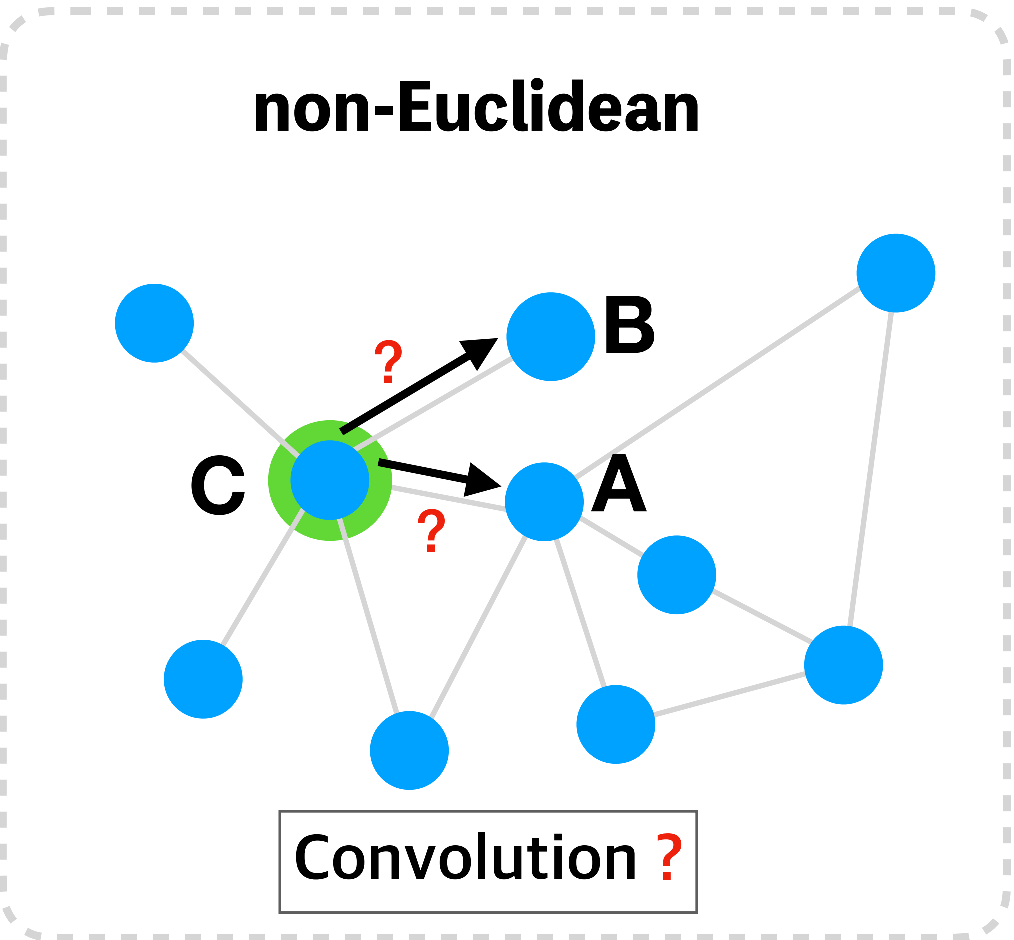
$$\hat{P}_5 = \sum_{i=1}^{9} P_i \cdot W_i$$

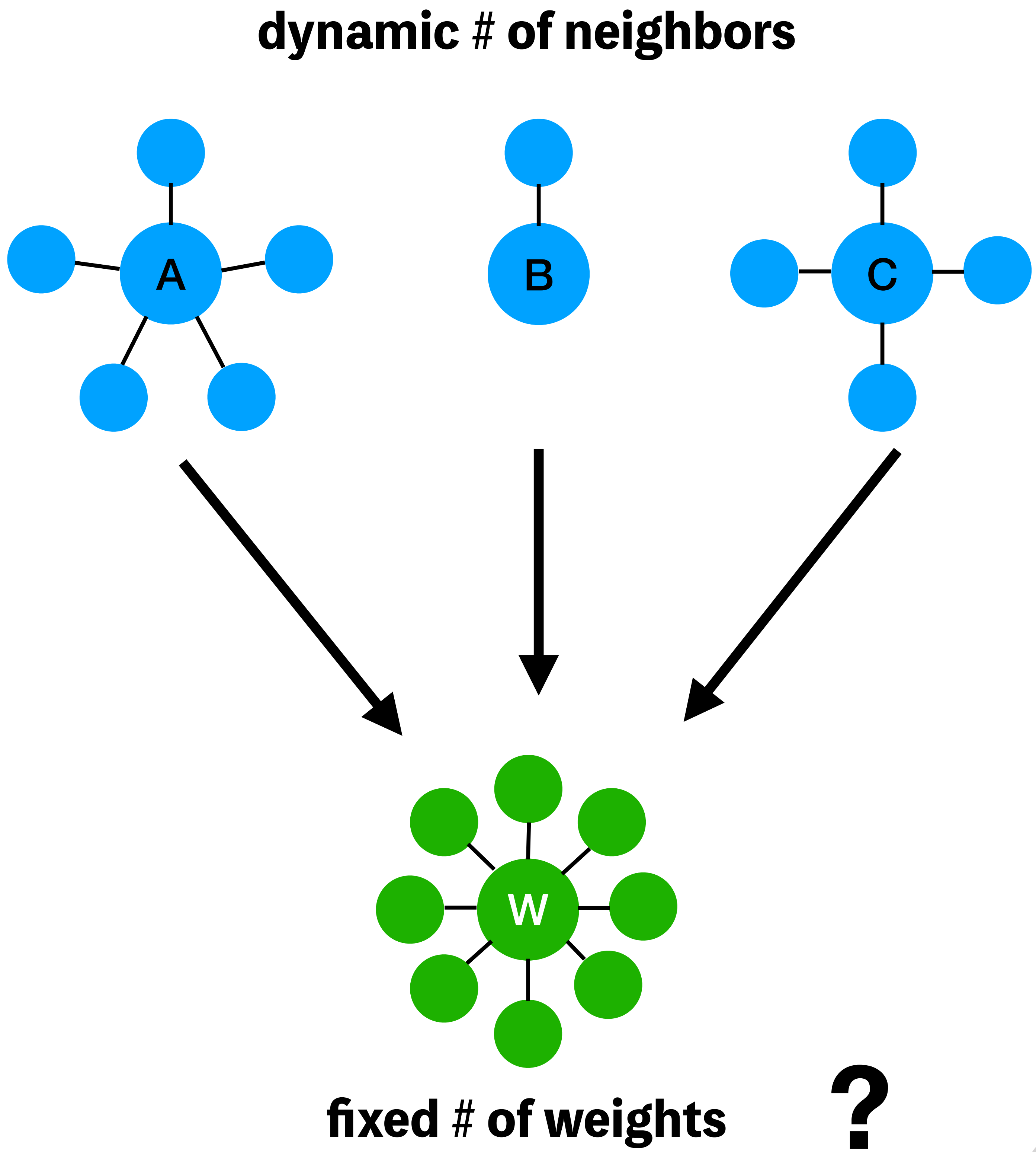
Each pixel has **fixed** number of neighbors

