# Spectral Basis of GNNs

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# GNN history

1997 Sperduti and Starita Supervised neural networks for the classification of structures

LeNet-5 1998

2005 Gori *et al.* A new model for learning in graph domains

2009 Scarselli *et al.* The graph neural network model

Hammond *et al.* Wavelets on graph via spectral graph theory

Micheli Neural networks for graph: A contextual constructive approach

2010 Gallicchio and Micheli Graph echo state networks

AlexNet (U of T) wins ILSVRC 2012

2013 Shuman *et al.* The emerging field of signal processing on graphs 2013

Bruna *et al.* Spectral networks and locally-connected networks on graphs

ZFNet (NYU) wins ILSVRC

GoogLeNet and VGGNet wins ILSVRC 2014

2015 Henaff *et al.* Deep convolutional networks on graph-structured data 2015

ResNet wins ILSVRC

2016 Defferrard *et al.* Convolutional neural networks on graphs with fast localized spectral filtering

Kipf and Welling Semi-supervised classification with graph convolutional networks

Atwood and Towsley Diffusion-convolutional neural networks

Niepert *et al.* Learning convolutional neural networks for graphs

2017 Gilmer *et al.* Neural message passing for quantum chemistry

2018 Battaglia *et al.* Relational inductive biases, deep learning, and graph networks

RecGNN
Graph Fourier Transform
Spectral ConvGNN
Spatial ConvGNN

# GNN history (significant eras)

1997 Sperduti and Starita Supervised neural networks for the classification of structures

LeN t-5 1998

2005 Gori *et al.* A new model for learning in graph domains

2009 Scarselli *et al.* The graph neural network model

Hammond *et al.* Wavelets on graph via spectral graph theory

Micheli Neural networks for graph: A contextual constructive approach

2010 Gallicchio and Micheli Graph echo state networks

- Theory of spectral domain filters
- Idea of graph-based convolution

AlexNet (U of T) wins ILS RC 2012

2013 Shuman *et al.* The emerging field of signal processing on graphs 2013

Bruna *et al.* Spectral networks and locally-connected networks on graphs

ZFNet (

GoogLeNet and VG

2015 Henaff *et al.* Deep convolutional networks on graph-structured data

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- Spectral domain filters as NNs and their approximation techniques

2016 Defferrard *et al.* Convolutional neural networks on graphs with fast localized spectral ering

Kipf and Welling Semi-supervised classification with graph convolutional networks

Atwood and Towsley Diffusion-convolutional neural networks

Niepert *et al.* Learning convolutional neural networks for graphs

RecGNN

n

N

N

- Adding up neighbors is all you need

2017 Gilmer *et al.* Neural message passing for quantum chemistry

2018 Battaglia *et al.* Relational inductive biases, deep learning, and graph networks

# GNN history (the people behind)

1997 Sperduti and Starita Supervised neural networks for the classification of structures

LeCun LeNet-5 1998

2005 Gori *et al.* A new model for learning in graph domains *(first use of the term GNN)*

2009 Scarselli *et al.* The graph neural network model

Hammond *et al.* Wavelets on graph via spectral graph theory

Micheli Neural networks for graph: A contextual constructive approach

2010 Gallicchio and Micheli Graph echo state networks

Sutskever+Hinton AlexNet (U of T) wins ILSVRC 2012

2013 Shuman *et al.* The emerging field of signal processing on graphs 2013

LeCun Bruna *et al.* Spectral networks and locally-connected networks on graphs

LeCun, sort of ZFNet (NYU) wins ILSVRC

LeCun Google GoogLeNet and VGGNet wins ILSVRC 2014

2015 Henaff *et al.* Deep convolutional networks on graph-structured data 2015

ResNet wins ILSVRC Microsoft

2016 Defferrard *et al.* Convolutional neural networks on graphs with fast localized spectral filtering

Google Kipf and Welling Semi-supervised classification with graph convolutional networks *(GCN)*

Atwood and Towsley Diffusion-convolutional neural networks

Niepert *et al.* Learning convolutional neural networks for graphs

2017 Gilmer *et al.* Neural message passing for quantum chemistry Google

2018 Battaglia *et al.* Relational inductive biases, deep learning, and graph networks Google

RecGNN
Graph Fourier Transform
Spectral ConvGNN
Spatial ConvGNN

# Graph Fourier transform

- Let $U$ be a eigenbasis of some Laplacian $L$
- Then $U^\top x$ is a projection of distribution $x$ on eigenbasis $U$
  - $$U^\top x = \begin{bmatrix} \leftarrow & \mu_1 & \rightarrow \\ \leftarrow & \mu_2 & \rightarrow \\ & \vdots & \end{bmatrix} x = \begin{bmatrix} \mu_1^\top x \\ \mu_2^\top x \\ \vdots \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} = \dot{x}$$
    where $a_i = \mu_i x$ is the projection onto $\mu_i$
  - The projected space is $\sum_i a_i \mu_i$

$x$ and $H$ will be used interchangeably here

dimension of Fourier space (= #eigenvectors)



