Math Behind GCN

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Overview

Graph Signal Processing (GSP)

Vertex Domain

Discrete Convolution

Convolutional Neural Networks (CNN)

Spectral Domain

Spectral Graph Convolution (SGC)

Graph Convolutional Networks (GCN)

Relational GCN (r-GCN)
Convolution → CNN

- Convolution: \[(f \ast g)(n) = \int_{-\infty}^{\infty} f(\tau)g(n-\tau)d\tau\]
- Discrete Convolution: \[(f \ast g)(a, b) = \sum_h \sum_k f(h, k)g(a - h, b - k)\]
  - In a way, **weighted** sum.
- \(g\) → the graph; \(f\) → the filter (kernel)
- **input** → \{convolution, activation, pooling\}∗ → **output**
  (e.g. classification: **output** → flatten → fully connected → softmax)
- Weight to be learned.
Vertex Domain v.s. Spectral Domain

Graph Signal Processing (GSP) → Vertex Domain

Spectral Domain → Convolution

Convolutional Neural Networks (CNN) → Spectral Graph Convolution (SGC)

Graph Convolutional Networks (GCN) → Relational GCN (r-GCN)
Vertex Domain v.s. Spectral Domain

- **Euclidean structure:**
  - matrix
  - e.g. image
  - Applying CNN, feature map could be extracted from the receptive field by using the kernel.

- **Non-Euclidean structure:**
  - graph $G = \langle V, E \rangle$
  - Couldn’t apply CNN: $n_{neighbors}$ is different, no fixed-sized kernel could apply; *translation invariance of discrete convolution is not guaranteed.*
  - How to extract features in general graphs?
    - **Vertex (spacial) domain:** (1) define receptive field (deal with each node); (2) extract features of neighbors (non-convolutional way)
    - **Spectral domain**
Graph Fourier Transformation

- Graph Signal Processing (GSP)
  - Vertex Domain
  - Spectral Domain
  - Discrete Convolution
  - Convolutional Neural Networks (CNN)
  - Spectral Graph Convolution (SGC)
  - Graph Convolutional Networks (GCN)
    - Relational GCN (r-GCN)
Graph Signal Processing (GSP)

Brief Intro

- Graph Signal Processing makes it possible to do convolution on generalized graphs. e.g. Graph Fourier transformation enables the formulation of fundamental operations on graphs, such as spectral filtering of graph signals.

- Convolution in the vertex domain is equivalent to multiplication in the graph spectral domain.
SGC $\rightarrow$ GCN

- Vertex Domain
- Spectral Domain
- Graph Signal Processing (GSP)
- Discrete Convolution
- Convolutional Neural Networks (CNN)
- Spectral Graph Convolution (SGC)
- Graph Convolutional Networks (GCN)
- Relational GCN (r-GCN)
Brief Intro

Graph Convolutional Networks (GCN) is a localized first-order approximation of Spectral Graph Convolution.
GCN \rightarrow r-GCN

Graph Signal Processing (GSP) \rightarrow \text{Vertex Domain} \rightarrow \text{Spectral Domain} \rightarrow \text{Discrete Convolution} \rightarrow \text{Convolutional Neural Networks (CNN)} \rightarrow \text{Spectral Graph Convolution (SGC)} \rightarrow \text{Graph Convolutional Networks (GCN)} \rightarrow \text{Relational GCN (r-GCN)}
Relational Graph Convolutional Networks (r-GCN) is an extension of Graph Convolutional Networks (GCN) on relational data.
The Emerging Field of Signal Processing on Graphs

- **Graph Signal Processing (GSP)**
- **Vertex Domain**
- **Spectral Domain**
- **Discrete Convolution**
- **Convolutional Neural Networks (CNN)**
- **Spectral Graph Convolution (SGC)**
- **Graph Convolutional Networks (GCN)**
- **Relational GCN (r-GCN)**
The Emerging Field of Signal Processing on Graphs

Objective

- To offer a tutorial overview of graph-based data analysis (especially arbitrary graphs, weighted graphs), from a signal-processing perspective.
- Examples of graph signals covers: transportation networks (e.g. epidemic), brain imaging (e.g. fMRI images), machine vision, automatic text classification.
- Irregular, high dimensional data domain; goal is to extracting information efficiently.
- Constructing, analyzing, manipulating graphs, as opposed to signals on graphs.
What corresponding relations can we get between signal processing tasks and graph data?

<table>
<thead>
<tr>
<th>Classical Discrete-Time Signal</th>
<th>Graph Signal</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$ samples with $N$ values</td>
<td>$N$ vertices (data points) with $N$ values</td>
</tr>
<tr>
<td>a classical discrete-time signal with $N$ samples: vector in $\mathbb{R}^N$</td>
<td>a graph signal with $N$ vertices: vector in $\mathbb{R}^N$</td>
</tr>
</tbody>
</table>

Modulating a signal on the real line by multiplying by a complex exponential corresponds to translation in the Fourier domain\(^1\).