Convolution



Challenge for non-Euclidean

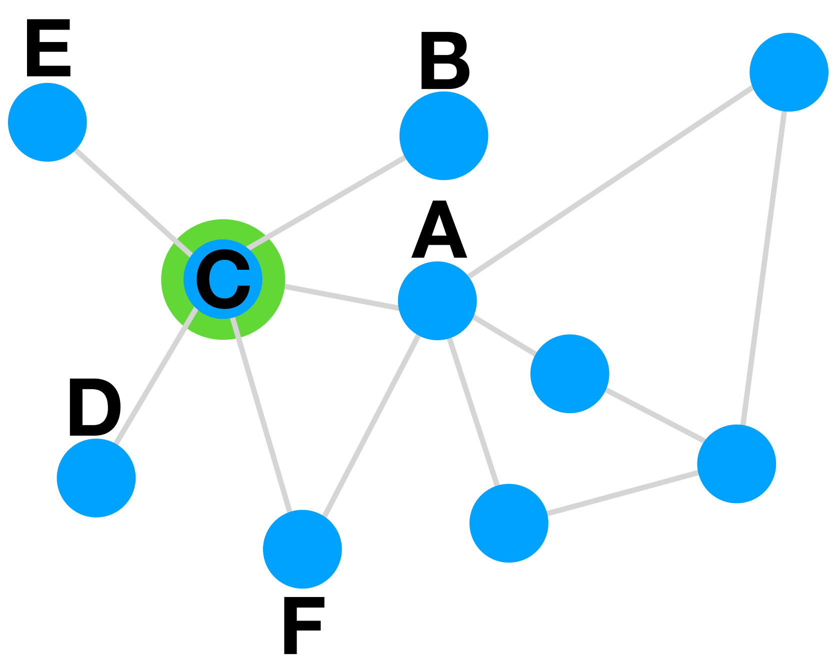




Challenge for non-Euclidean

Task: Infer the value of C

Graph Structure



+

Graph Signal
(Feature Matrix)