Hammond *et al.* Wavelets on graphs via spectral graph theory, 2009

# Graph Fourier transform

- Let $U$ be a eigenbasis of some Laplacian $L$
- Then $U^{\top}x$ is a projection of distribution $x$ on eigenbasis $U$
- An application of $U$ would transform $\dot{x}$ back into $x$

$$U\dot{x} = \begin{bmatrix} \uparrow & \uparrow & \\ \mu_1 & \mu_2 & \dots \\ \downarrow & \downarrow & \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} \mu_{11}a_1 + \mu_{21}a_2 + \cdots \\ \mu_{12}a_1 + \mu_{22}a_2 + \cdots \\ \vdots \end{bmatrix}$$

$$= \mu_1 a_1 + \mu_2 a_2 + \cdots = \mu_1 \mu_1^{\top} x + \mu_2 \mu_2^{\top} x + \cdots$$

$$= \left(\sum_i \mu_i \mu_i^{\top}\right) x = Ix = x$$

Homework: prove $\sum_i \mu_i \mu_i^{\top} = I$

# Graph Fourier transform

- Let $U$ be a eigenbasis of some Laplacian $L$
- Then $U^\top x$ is a projection of distribution $x$ on eigenbasis $U$
- An application of $U$ would transform $\dot{x}$ back into $x$, $U(\dot{x}) = U(U^\top x) = x$ (obvious since $UU^\top = I$)
- Denote $U^\top x$ as $F(x)$ and $U\dot{x}$ as $F^{-1}(\dot{x})$

# Graph Fourier transform

- A convolution of $x$ in the Fourier domain of a graph $G$ is $x * g = F^{-1}\big(F(x) \odot F(g)\big) = U(U^\top x \odot U^\top g)$ where $U$ is the eigenbasis of some Laplacian of $G$, $g$ is some filter that works on the eigenbasis $U$, and $\odot$ is the element-wise (Hadamard) product
- Suppose $U^\top g = \begin{bmatrix} g_1 \\ g_2 \\ \vdots \end{bmatrix}$. Let $g_\theta = \mathrm{diag}(U^\top g) = \begin{bmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix}$

  Then we can write $x * g = U g_\theta U^\top x$ (shown below)
  - Each $g_i$ weights the significance of the eigenvector $\mu_i$
  - $g_\theta$ is to be inferred
  - This inference task results in the spectral GNNs

$$U^\top x \odot U^\top g = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} \odot \begin{bmatrix} g_1 \\ g_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} a_1 g_1 \\ a_2 g_2 \\ \vdots \end{bmatrix}$$

$$g_\theta U^\top x = \begin{bmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} a_1 g_1 \\ a_2 g_2 \\ \vdots \end{bmatrix}$$

Henaff *et al.* Deep Convolutional Networks on Graph-Structured Data, 2013

# Spectral GNN

- **The spectral GNN task of learning a function $f$ and filter $g$ for graph $G$, is to infer $f$ and the coefficients $g_1$, $g_2$, …, such that for each $x$, $f(Ug_\theta U^\top x)$ matches the desired output**
  - These GNNs work in the spectral domain as opposed to the spatial domain of the graph
  - $g_\theta$ is to be independent of the eigenvectors $U$
    - That is, $g_\theta(L) = g_\theta(U\Lambda U^\top) = Ug_\theta(\Lambda)U^\top x$ where $L$ is some Laplacian for $G$
    - Of course, $g_\theta$ may turn out to be independent of $\Lambda$
      - In which case, $g_\theta$ is inferred solely from the examples
- In spectral GNNs we learn which eigenvectors to use from examples in a supervised learning
  - In spectral clustering we take the eigenvectors of the slowest growth (hence more “global”) and perform unsupervised learning with those vectors

# Chebyshev approximation for $U$

- However, computing $U$ is $O(N^3)$ and computing $U^\top x$ is $O(N^2)$ ⇒ expensive
- Approximate $g_\theta$ with Chebyshev polynomials

$$g_\theta(\Lambda) \approx g_{\theta'}(\Lambda) = \sum_{i=0}^{K} \theta_i' T_i(\tilde{\Lambda})$$

where

- $\tilde{\Lambda} = \frac{2}{\lambda_{\max}}\Lambda - I$ ($\lambda_{\max}$ is the largest eigenvalue)
- $\theta' \in \mathbb{R}^K$ are Chebyshev coefficients, and
- The polynomials $T_i(x)$ are computed with a recurrence relation
  - $T_0(x) = 1, T_1(x) = x$ (base case)
  - $T_{n+1}(x) = 2x\, T_n(x) - T_{n-1}(x)$
- $K$ is the number of expansion terms



Defferrard *et al.* Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering, 2016

# Chebyshev approximation for $U$

- However, computing $U$ is $O(N^3)$ and computing $U^\top x$ is $O(N^2) \Rightarrow$ expensive
- Approximate $g_\theta$ with Chebyshev polynomials

$$g_\theta(\Lambda) \approx g_{\theta'}(\Lambda) = \sum_{i=0}^{K} \theta_i' \, T_i(\tilde{\Lambda})$$

- Then

$$x * g_\theta = U g_\theta U^\top x \approx U \left( \sum_{i=0}^{K} \theta_i' \, T_i(\tilde{\Lambda}) \right) U^\top x$$

- Since $UT(\tilde{\Lambda})U^\top = \frac{2}{\lambda_{\max}} U\Lambda U^\top - IUU^\top = \frac{2}{\lambda_{\max}} L - I$

Write $\tilde{L} = \frac{2}{\lambda_{\max}} L - I$ and $\boxed{x * g_\theta \approx \sum_{i=0}^{K} \theta_i' \, T_i(\tilde{L}) \, x}$

Chebyshev approximation

# Chebyshev approximation for $U$

- $T_n$, the $n^{\text{th}}$ order coefficient of the Chebyshev polynomials **of the first kind**, is

$$T_n(\cos\theta) = \cos n\theta$$

  - The coefficients can be obtained using the recurrence relation

$$\cos(n+1)\theta + \cos(n-1)\theta = 2\cos\theta\cos n\theta$$
$$\Rightarrow T_{n+1}(x) = 2x\,T_n(x) - T_{n-1}(x)$$