What makes the problem settings different?

- A discrete-time signal ignores key dependencies in irregular data domain.
- Different in fundamental, non-trivial properties.

\(^1\)Modulation and Sampling. Click here link to some EE slides.
Challenge # 1: Shifting

Weighted graphs are irregular structures that lack a shift-invariant notion of translation. $f(t - n)$ no longer makes sense. $^a_b$

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$^a$Special case: ring graph, where Laplacians are circulant and the graphs are highly regular.

$^b$Thus convolution could not be applied directly.
Challenge # 2: Transform

The analogous spectrum in the graph setting is discrete and irregularly spaced. Recall that:

Modulating a signal on the real line by multiplying by a complex exponential corresponds to translation in the Fourier domain.

“Transformation” to the graph spectral domain is needed, otherwise convolution could not be applied.
Challenge # 3: Downsampling

Downsampling means “delete every other data point” for a discrete-time signal. But what is downsampling for graph signal? What is “every other vertex”?

Essential for pooling.
Challenge # 4: Multiresolution

With a fixed notion of downsampling, we still need a method to generate coarser version of the graph to achieve multiresolution. And the coarse version should still capture the structural properties embedded in the original graph. Essential for pooling.
Analyzing signals defined on an undirected, connected, weighted graph $G = \{V, E, W\}$, where set of vertices is finite $|V| = N$, edges is represented by $E$ and $W$ is a weighted adjacency matrix.

- Edge $e = (i, j)$ connects vertices $v_i$ and $v_j$, the entry $W_{i,j}$ represents the weight of the edge. If $e = (i, j)$ does not exists then $W_{i,j} = 0$.

- If the graph $G$ is not fully connected and has $M > 1$ connected components, separate the graph into $M$ parts and independently process the separated signals on each subgraph.

- A signal / function defined on the vertices of the graph: $f : V \rightarrow \mathbb{R}$ may be represented as a vector $f \in \mathbb{R}^N$, where $f_i$ represents the function value at $v_i$. 
Problem Definition (2/2)

- $W_{i,j}$ could be naturally given by the application, or defined by ourselves. One common way is the \textbf{threshold Gaussian kernel} (for some parameters $\theta$ and $\kappa$):

$$W_{i,j} = \begin{cases} 
\exp \left( -\frac{[\text{dist}(i,j)]^2}{2\theta^2} \right) & \text{if } \text{dist}(i,j) \leq \kappa \\
0 & \text{otherwise}
\end{cases}$$

\textbf{Solution:} define operations on weighted graphs differently.
The Emerging Field of Signal Processing on Graphs

Other topics mentioned in the paper: Translation, Modulation & Dilation, Graph Coarsening & Downsampling & Reduction (Challenge # 3 and 4), vertex domain design, etc.
The classic Fourier transform:

\[ \hat{f}(\xi) = \langle f, e^{2\pi i \xi t} \rangle = \int_{\mathbb{R}} f(t) e^{2\pi i \xi t} dt \]

is the expansion of \( f \) in terms of the complex exponentials \( (e^{2\pi i \xi t}) \); the expansion results are the eigenfunctions\(^2\) of 1-d Laplace operator \( \Delta \):

\[ -\Delta (e^{2\pi i \xi t}) = -\frac{\partial^2}{\partial t^2} e^{2\pi i \xi t} = (2\pi \xi)^2 e^{2\pi i \xi t} \]

or, in other ways,

\[ \hat{f}(\omega) = \int f(t) e^{-i\omega t} dt, \quad \Delta(e^{-i\omega t}) = -\omega^2 e^{-i\omega t} \]

\[ e^{i\omega t} = \cos(\omega n) + i \sin(\omega n), \quad i = \sqrt{-1} \]

\(^2\)Should correspond to eigenvectors in graph settings.
The Emerging Field of Signal Processing on Graphs

Graph Fourier transform $\hat{f}$: of any $f \in \mathbb{R}^N$, of all vertices of $G$, expansion of $f$:

$$\hat{f}(\lambda_l) = \langle f, u_l \rangle = \sum_{i=1}^{N} f(i)u^*_l(i)$$

$u^*_l(i)$ is the conjugate of $u_l(i)$ in the complex space.

The inverse graph Fourier transform is then given by:

$$f(i) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l)u_l(i)$$

Intuitive understanding of inverse Fourier transform$^3$: we know all frequency and phase information about a signal then we may reconstruct the original signal precisely.