$$C = \frac{A+B+D+E+F}{5}$$

Simple

$$C = \boxed{f(A, B, D, E, F \,|\, Graph)}$$

Real-World

Overview of Graph Research

Graph Neural Networks

Theory

Theoretical understanding is limited

- **<u>White-box: Graph Theory</u>**
- Black-box: XAI for Graph

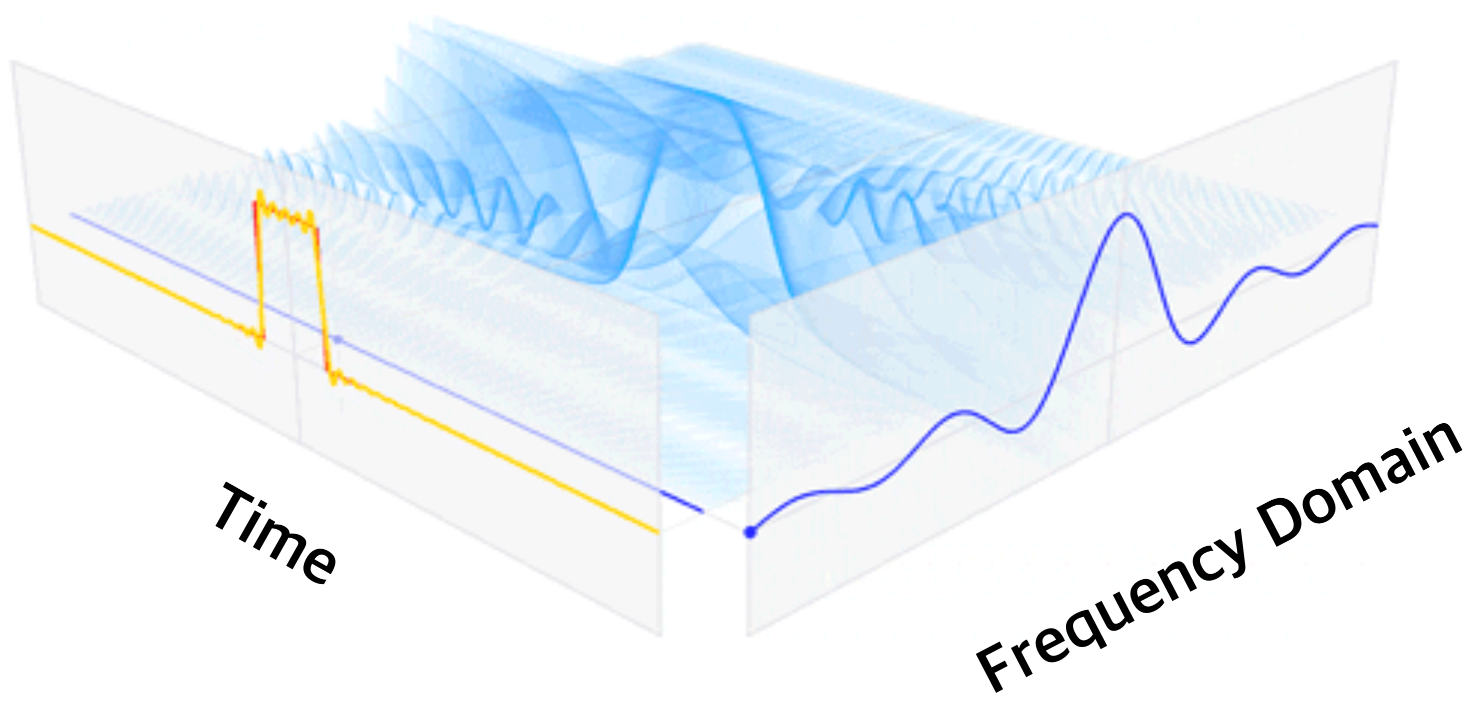
Application

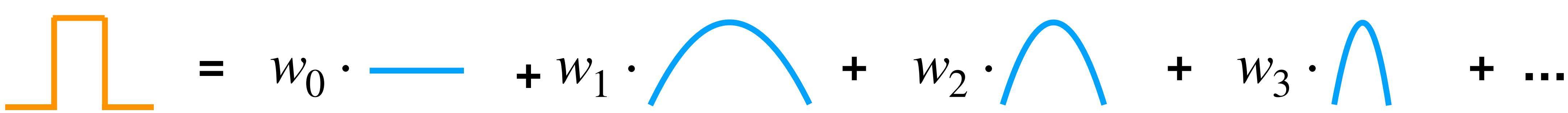
Limited in social networks

- Transportation Network
- Circuit Modeling
- Brain Network
- Disease Spreading

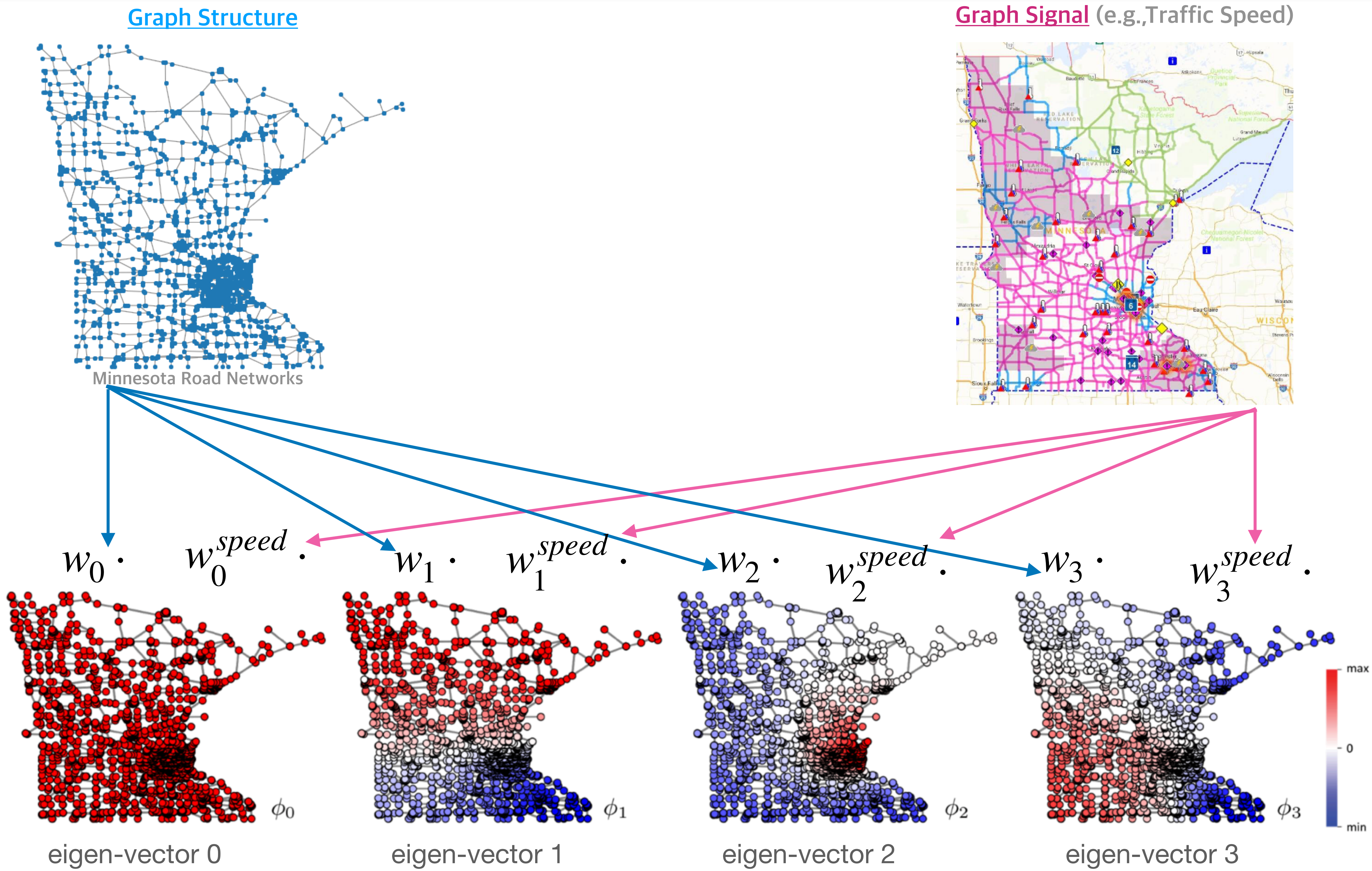
Spectral Analysis

credit: giphy



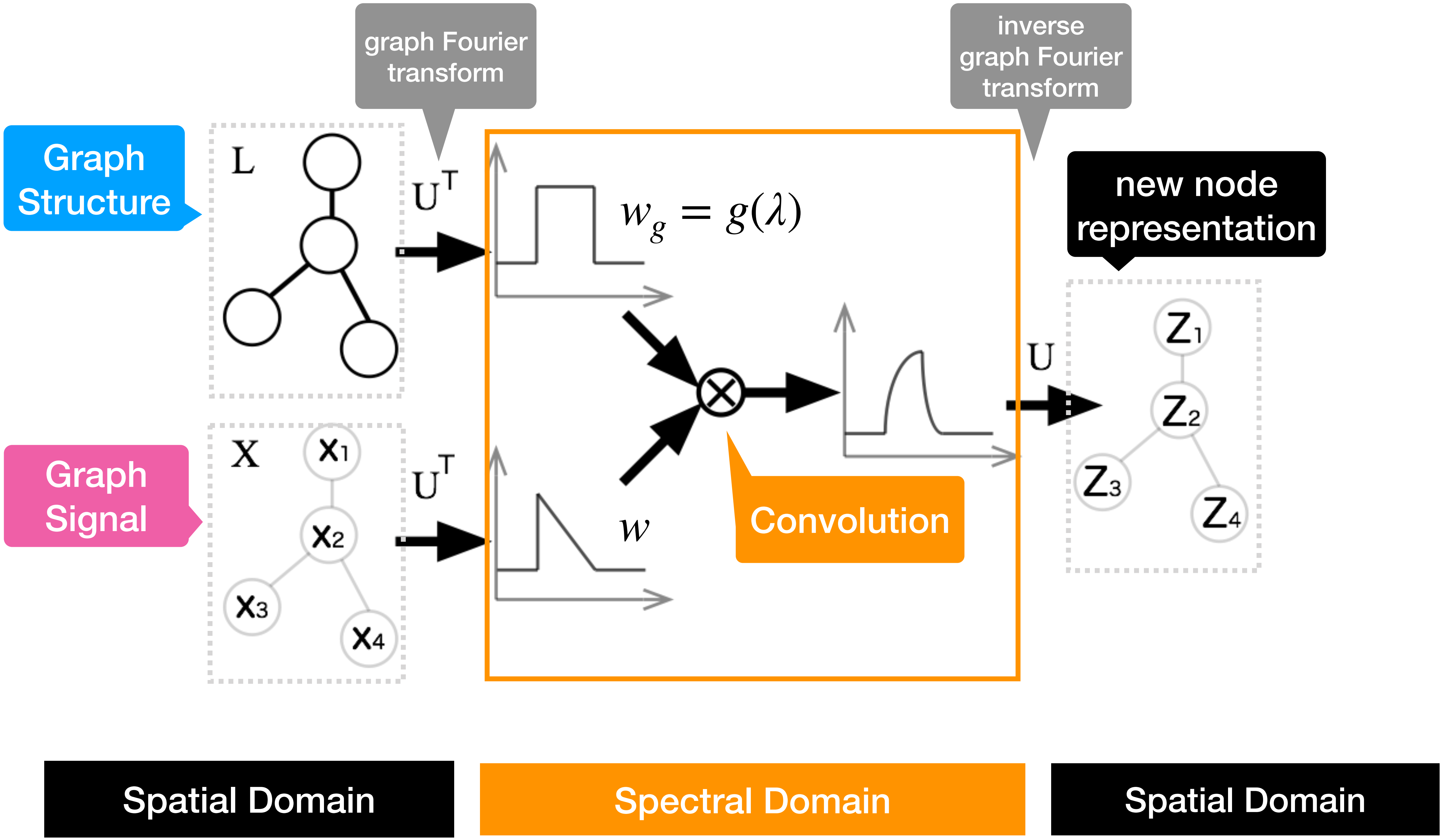


Spectral Analysis for Graph

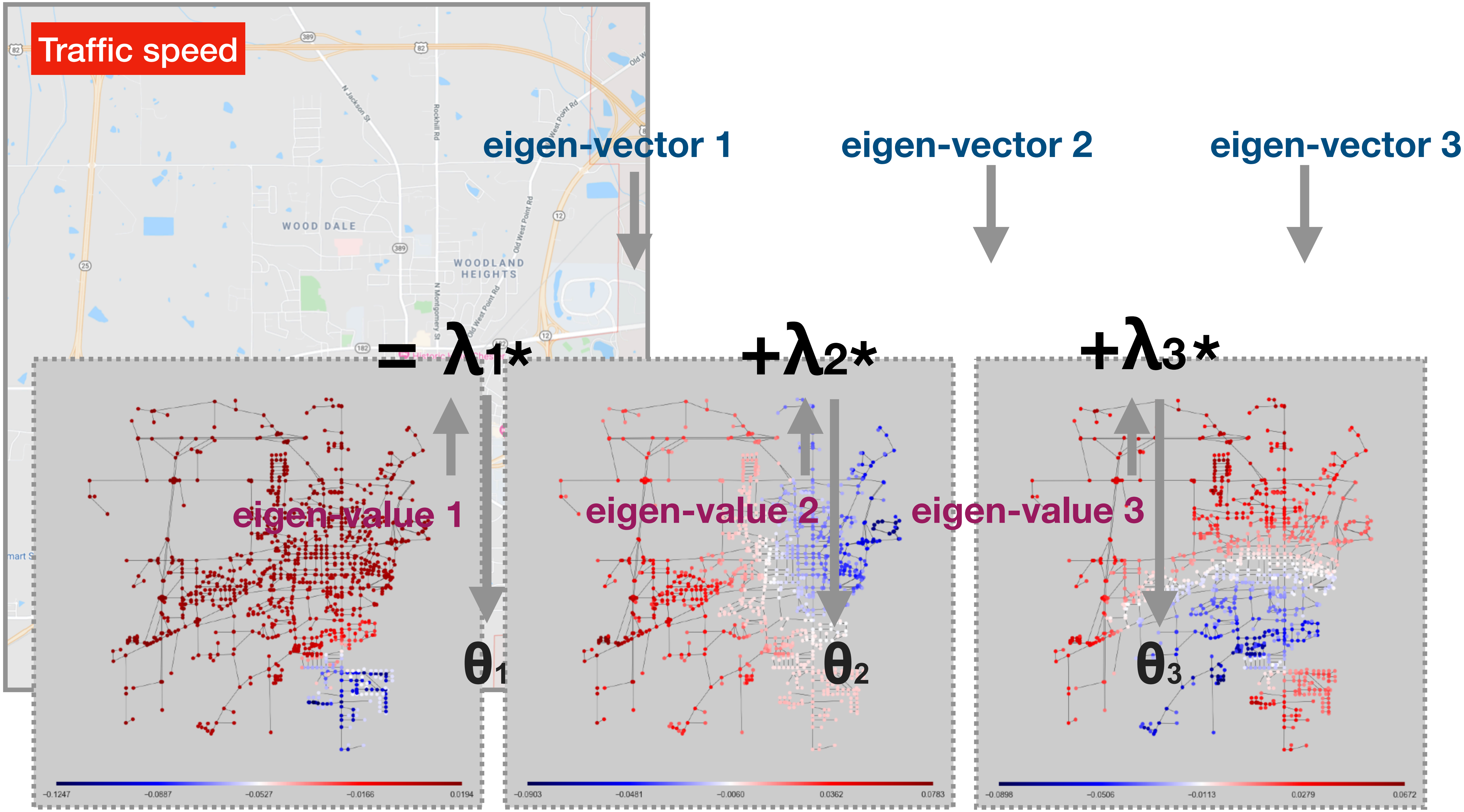


Graph Fourier Transform (Spectral Decomposition)

What is Graph Convolution



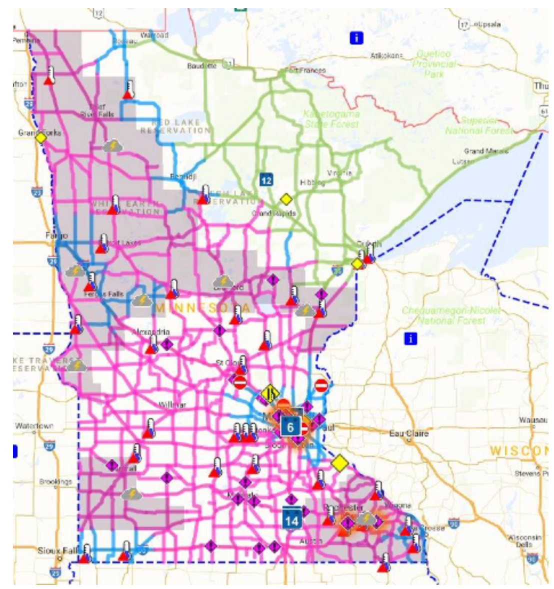
What is Spectral Graph



What is Graph Convolution

Graph Structure

Graph Signal (e.g.,Traffic Speed)



$$g_\theta \star x = U g_\theta U^\top x = \mathbf{P}(\mathbf{L})\, x$$ (polynomial approximation)

1 graph Fourier transform