0th order
  - $\cos 0\theta = 1 \quad \Rightarrow T_0(x) = 1$

1st order
  - $\cos 1\theta = \cos\theta \quad \Rightarrow T_1(x) = x$

2nd order
  - $\cos 2\theta = 2\cos^2\theta - 1 \quad \Rightarrow T_2(x) = 2x^2 - 1$

3rd order
  - $\cos 3\theta = 4\cos^3\theta - 3\cos\theta \quad \Rightarrow T_3(x) = 4x^3 - 3x$

# Chebyshev approximation for $U$

- Chebyshev approximation has $x * g_\theta \approx \sum_{i=0}^{K} \theta_i' \, T_i(\tilde{L}) \, x$
- To compute $T_i(\tilde{L})$, use the Chebyshev recurrence

$$T_0(\tilde{L}) = 1,\ T_1(\tilde{L}) = \tilde{L},\ T_{n+1}(\tilde{L}) = 2\,\tilde{L}\,T_n(\tilde{L}) - T_{n-1}(\tilde{L})$$

- Denote $\bar{x}_k = T_k(\tilde{L})\,x$, this becomes

$$\bar{x}_{n+1} = 2\,\tilde{L}\,\bar{x}_n - \bar{x}_{n-1} \text{ (or } \bar{x}_n = 2\,\tilde{L}\,\bar{x}_{n-1} - \bar{x}_{n-2}\text{)}$$

- Then, $x * g_\theta \approx \sum_{i=0}^{K} \theta_i' \; T_i(\tilde{L})\,x = [\theta_0' \quad \dots \quad \theta_K'] \begin{bmatrix} \bar{x}_0 \\ \vdots \\ \bar{x}_K \end{bmatrix}$
  - Can be computed in $O(K|E|)$ time from $\tilde{L}$
- Precompute the $K$ vectors $\bar{x}_0, \dots, \bar{x}_K$, with the recurrence relation, and learn the scalars $\theta_0', \dots, \theta_K'$

# $K = 1$ (GCN) approximations

- Chebyshev approximation has $x * g_\theta \approx \sum_{i=0}^{K} \theta_i' T_i(\tilde{L}) x$
- GCN takes $K = 1$ to obtain

$$x * g_{\theta'} \approx \theta_0' x + \theta_1' \tilde{L} x = \theta_0' x + \theta_1' \left( \frac{2}{\lambda_{\max}} L - I_N \right) x$$

- Since $\lambda_{\max} = 2$ we get $x * g_{\theta'} \approx \theta_0' x + \theta_1' (L - I_N) x$
  - $\theta_0'$ and $\theta_1'$ are parameters to be learned
- On the unweighted normalized Laplacian $L = D^{-1/2}(D - A)D^{-1/2} = I - D^{-1/2} A D^{-1/2}$, this becomes

$$x * g_{\theta'} = \theta_0' x - \theta_1' D^{-1/2} A D^{-1/2} x$$

- Further constraint the number of parameters by letting $\theta_0' = -\theta_1' = \theta$

$$x * g_{\theta'} = \theta \left( I + D^{-1/2} A D^{-1/2} \right) x$$

GCN 1st order approximation



Kipf and Welling. Semi-Supervised Classification with Graph Convolutional Networks, 2016

# $K = 1$ (GCN) approximations

- However, since $L = I - D^{-1/2}AD^{-1/2}$

  $\Rightarrow x * g_{\theta'} = \theta\left(I + D^{-1/2}AD^{-1/2}\right)x = \theta(2I - L)x$
- Then, multiple applications of $\theta(2I - L)$ would result in

  $$\theta^k(2I - L)^k x = \theta^k U(2 - \Lambda)^k U^\top x$$

  where $\Lambda/U$ are the eigenvalues/eigenvectors for $L$

  (GCN places non-linear functions between layers which we ignore in this derivation)
  - Since $L$ has eigenvalues in $[0, \lambda_{\max}]$ (where $\lambda_{\max} \leq 2$ is the largest eigenvalue of $L$)

    $\Rightarrow (2 - \Lambda)^k$ has range of $[(2 - \lambda_{\max})^k, 2^k]$

    $\Rightarrow$ Exponentially large spectral coefficients at higher $k$
- Solution: Let $\hat{A} = A + I$ (augmentation) and normalize $\hat{A}$ (renormalization)

  Augmented adjacency matrix

  That is, $x * g_{\theta'} = \theta\widehat{D}^{-1/2}\hat{A}\widehat{D}^{-1/2}x$ where $\widehat{D}_{ii} = \sum_i \hat{A}_{ij}$



Kipf and Welling. Semi-Supervised Classification with Graph Convolutional Networks, 2016

# How legit are GCN approximations

- Consider the two approximations of $x * g_\theta$ in GCN

  1. $S_{\text{1-order}} = \theta\left(I + D^{-1/2} A D^{-1/2}\right)$, or
  2. $\hat{S}_{\text{adj}} = \theta \widehat{D}^{-1/2} \hat{A} \widehat{D}^{-1/2}$ $(\hat{A} = A + I)$

  where $\theta$ is a scalar to be learned

- Evaluate how well they approximate $x * g_\theta$ in the case that $g_\theta = \mathrm{diag}(\Lambda)$, that is,

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

- First, letting $\theta_0' = -\theta_1'$ (case of $S_{\text{1-order}}$) or $\theta_0' = \theta_1'$ would result in $x * g_{\theta'}$ having the same eigenvectors as $L$, that is,
  - $\theta_0' = -\theta_1' \Rightarrow x * g_{\theta'} = \theta(2I - L)x$
    $\Rightarrow$ same eigenvectors but eigenvalues become $2 - \lambda$
  - $\theta_0' = \theta_1' \Rightarrow x * g_{\theta'} = \theta L x$
    $\Rightarrow$ same eigenvalues/ eigenvectors