With $\otimes$ for convolution, $\odot$ for simple multiplication:

$$\mathcal{X} \otimes \mathcal{Y} = \text{Fourier}_{\text{inverse}}(\text{Fourier}(\mathcal{X}) \odot \text{Fourier}(\mathcal{Y}))$$

---

$^3$Yunsheng’s slides: change of basis
Filtering in the frequency domain:

\[ \hat{f}_{\text{out}}(\xi) = \hat{f}_{\text{in}}(\xi) \hat{h}(\xi) \]

its inverse Fourier transform:

\[ f_{\text{out}}(t) = (f_{\text{in}} \ast h)(t) = \int_{\mathbb{R}} \hat{f}_{\text{in}}(\xi) \hat{h}(\xi) e^{2\pi i \xi t} d\xi \]

**Convolution on Graph**: frequency filtering with the complex exponentials replaced by the graph Laplacian eigenvectors \((u_l(i))\).

\[ f_{\text{out}}(i) = (f \ast h)(i) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l) \hat{h}(\lambda_l) u_l(i) \]

where \( \hat{h}(\cdot) \) is the transfer function of the filter, \( f_{\text{in}} \) omitted in to be \( f \).

\(^4\)Yunsheng’s slides: feature aggregation; Defferrard’s work: convolution + non-linear activation.
The Emerging Field of Signal Processing on Graphs

1-d Laplacian $\triangle$: the second derivative

Graph Laplacian: A difference operator that satisfies

$$(Lf)(i) = \sum_{j \in \mathcal{N}_i} W_{i,j} [f(i) - f(j)]$$

where $\mathcal{N}_i$ is the set of vertices connected to vertex $i$ by an edge.
The Emerging Field of Signal Processing on Graphs

Graph Laplacian

What

- \( D \): diagonal matrix whose \( i^{th} \) diagonal element \( d_i \) is equal to the sum of the weights of all the edges incident to \( v_i \)
- **combinatorial graph Laplacian** / non-normalized graph Laplacian:
  \[
  L = D - W
  \]
- normalized graph Laplacian / symmetric normalized Laplacian:
  \[
  \tilde{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I_N - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}. \]
- asymmetric graph Laplacian: \( L_a = I_N - P \), where \( P = D^{-1}W \) is the random walk matrix

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\( ^a I_N \) is \( N \times N \) identity matrix.

\( ^b P_{i,j} \) describes the probability of going from \( v_i \) to \( v_j \) in one step of a Markov random walk on \( G \).
The Emerging Field of Signal Processing on Graphs

Graph Laplacian

What - in other words

- \( L = D - W \) (when \( W \) is \( A \), which means that each edge has weight 1):
  \[
  L(u, v) = \begin{cases} 
  d_v & \text{if } u = v \text{ (} d_v \text{ is the degree of node } v) \\
  -1 & \text{if } u \neq v, (u, v) \in \mathcal{E} \\
  0 & \text{otherwise}
  \end{cases}
  \]

- \( \tilde{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I_N - D^{-\frac{1}{2}}WD^{-\frac{1}{2}} \) (when \( W \) is \( A \)):
  \[
  \tilde{L}(u, v) = \begin{cases} 
  1 & \text{if } u = v, d_v \neq 0 \text{ (} d_v \text{ is the degree of node } v) \\
  -\frac{1}{\sqrt{d_u d_v}} & \text{if } u \neq v, (u, v) \in \mathcal{E} \\
  0 & \text{otherwise}
  \end{cases}
  \]
Graph Laplacian

What - more

- The normalized and non-normalized graph Laplacians are both examples of generalized graph Laplacians. Generalization: any symmetric matrix whose $i, j^{th}$ entry is negative if there’s an edge connecting $v_i, v_j$, zero if $i \neq j$ and $v_i, v_j$ not connected, may be anything when $i = j$.

- $L_a$ has the same set of eigenvalues as $\tilde{L}^b$.

- Laplacian of a graph is also sometimes called: admittance matrix, discrete Laplacian or Kirchoff matrix.

- It remains no clear answer when should we use which Laplacian matrix.

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Supplementary notes:

- Also called discrete Schrödinger operators.

- If $\tilde{u}_l$ is an eigenvector of $\tilde{L}$ associated with $\tilde{\lambda}_l$, then $D^{-1/2} \tilde{u}_l$ is an eigenvector of $L_a$ associated with the eigenvalue $\tilde{\lambda}_l$.
An example of non-normalized $L$ with $W = A$, $L = D - A$:
Graph Laplacian properties:

- (normalized / non-normalized) graph Laplacian ($L$, or $\tilde{L}$) is a real symmetric matrix, with a complete set of orthonormal eigenvectors\(^5\), which we denote by \(\{u_l\}\) where \(l = 0, 1, \ldots, N - 1\).
- \(\{u_l\}\) has associated real non-negative eigenvalues \(\{\lambda_l\}\).
- \(Lu_l = \lambda_l u_l\)
- The amount of eigenvalues that appears to be 0 is equal to the number of connected components of the graph.
- Considering connected graphs only, we could order the eigenvalues as \(0 = \lambda_0 \leq \lambda_1 \cdots \leq \lambda_{N-1}\).
- The entire spectrum could be denoted as:

\[
\sigma(L) = \{\lambda_0, \lambda_1, \ldots, \lambda_{N-1}\}
\]