2 convolution (theorem)

3 Inverse graph Fourier transform

GNN, What else?

Spectral Graph | Message Passing

Page Rank | Random Walk

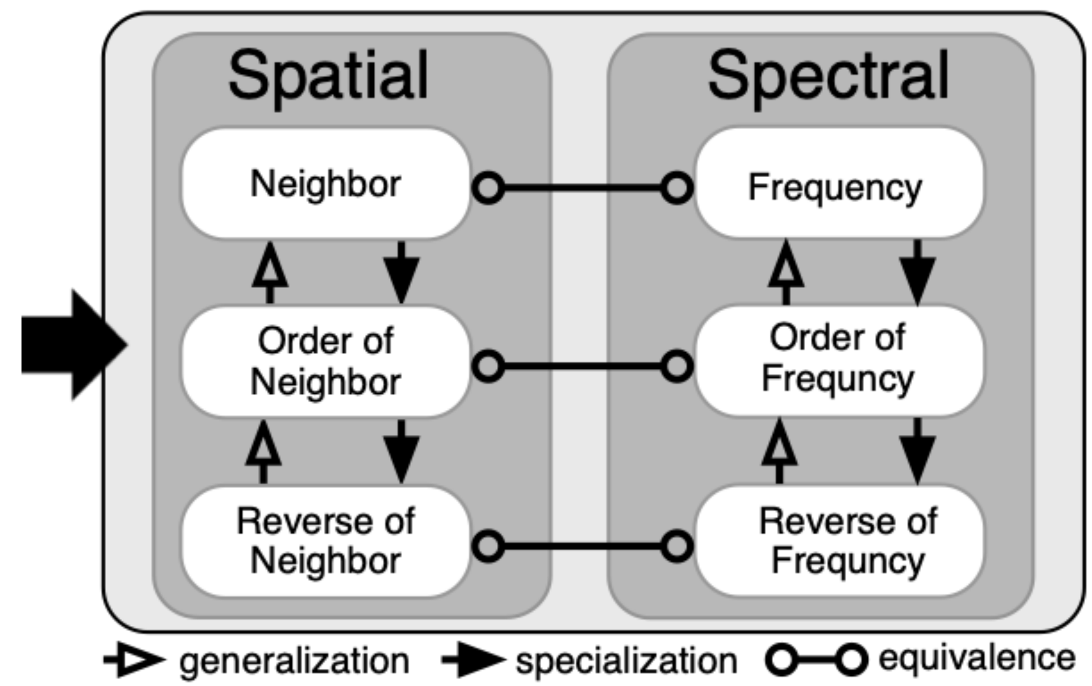
Heat Diffusion | Low-pass Filter

Heat Diffusion | Attention Model

DSF/BSF | ARMA filter

Weisfeiler-Lehman | Laplacian Smooth

30+

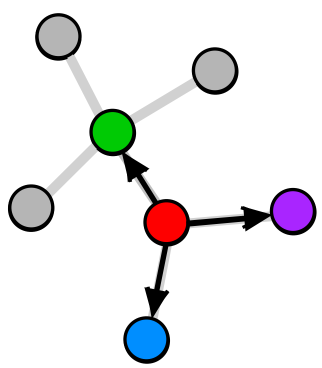


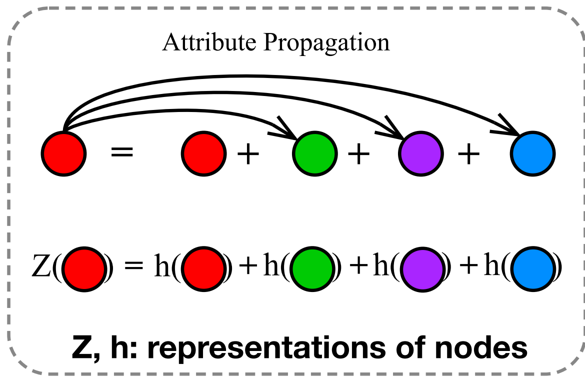
- A large number of graph neural networks, with different mechanisms
- **Challenge for research**: no uniform framework to compare them

Analysis 1: Spatial-based GNN

function of Adjacency

Linear





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

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

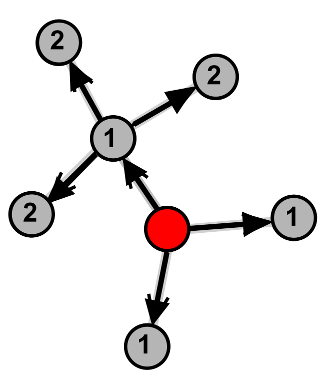
GraphSAGE *Will Hamilton et al. (2017)*

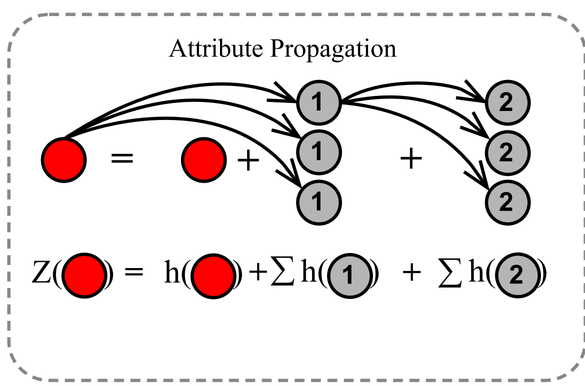
$$\mathbf{Z} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{I}+\mathbf{A})\mathbf{D}^{-\frac{1}{2}}\mathbf{X} = (\mathbf{I}+\tilde{\mathbf{A}})\mathbf{X}$$