# How legit are GCN approximations

- Use the Karate club graph for $L$
- Comparison of eigenvectors/ eigenvalues

| Filter | Eigenvalues | Eigenvector (corr. to smallest eigenvalue in $L$) |
|---|---|---|
| $L$ | 1.71, 1.61, 1.58, 1.57, ..., .39, .29, .13, 0 | -.32, -.24, -.25, -.2, -.14, -.16, -.16, -.16, -.18, -.11, ..., -.14, -.14, -.11, -.16, -.14, -.16, -.16, -.2, -.28, -.33 |
| $S_{\text{1-order}}$ | 2., 1.87, 1.71, 1.61, 1.39, ..., .5, .43, .42, .39, .29 | .32, .24, .25, .2, .14, .16, .16, .16, .18, .11, ..., .14, .14, .11, .16, .14, .16, .16, .2, .28, .33 |
| $\hat{S}_{\text{adj}}$ | 1., .9, .77, .7, .55, ..., -.21, -.22, -.27, -.31, -.42 | .3, .23, .24, .19, .15, .16, .16, .16, .18, .13, ..., .15, .15, .13, .16, .15, .16, .16, .19, .26, .31 |

  - $L$ and $S_{\text{1-order}}$ share the same eigenvectors
  - Eigenvectors of $\hat{S}_{\text{adj}}$ closely resembles those of $L$ and $S_{\text{1-order}}$
- Evaluate MSE($S_{\text{1-order}}x$, $Lx$) and MSE($\hat{S}_{\text{adj}}x$, $Lx$) on randomly generated $x$
  - MSE($S_{\text{1-order}}x$, $Lx$) $= 0.159$ (obtained at $\theta \sim 0.1$)
  - MSE($\hat{S}_{\text{adj}}x$, $Lx$) $= 0.166$ (obtained at $\theta \sim 0.07$)
  - MSE(random vector, $Lx$) $= 0.413$
  - Better than random but lackluster performance due to differences in eigenvalues which were not remedied downstream

# Matrices introduced so far

| | Name | Eigenvalues range |
|---|---|---|
| $A$ | Adjacency matrix | [-$\max(A)$, $\max(A)$] (also see Bhunia *et al.* 2019) |
| $D - A$ | Laplacian | [0, 2 $\max(A)$] |
| $I - D^{-1/2}AD^{-1/2}$ (or $D^{-1/2}(D-A)D^{-1/2}$) | Normalized Laplacian | [0, 2] |
| $D^{-1/2}AD^{-1/2}$ | Normalized adjacency matrix (Ng, Jordan, Weiss. 2001) | [-1, 1] |
| $I - D^{-1}A$ | Random Walk Laplacian | (non-symmetric) |
| $I + D^{-1/2}AD^{-1/2}$ | 1st order approximation GCN (Kipf and Welling. 2016) | [0, 2] |
| $\hat{A} = I + A$ | Augmented adjacency matrix | [-$\max(\hat{A})$, $\max(\hat{A})$] |
| $\hat{D} - \hat{A} = (D + I) - (A + I) = D - A$ | (Augmented) Laplacian | [0, 2 $\max(A)$] |
| $I - \hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}$ | Normalized augmented Laplacian | [0, 2] |
| $\hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}$ | Normalized augmented adjacency matrix GCN (Kipf and Welling. 2016) | [-1, 1] |

# Matrices introduced so far

| | Name | Eigenvalues range |
|---|---|---|
| $A$ | Adjacency matrix | [-max$(A)$, max$(A)$] (also see Bhunia *et al.* 2019) |
| $D - A$ | Laplacian | [0, 2 max$(A)$] |
| $I - D^{-1/2}AD^{-1/2}$ (or $D^{-1/2}(D-A)D^{-1/2}$) | Normalized Laplacian | [0, 2] |
| $D^{-1/2}AD^{-1/2}$ | Normalized adjacency matrix (Ng, Jordan, Weiss. 2001) | |
| $I - D^{-1}A$ | Random Walk Laplacian | |
| $I + D^{-1/2}AD^{-1/2}$ | 1st order approximation GCN (Kipf and Welling. 2016) | |
| $\hat{A} = I + A$ | Augmented adjacency matrix | |
| $\hat{D} - \hat{A} = (D + I) - (A + I) = D - A$ | (Augmented) Laplacian | |
| $I - \hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}$ | Normalized augmented Laplacian | |
| $\hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}$ | Normalized augmented adjacency matrix GCN (Kipf and Welling. 2016) | [-1, 1] |

These have similar eigenvectors (but differ in eigenvalues)

# Goodness of adjacency matrices

- The use of adjacency matrix $\hat{S}_{\text{adj}} = \theta\widehat{D}^{-1/2}\hat{A}\widehat{D}^{-1/2}$ allows GCN to be consider as spatial GNN (Gilmer *et al*. 2017)
  - Rewrite $\theta\widehat{D}^{-1/2}\hat{A}\widehat{D}^{-1/2}x$ as $\hat{A}HW$ it is clear that the method is spatial

- $\hat{S}_{\text{adj}} = \theta\widehat{D}^{-1/2}\hat{A}\widehat{D}^{-1/2}$ as low-pass filter (Wu *et al*. 2019)
  - A filter $x * g = Ug_\theta U^\top x$ projects $x$ into the eigenbasis $U$
    - Adjacency matrices filters $x$ through only the low frequency (global) eigenvectors
  - Two contributing factors
    1. Effects of stacking multiple layers
    2. Effects of augmentation

# Goodness of adjacency matrices

- $\hat{S}_{\text{adj}} = \theta \widehat{D}^{-1/2} \hat{A} \widehat{D}^{-1/2}$ as low-pass filter (Wu *et al.* 2019)

1. Effects of stacking multiple layers
   - As mentioned, $\left(\hat{S}_{\text{adj}}\right)^k = \theta^k U (2-\Lambda)^k U^\top$
   - At high $k$, values of $(2-\Lambda)^k$ for $(2-\Lambda) \ll 1$ diminish

| Filter | Eigenvalues (using the Karate club graph for $L$) |
|---|---|
| $L^6$ | 25.41, 17.54, 15.76, 14.95, 11.26, 9.24, 8.09, 7.31, 6.1, 4.16, 2.43, 1.82, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0.56, 0.42, 0.31, 0.21, 0.16, 0.13, 0.07, 0.05, 0, 0, 0, 0 |
| $(S_{\text{1-order}})^6$ | 64, 42.45, 25.26, 17.59, 7.14, 6.08, 4.67, 4., 3.45, 2.66, 2.14, 1.71, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0.51, 0.35, 0.15, 0.07, 0.05, 0.04, 0.03, 0.02, 0.01, 0.01, 0, 0 |
| $(\hat{S}_{\text{adj}})^6$ | 1, 0.52, 0.22, 0.12, 0.03, 0.02, 0.01, 0.01, 0.01, 0.01, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 |

- Eigenvalue of 1 for $(\hat{S}_{\text{adj}})^6$ corresponds to the eigenvalue of 0 for $L \Rightarrow$ low frequency (low-pass) filter
- The same cannot be achieved with $L$ because of the range of eigenvalues

# Goodness of adjacency matrices

- $\hat{S}_{\text{adj}} = \theta \widehat{D}^{-1/2} \hat{A} \widehat{D}^{-1/2}$ as low-pass filter (Wu *et al.* 2019)

  2. Effects of augmentation

     - An adjacency matrix with augmentation (self-loops) has a smaller spectrum than one without (that is, the normalized adjacency matrix $D^{-1/2} A D^{-1/2}$)
     - **Theorem** (Wu *et al.* 2019). Let $A$ (and $D$) be the adjacency matrix (and degree matrix) of an undirected, weighted, simple connected graph $G$. Let $\hat{A} = A + \gamma I$, $\gamma > 0$ and let $\widehat{D}$ be its degree matrix. Let
       - $\lambda_n / \lambda_1$ be the min/max eigenvalues of $D^{-1/2} A D^{-1/2}$
       - $\hat{\lambda}_n / \hat{\lambda}_1$ be the min/max eigenvalues of $\widehat{D}^{-1/2} \hat{A} \widehat{D}^{-1/2}$

       Then $\lambda_n < \hat{\lambda}_n < \hat{\lambda}_1 = \lambda_1 = 1$

     ⇒ Eigenvalues of $\widehat{D}^{-1/2} \hat{A} \widehat{D}^{-1/2}$ range in $[\lambda, 1]$ for some $\lambda > -1$ ⇒ No exponential increase at large $k$

# More levels of augmentation

- Extend augmentation $\hat{A} = A + I$ to more levels
  - Consider $\hat{A}_\gamma = A + \gamma I$ for different values of $\gamma$
    - The larger the value $\gamma$, the smaller the spectrum

      **Theorem** (Hoang and Maehara, 2019). Let
      - $\hat{A}_\gamma = A + \gamma I$ for $\gamma > 0$
      - $\widehat{D}_\gamma$ be the degree matrix for $\hat{A}_\gamma$
      - $\lambda_\gamma^{(i)}$ be the $i^{\text{th}}$ largest eigenvalue of $\widehat{D}_\gamma^{-1/2} \hat{A}_\gamma \widehat{D}_\gamma^{-1/2}$

      Then for $0 \le \gamma' < \gamma$, $\lambda_{\gamma'}^{(i)} < \lambda_\gamma^{(i)} \le \lambda_{\gamma'}^{(1)} = \lambda_\gamma^{(1)} = 1$

      **Corollary.** $\gamma > \gamma' \Rightarrow [\lambda_\gamma^{(n)}, \lambda_\gamma^{(1)}]$ is smaller than $[\lambda_{\gamma'}^{(n)}, \lambda_{\gamma'}^{(1)}]$
    - Eigenvectors would change as well but that trend is less well understood

# Eigenvalues after augmentation

- Eigenvalues of $\widehat{D}_\gamma^{-1/2}\hat{A}_\gamma\widehat{D}_\gamma^{-1/2}$ for the Karate club
  - All eigenvalues except 1 diminishes quickly when raised to some power
  - Negative eigenvalues will dovetail between negative and positive as the power changes between odd and even numbers
- **At some $\gamma$ value, the range becomes close to [0, 1]**
  - In the present example, $\gamma = 4.5$