GIN *Xukeyu Lu et al. (2019)*

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

Polynomial





DeepWalk *Bryan Perozzi et al. (2014)*

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

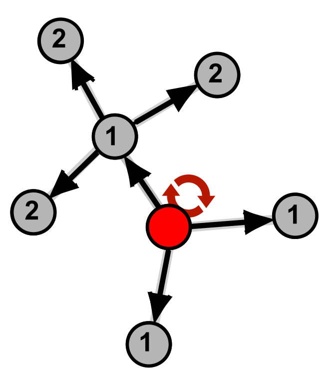
ChebyNet *Defferrard, Michael et al. (2016)*

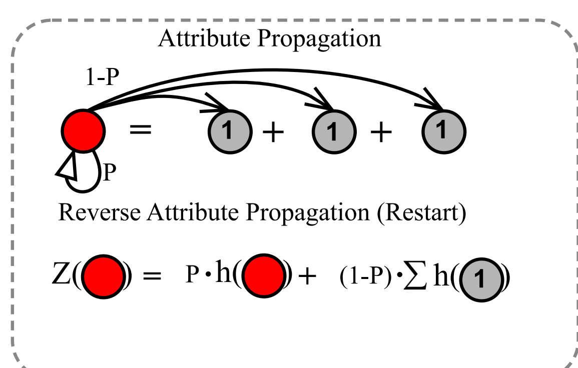
$$\mathbf{Z} = \sum_{k=0}^{K-1}\theta_k T_k(\tilde{\mathbf{L}})\mathbf{X} = \left[\tilde{\theta}_0\mathbf{I}+\tilde{\theta}_1(\mathbf{I}-\tilde{\mathbf{A}})+\tilde{\theta}_2(\mathbf{I}-\tilde{\mathbf{A}})^2+\ldots\right]\mathbf{X} = \left(\phi\mathbf{I}+\sum_{i=1}^{k}\psi_i\tilde{\mathbf{A}}^i\right)\mathbf{X}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

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)*

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

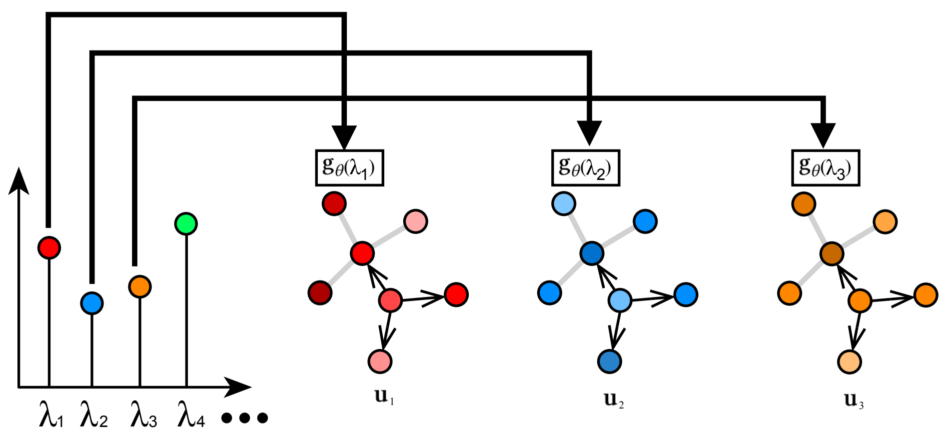
Auto Regressive Filter *Qimai Li et al. (2019)*

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

Analysis 2: Spectral-based GNN

function of Eigenvalues

Linear



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

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

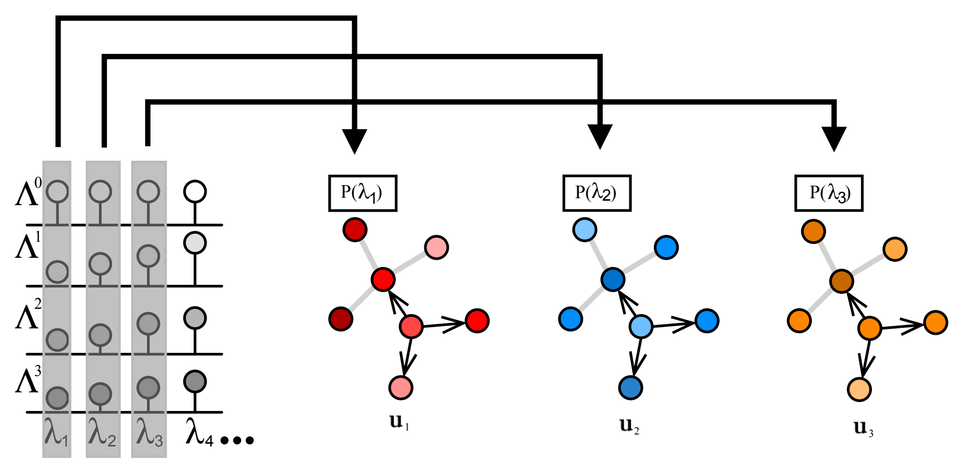
GraphSAGE *Will Hamilton et al. (2017)*

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

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)*

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

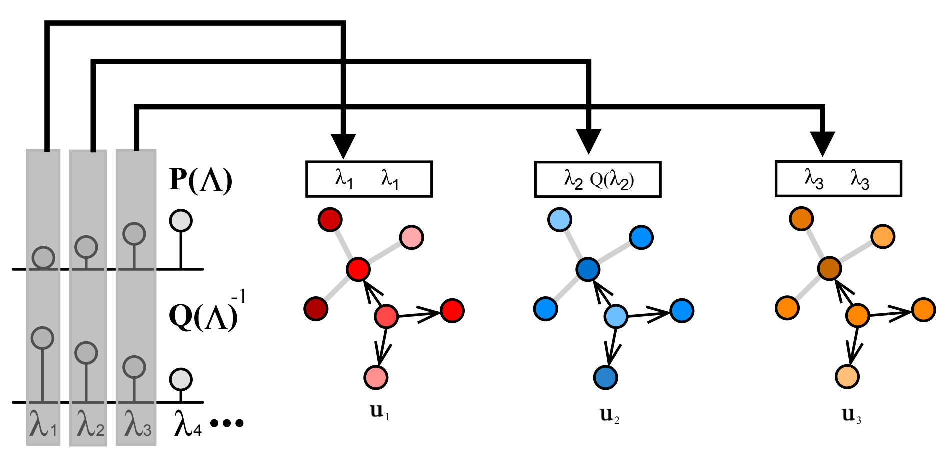
ChebyNet *Defferrard, Michael et al. (2016)*