| $\gamma$ | Eigenvalues of $\widehat{D}_\gamma^{-1/2}\hat{A}_\gamma\widehat{D}_\gamma^{-1/2}$ | Range |
|---|---|---|
| 0.0 | 1.0, 0.868, 0.713, ..., -0.583, -0.612, -0.715 | [-0.715, 1.0] |
| 0.5 | 1.0, 0.884, 0.747, ..., -0.391, -0.435, -0.542 | [-0.542, 1.0] |
| **1.0** | **1.0, 0.896, 0.774, ..., -0.271, -0.312, -0.420** | **[-0.420, 1.0]** |
| 1.5 | 1.0, 0.906, 0.796, ..., -0.182, -0.220, -0.325 | [-0.325, 1.0] |
| 2.0 | 1.0, 0.915, 0.815, ..., -0.113, -0.149, -0.249 | [-0.249, 1.0] |
| 2.5 | 1.0, 0.922, 0.830, ..., -0.057, -0.089, -0.184 | [-0.184, 1.0] |
| 3.0 | 1.0, 0.928, 0.843, ..., -0.010, -0.039, -0.129 | [-0.129, 1.0] |
| 3.5 | 1.0, 0.933, 0.854, ..., 0.032, 0.004, -0.080 | [-0.080, 1.0] |
| 4.0 | 1.0, 0.937, 0.864, ..., 0.069, 0.042, -0.037 | [-0.037, 1.0] |
| **4.5** | **1.0, 0.941, 0.873, ..., 0.103, 0.076, 0.000** | **[ 0.000, 1.0]** |
| 5.0 | 1.0, 0.945, 0.881, ..., 0.134, 0.106, 0.036 | [ 0.036, 1.0] |
| 5.5 | 1.0, 0.948, 0.888, ..., 0.163, 0.133, 0.067 | [ 0.067, 1.0] |
| 6.0 | 1.0, 0.950, 0.894, ..., 0.190, 0.158, 0.096 | [ 0.096, 1.0] |
| 6.5 | 1.0, 0.953, 0.899, ..., 0.215, 0.181, 0.123 | [ 0.123, 1.0] |
| 7.0 | 1.0, 0.955, 0.904, ..., 0.239, 0.203, 0.148 | [ 0.147, 1.0] |
| 7.5 | 1.0, 0.957, 0.909, ..., 0.261, 0.223, 0.170 | [ 0.170, 1.0] |
| 8.0 | 1.0, 0.959, 0.913, ..., 0.282, 0.242, 0.192 | [ 0.192, 1.0] |

# Eigenvectors after augmentation

- Eigenvectors of $\widehat{D}_\gamma^{-1/2}\hat{A}_\gamma\widehat{D}_\gamma^{-1/2}$ for the Karate club
- Deviation from $D^{-1/2}AD^{-1/2}$ becomes very significant as $\gamma$ increases beyond 1

| $\gamma$ | Eigenvector of $\widehat{D}_\gamma^{-1/2}\hat{A}_\gamma\widehat{D}_\gamma^{-1/2}$ of largest eigenvalue (=1) |
|---|---|
| 0.0 | 0.320, 0.240, 0.253, 0.196, ..., 0.160, 0.196, 0.277, 0.330 |
| 0.5 | 0.309, 0.234, 0.246, 0.194, ..., 0.161, 0.194, 0.269, 0.318 |
| **1.0** | **0.299, 0.229, 0.241, 0.192, ..., 0.162, 0.192, 0.262, 0.308** |
| 1.5 | 0.291, 0.225, 0.236, 0.190, ..., 0.163, 0.190, 0.255, 0.299 |
| 2.0 | 0.283, 0.222, 0.231, 0.189, ..., 0.164, 0.189, 0.250, 0.291 |
| 2.5 | 0.277, 0.218, 0.228, 0.188, ..., 0.164, 0.188, 0.245, 0.284 |
| 3.0 | 0.271, 0.216, 0.224, 0.187, ..., 0.165, 0.187, 0.241, 0.278 |
| 3.5 | -0.266, -0.213, -0.222, -0.186, ..., -0.165, -0.186, -0.237, -0.273 |
| 4.0 | -0.262, -0.211, -0.219, -0.185, ..., -0.166, -0.185, -0.234, -0.268 |
| **4.5** | **-0.258, -0.209, -0.217, -0.184, ..., -0.166, -0.184, -0.231, -0.264** |
| 5.0 | -0.254, -0.207, -0.215, -0.184, ..., -0.166, -0.184, -0.228, -0.260 |
| 5.5 | -0.250, -0.206, -0.213, -0.183, ..., -0.166, -0.183, -0.226, -0.256 |
| 6.0 | -0.247, -0.204, -0.211, -0.183, ..., -0.167, -0.183, -0.224, -0.253 |
| 6.5 | -0.244, -0.203, -0.209, -0.182, ..., -0.167, -0.182, -0.222, -0.250 |
| 7.0 | -0.242, -0.202, -0.208, -0.182, ..., -0.167, -0.182, -0.220, -0.247 |
| 7.5 | 0.239, 0.200, 0.206, 0.181, ..., 0.167, 0.181, 0.218, 0.244 |
| 8.0 | -0.237, -0.199, -0.205, -0.181, ..., -0.167, -0.181, -0.216, -0.242 |

# Eigenvectors after augmentation

- Eigenvectors of $\widehat{D}_\gamma^{-1/2} \hat{A}_\gamma \widehat{D}_\gamma^{-1/2}$ for the Karate club
- Deviation from $D^{-1/2} A D^{-1/2}$ becomes very significant as $\gamma$ increases beyond 1