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

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)*

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

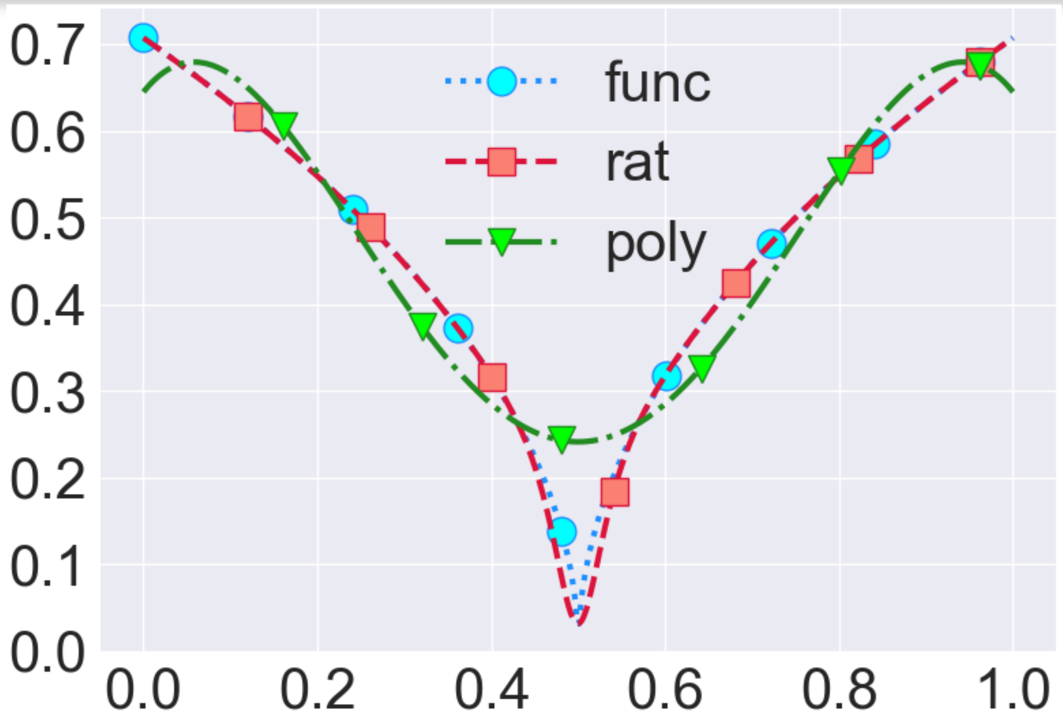
ARMA Filter *Filippo Maria Bianchi et al. (2018)*

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

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

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

Theoretical Support



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

Polynomial approximation

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

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

easy to compute
hard to be accurate

Rational approximation

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

moderately **simple** form, not well-known properties

moderately **easy** to handle computationally

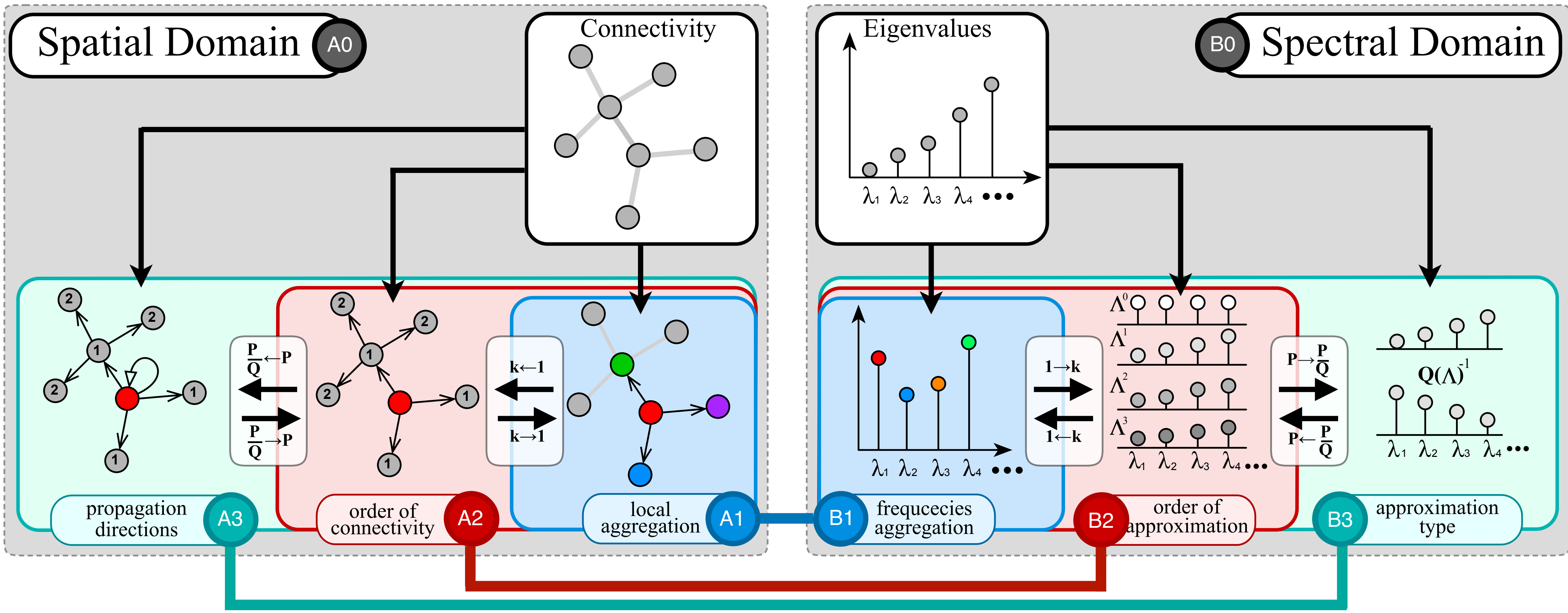
excellent for oscillations between exact-fit value

model **complicated** structure with a fairly low degree

excellent interpolatory/extrapolatory/asymptotic properties

moderately easy to compute
easy to be accurate

Analysis 3: The Framework



	Linear	Polynomial	Rational
Spatial			
Spectral			

Complex, Powerful

GNNs

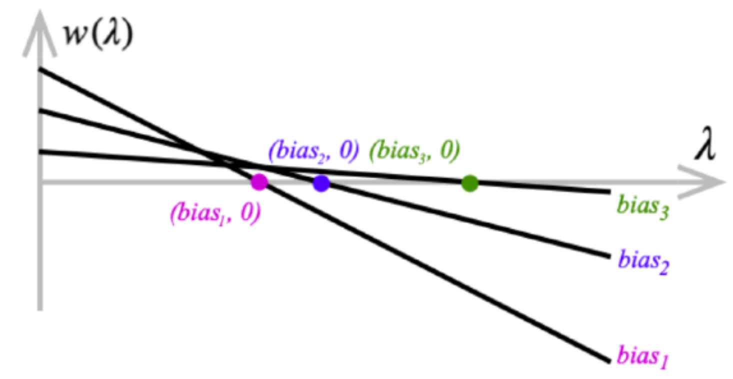
	Spatial-based (**A0**)	Spectral-based (**B0**)
	$f(\mathbf{A})$ in $\mathbf{Z} = f(\mathbf{A})\,\mathbf{X}$	$\mathrm{g}(\boldsymbol{\Lambda})$ in $\mathbf{Z} = \mathbf{U}\,\mathrm{g}(\boldsymbol{\Lambda})\,\mathbf{U}^{\intercal}\,\mathbf{X}$
	linear function of $\mathbf{A}$ (**A1**)	linear function of $\boldsymbol{\Lambda}$ (**B1**)
GCN	$\mathbf{I} + \tilde{\mathbf{A}}$	$2 - \boldsymbol{\Lambda}$
GraphSAGE	$\hat{\mathbf{D}}^{-1} + \tilde{\mathbf{A}}$	$2 - \boldsymbol{\Lambda}$
GIN	$(1 + \epsilon)\,\mathbf{I} + \mathbf{A}$	$2 + \epsilon - \boldsymbol{\Lambda}$
	polynomial function of $\mathbf{A}$ (**A2**)	polynomial function of $\boldsymbol{\Lambda}$ (**B2**)
ChebNet	$\phi\mathbf{I} + \sum_{i=1}^{k} \psi_i \tilde{\mathbf{A}}^i$	$\tilde{\theta}_0 \cdot 1 + \tilde{\theta}_1\boldsymbol{\Lambda} + \tilde{\theta}_2\boldsymbol{\Lambda}^2 + \ldots$
DeepWalk	$\frac{1}{t+1}\left(\mathbf{I} + \tilde{\mathbf{A}} + \tilde{\mathbf{A}}^2 + \ldots + \tilde{\mathbf{A}}^t\right)$	$\frac{1}{t+1}[\ldots + \left((-1)^{t-1} + \begin{pmatrix} 1 \\ t \end{pmatrix}(-1)^{t-1}\right) + \ldots]$
DCNN	$\psi_1\tilde{\mathbf{A}} + \psi_2\tilde{\mathbf{A}}^2 + \psi_3\tilde{\mathbf{A}}^3 + \ldots$	$\theta_1\boldsymbol{\Lambda} + \theta_2\boldsymbol{\Lambda}^2 + \theta_3\boldsymbol{\Lambda}^3 + \ldots$
Node2Vec	$\frac{1}{p}\mathbf{I} + \left(1 - \frac{1}{q}\right)\tilde{\mathbf{A}} + \frac{1}{q}\tilde{\mathbf{A}}^2$	$\left(1 + \frac{1}{p}\right) - \left(1 + \frac{1}{q}\right)\boldsymbol{\Lambda} + \frac{1}{q}\boldsymbol{\Lambda}^2$
SGC	$0 \cdot \mathbf{I} + 0 \cdot \tilde{\mathbf{A}} + 0 \cdot \tilde{\mathbf{A}}^2 + \ldots + 1 \cdot \tilde{\mathbf{A}}^K$	$\begin{pmatrix} K \\ 0 \end{pmatrix} + \begin{pmatrix} K \\ 1 \end{pmatrix}\boldsymbol{\Lambda}^1 + \begin{pmatrix} K \\ 2 \end{pmatrix}\boldsymbol{\Lambda}^2 + \cdots + \boldsymbol{\Lambda}^n$
	rational function of $\mathbf{A}$ (**A3**)	rational function of $\boldsymbol{\Lambda}$ (**B3**)
Auto-Regress	$\mathbf{I}/[(1 + \alpha)\,\mathbf{I} - \alpha\,\tilde{\mathbf{A}}]$	$1/[1 + \alpha(1 - \boldsymbol{\Lambda})]$
PPNP	$\alpha/[\mathbf{I} - (1 - \alpha)\,\tilde{\mathbf{A}}]$	$\alpha/[\alpha\mathbf{I} + (1 - \alpha)\boldsymbol{\Lambda}]$
ARMA	$b/(\mathbf{I} - a\,\tilde{\mathbf{A}})$	$b/(1 - a + a\boldsymbol{\Lambda})$

Analysis 4: Bias of Linear Model

Bias: 2 for *GCN*, 2 for *GraphSAGE*, and 2+ε for *GIN*

GCN	$2 - \Lambda$
GraphSAGE	$2 - \Lambda$
GIN	$2 + \epsilon - \Lambda$

Why is 2?



Ratio of each spectral component using spectral filtering function

Ratio -> Adjusted Ratio

$$w\left(\lambda_i\right) = \frac{\left|bias - \lambda_i\right|}{\sum_j \left|bias - \lambda_j\right|}$$

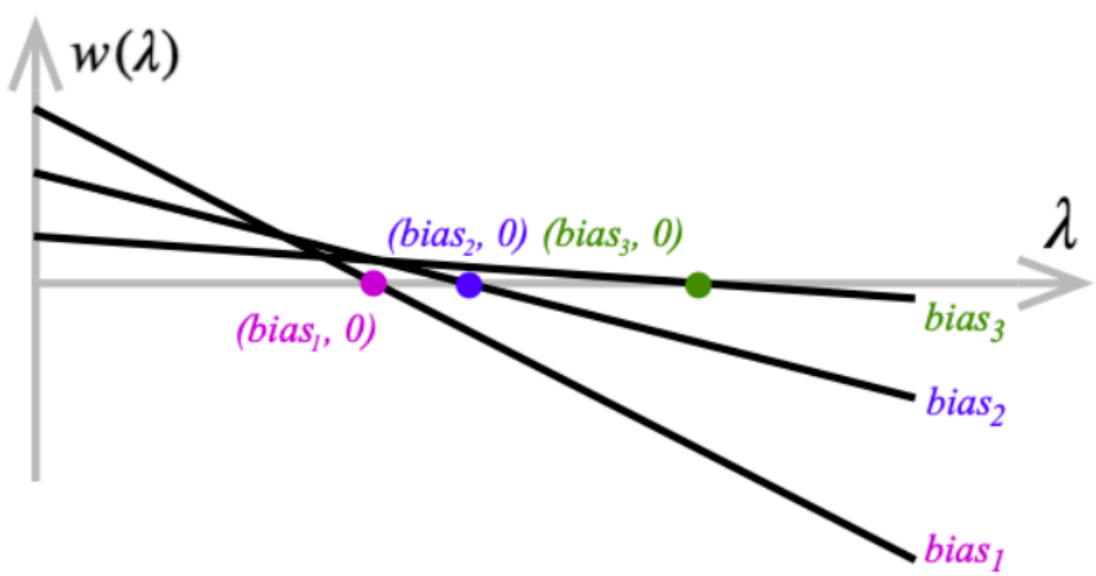
Analysis 4: Design of Linear Model

Eigenvalue is in [0, 2) for the normalized graph Laplacian matrix:

$$\lim_{N\to\infty} \sup \lambda = 2$$

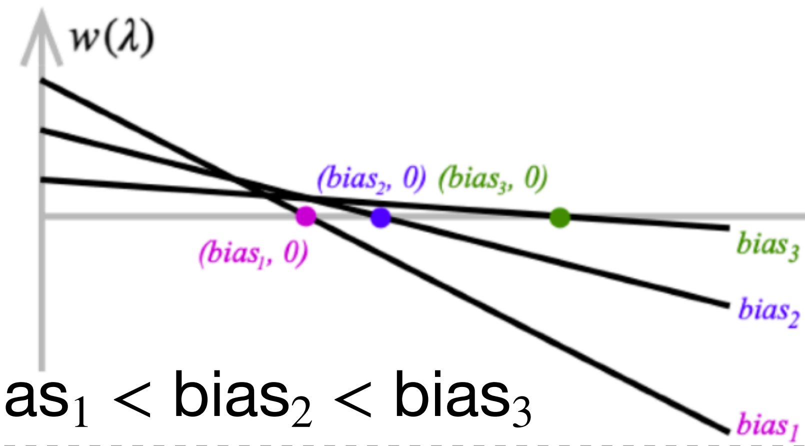
if bias>**2**, we have: $bias - \lambda > 0$

$$w(\lambda_i) = \frac{|bias - \lambda_i|}{\sum_j |bias - \lambda_j|} = \frac{bias - \lambda_i}{N \cdot bias - \sum_j \lambda_j} = \overbrace{\boxed{\frac{-1}{N \cdot bias - \sum_j \lambda_j}}}^{slope} \lambda_i + \overbrace{\frac{bias}{N \cdot bias - \sum_j \lambda_j}}^{intercept},$$