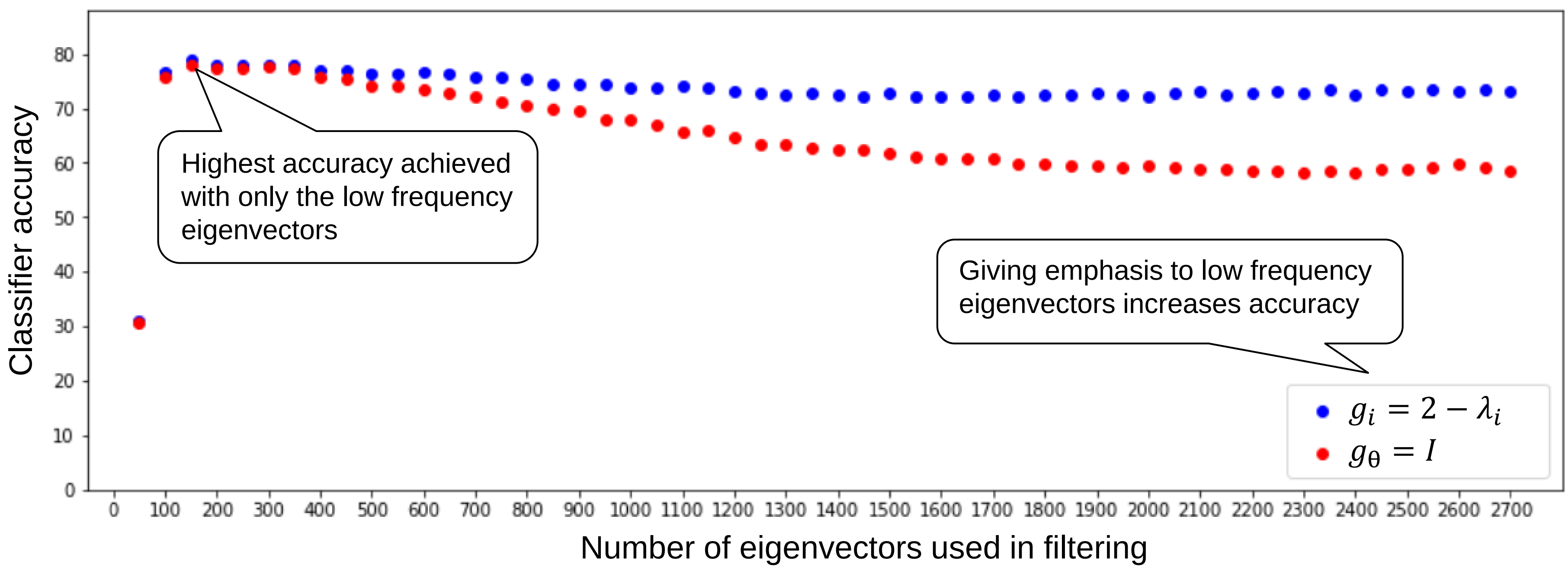
| $\gamma$ | Eigenvector of $\widehat{D}_\gamma^{-1/2} \hat{A}_\gamma \widehat{D}_\gamma^{-1/2}$ of smallest eigenvalue |
|---|---|
| 0.0 | 0.221, 0.185, 0.035, 0.019, ..., -0.164, -0.199, 0.410, 0.473 |
| 0.5 | 0.247, 0.198, 0.033, 0.015, ..., -0.169, -0.228, 0.410, 0.501 |
| **1.0** | **0.273, 0.197, 0.031, 0.009, ..., -0.166, -0.242, 0.404, 0.524** |
| 1.5 | 0.295, 0.190, 0.029, 0.004, ..., -0.161, -0.249, 0.396, 0.545 |
| 2.0 | -0.315, -0.180, -0.028, 0.001, ..., 0.154, 0.251, -0.386, -0.566 |
| 2.5 | 0.333, 0.168, 0.027, -0.006, ..., -0.147, -0.250, 0.373, 0.585 |
| 3.0 | 0.349, 0.157, 0.027, -0.009, ..., -0.141, -0.247, 0.358, 0.604 |
| 3.5 | 0.364, 0.145, 0.027, -0.012, ..., -0.135, -0.243, 0.342, 0.621 |
| 4.0 | 0.377, 0.134, 0.027, -0.015, ..., -0.129, -0.239, 0.326, 0.637 |
| **4.5** | **-0.388, -0.124, -0.028, 0.017, ..., 0.124, 0.234, -0.308, -0.653** |
| 5.0 | -0.398, -0.114, -0.029, 0.019, ..., 0.119, 0.229, -0.291, -0.667 |
| 5.5 | -0.406, -0.105, -0.030, 0.020, ..., 0.115, 0.224, -0.274, -0.680 |
| 6.0 | -0.413, -0.097, -0.031, 0.021, ..., 0.110, 0.219, -0.257, -0.692 |
| 6.5 | -0.418, -0.089, -0.031, 0.022, ..., 0.107, 0.214, -0.241, -0.703 |
| 7.0 | -0.422, -0.082, -0.032, 0.023, ..., 0.104, 0.209, -0.226, -0.714 |
| 7.5 | 0.425, 0.076, 0.033, -0.024, ..., -0.101, -0.204, 0.211, 0.723 |
| 8.0 | -0.427, -0.070, -0.034, 0.024, ..., 0.098, 0.200, -0.197, -0.733 |

# Low-pass filter performance

- We need to first find out how well a low-pass filter perform
- Construct such a filter (of only low frequency eigenvectors)
  - Recall that $x * g = U g_\theta U^\top x$ where $U = [\mu_1, \mu_2, \ldots]$
    - $g_\theta = \text{diag}(U^\top g) = \begin{bmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix}$
    - Each $g_i$ weights the significance of eigenvector $\mu_i$
  - Obtain $U$ from decomposition of normalized Laplacian
    - The eigenvalues are in the range of $[0,2]$ where $0$ has the lowest frequency (global) and $2$ has the highest frequency
    - Sort eigenvectors by the eigenvalues and include only low frequency eigenvectors in filter $UIU^\top$ (details in later slide)
      - The use of $I$ as $g_\theta$ implies that all eigenvectors included are equal
      - Alternatively let $g_i = 2 - \lambda_i$ so smaller eigenvalues are more significant
    - Compare effects of including only low frequency eigenvectors versus using all eigenvectors