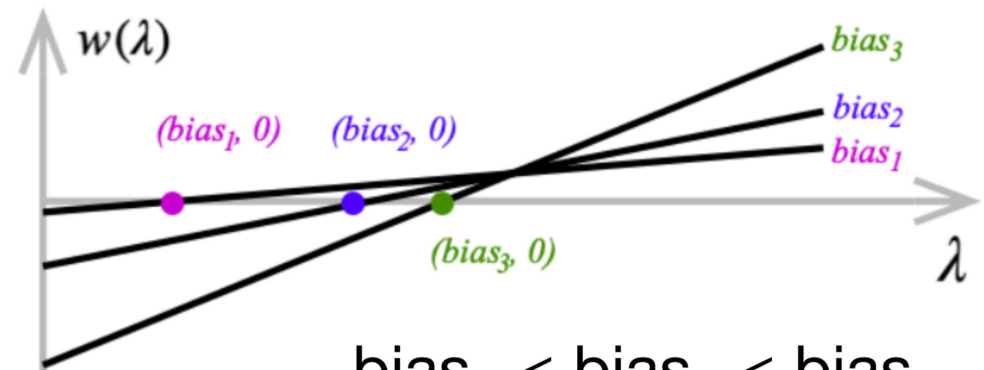
Analysis 4: Design of Linear Model

Low-pass
More weight on low-frequency
Neighbors are similar



$\text{bias}_1 < \text{bias}_2 < \text{bias}_3$

High-pass
More weight on high-frequency
Neighbors are dissimilar



$\text{bias}_1 < \text{bias}_2 < \text{bias}_3$

Conclusion: Magic number "**2**" ensure that

- Each adjusted weight is positive
- Filtering function is low-pass

Analysis 5: Effect of Rational Model

Polynomial

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

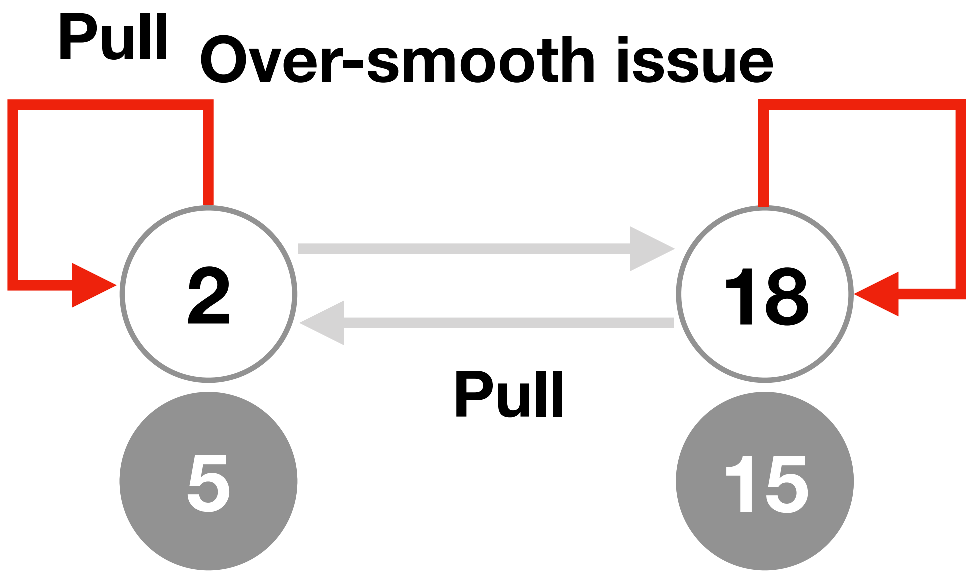
Label propagation

Rational

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

Label propagation

Reverse Label propagation



Analysis 5: Effect of Rational Model

Johannes Klicpera et al. (2018)

Personalized Page Rank (information retrieval)

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

$(1-\alpha)$ α

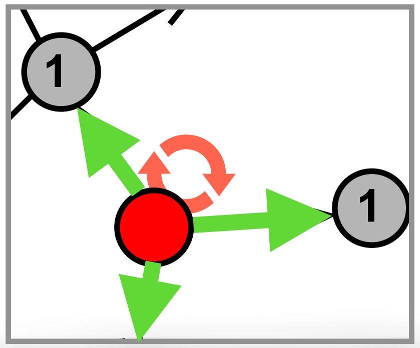
Filippo Maria Bianchi et al. (2018)

ARMA (time series)

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

a b

next $= \alpha$ current $+ \beta$ original



Summary

- **Analysis 1**: Spatial-based GNNs
  - Feature is a Function of Graph Adjacency
- **Analysis 2**: Spectral-based GNNs
  - Feature is a Function of Eigenvalues
- **Analysis 3**: A Unified Framework
  - Connect Spatial- and Spectral-based GNNs
- **Analysis 4**: Linear Model
  - Effect of Different Bias Design
- **Analysis 5**: Rational Model
  - Effect of Rational Model

Convergence rate

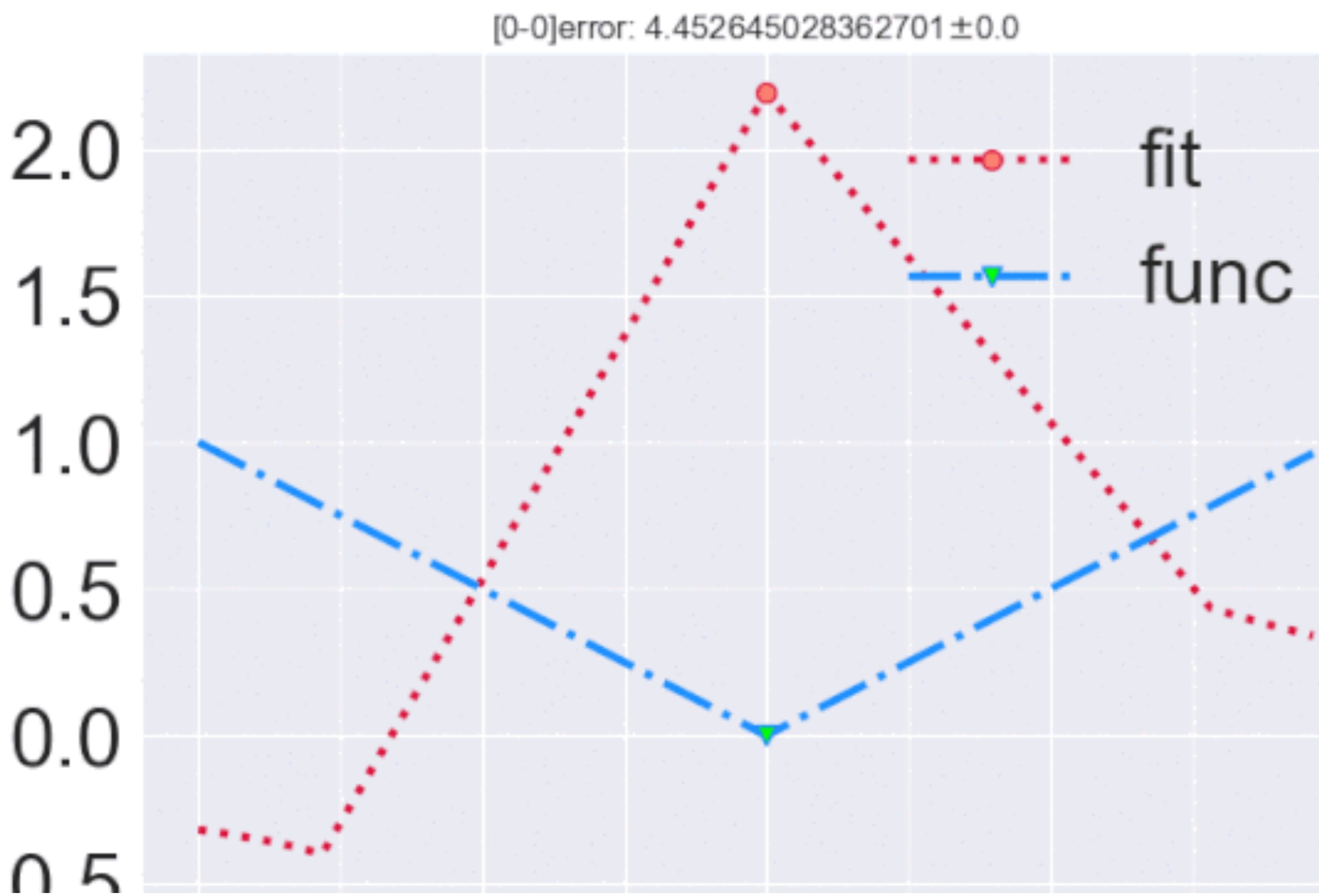
Theorem: Given n>5, there exists a rational function of degree n that satisfies:

$$\sup_{x\in[-c,c]} |f_{1,2} - R_n(x)| \leq Ce^{-\sqrt{n}}.$$

When the order is greater than 5
RemezNet is more accurate than GCN/ChebNet

$$\mathcal{O}(\textbf{poly}\ \textbf{log}(\mathbf{1}/\epsilon)) \quad < \quad \Omega(\textbf{poly}(\mathbf{1}/\epsilon))$$

Evaluation: Approximation Demo



[Screenshots in every 100 epochs]

RemezNet: iteratively close to the target

Questions or Comments?