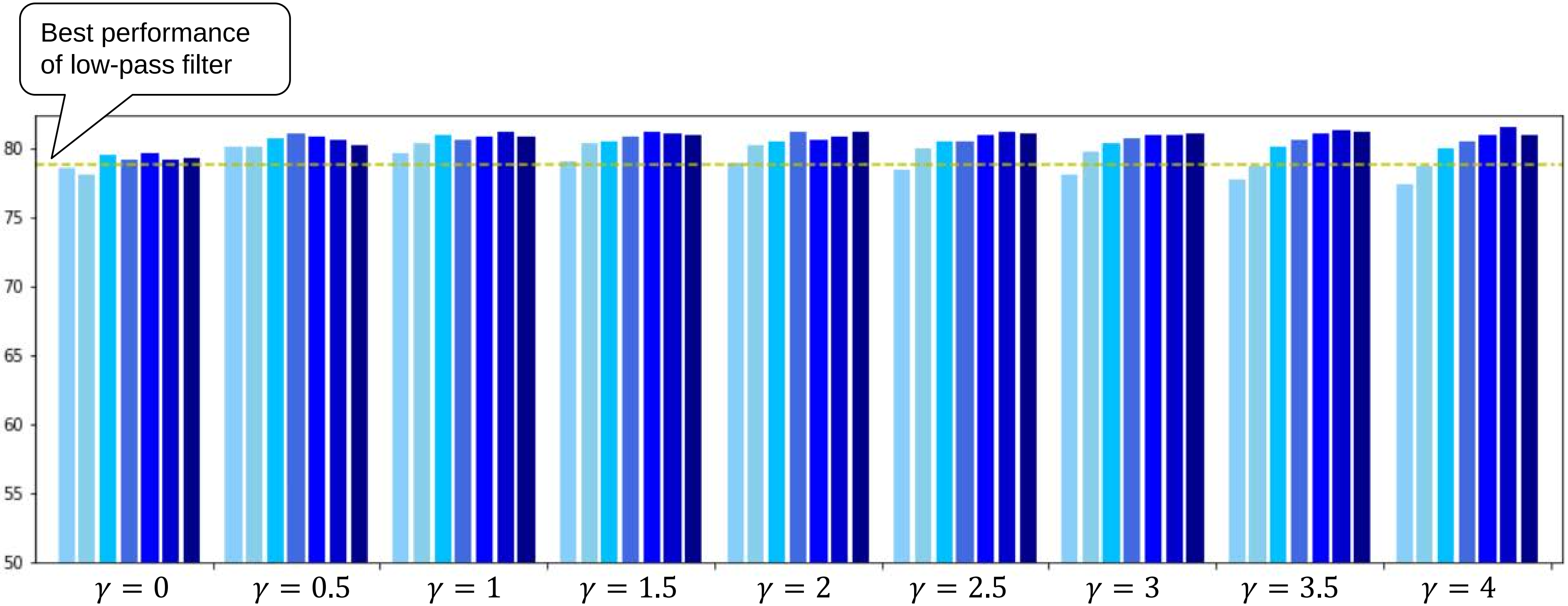
# Low-pass filter performance

- Cora dataset
  - Nodes: 2708 scientific publications
  - Links: 5429
  - Feature: 1433 word embedding
  - Classes: 7
- Procedure
  - Filter features with 50, 100, 150, … eigenvectors of the lowest frequencies
  - Train a 2-layer MLP to classify with the filtered features



# Adjacency matrix performance

- Repeat test with $\widehat{D}_\gamma^{-1/2}\hat{A}_\gamma\widehat{D}_\gamma^{-1/2}$ where $\hat{A}_\gamma = A + \gamma I$ as filter




- Accuracies obtained comparable to low-pass filters
- Increasing amount of augmentation $\gamma$ improves accuracy
- Stacking more layers helps but only to a certain extend

# Filter with only subset eigenvectors

- Recall from earlier slide

$$U^\top x = \begin{bmatrix} \leftarrow & \mu_1 & \rightarrow \\ \leftarrow & \mu_2 & \rightarrow \\ & \vdots & \end{bmatrix} x = \begin{bmatrix} \mu_1^\top x \\ \mu_2^\top x \\ \vdots \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}$$

- Examine the exact form of $a_i$
  - Denote $x = \begin{bmatrix} \leftarrow & x_1 & \rightarrow \\ \leftarrow & x_2 & \rightarrow \\ & \vdots & \end{bmatrix}$, where each $x_i = [x_{i1} \quad x_{i2} \quad \cdots \quad x_{iM}]$

$$U^\top x = \begin{bmatrix} \leftarrow & \mu_1 & \rightarrow \\ \leftarrow & \mu_2 & \rightarrow \\ & \vdots & \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1M} \\ x_{21} & x_{22} & \cdots & x_{2M} \\ & \vdots & & \end{bmatrix} = \begin{bmatrix} \mu_1^\top x_{*1} & \mu_1^\top x_{*2} & \cdots & \mu_1^\top x_{*M} \\ \mu_2^\top x_{*1} & \mu_2^\top x_{*2} & \cdots & \mu_2^\top x_{*M} \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

$$\Rightarrow a_i = [\mu_i^\top x_{*1} \quad \mu_i^\top x_{*2} \quad \cdots \quad \mu_i^\top x_{*M}]$$

  - $a_i$ is computed from all rows and columns of $x$
  - For $\mu_i^\top x_{**}$ to compute correctly indices of $\mu_i^\top$ and $x_{**}$ must match
  - However, the **ordering of** $\mu_1, \mu_2, \ldots$ **in** $\begin{bmatrix} \leftarrow & \mu_1 & \rightarrow \\ \leftarrow & \mu_2 & \rightarrow \\ & \vdots & \end{bmatrix}$ **does not matter**
    - To use only some eigenvectors, simply **zero out the unused eigenvectors** (corresponding $a_i$s will become zero)
    - Or just **remove those unused eigenvectors**