\(^5\)Also known as graph Fourier modes.
Graph Laplacian another expression:

\[ L = U \begin{bmatrix} \lambda_0 & 0 & \cdots & 0 \\ 0 & \lambda_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_{N-1} \end{bmatrix} U^{-1} = U \begin{bmatrix} \lambda_0 & 0 & \cdots & 0 \\ 0 & \lambda_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_{N-1} \end{bmatrix} U^T \]

where \( \lambda_i \) is eigenvalue, and \( U = (\vec{u}_0, \vec{u}_1, \ldots, \vec{u}_N) \), \( \vec{u}_i \) is column vector, and is unit eigenvector. \( U^{-1} \) could be replaced by \( U^T \) because \( UU^T = I_N \).

Fourier transformation could be expressed as:

\[ \hat{h}(L) = U \begin{bmatrix} \hat{h}(\lambda_0) & 0 & \cdots & 0 \\ 0 & \hat{h}(\lambda_1) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \hat{h}(\lambda_{N-1}) \end{bmatrix} U^T, \quad f_{out} = \hat{h}(L)f_{in} \]
Graph Coarsening: \((G = \{V, E, W\})\)

1. Graph reduction: identify a reduced set of vertices \(V^{\text{reduced}}\)
2. Graph contraction: assign edges and weights to connect the new set of vertices, \(E^{\text{reduced}}\) and \(W^{\text{reduced}}\).
The convolution theorem defines convolutions as linear operators that diagonalize in the Fourier basis (represented by the eigenvectors of the Laplacian operator)\textsuperscript{6}.

Fourier transform localize signals in frequency domain but not in time domain.

Indeterminacy principles: one cannot be arbitrarily accurate in local both in time and frequency.

The meaning of localize: to find where the signal is mostly concentrated, and with what precision.

Vertex domain filtering ($\mathcal{N}(i, k)$ is $i$’s neighbors within K-hop):

$$f_{out}(i) = b_{i,i} f_{in}(i) + \sum_{j \in \mathcal{N}(i,K)} b_{i,j} f_{in}(j)$$

\textsuperscript{6}Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering (NIPS 2016)
Problem Settings

1. Data sets: MNIST and 20NEWS
2. $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{W}\}$, undirected connected weighted graph.
3. Focus on filtering, other parts remain default (such as the activation, ReLU).

Contributions

1. A spectral graph theoretical formulation of CNNs on graphs;
2. Strictly localized spectral filters, limited to a radius of $K$ ($K$ hops from the central vertex);
3. Low computational complexity, $O(K\mathcal{E})$.
4. Low storage cost, stores the data and Laplacian (sparse, $|\mathcal{E}|$ values).
5. Efficient pooling strategy\(^a\).

\(^a\)Rearrange into binary tree, analog to pooling of 1D signals
Fast localized spectral filters:

**Why?**

- Why not spatial filter, why spectral filter? - Spatial domain filter is naturally localized, but spectral domain could also achieve localization, while having more mathematically-supported operators, etc.

- Why emphasize “fast”? - A filter defined in the spectral domain is not naturally localized, translations are costly due to the $O(n^2)$ multiplication with the graph Fourier basis.

**How?**

A special choice of filter parametrization.
Starting from signal processing:

- Recall that: The Laplacian is indeed diagonalized by the Fourier basis (the orthonormal eigenvectors) \( U = [u_0, u_1, \ldots, u_{N-1}] \in \mathbb{R}^{N \times N} \).
- Let \( \Lambda = \text{diag}(\lambda_0, \ldots, \lambda_{N-1}) \), then we have \( L = U \Lambda U^T \).
- The graph Fourier transform of a signal \( x \in \mathbb{R}^N \) is then defined as \( \hat{x} = U^T x \in \mathbb{R}^N \), with inverse \( x = U \hat{x} \). This transformation enables the formation of fundamental operations, such as filtering, just as on Euclidean spaces.
- Recall that: \( \mathcal{X} \otimes \mathcal{Y} = \text{Fourier}_{\text{inverse}}(\text{Fourier}(\mathcal{X}) \odot \text{Fourier}(\mathcal{Y})) \)
- Definition of convolutional operator:

\[
(f \ast h)(\ast G) = U((U^T f) \odot (U^T h))
\]

where \( \odot \) is the element-wise Hadamard product\(^7\).

\(^7\)Hadamard product: \((A \odot B)_{i,j} = A_{i,j} \times B_{i,j}\)
A signal $x$ filtered by $g_\theta$ as

$$y = g_\theta(L)x = g_\theta(U\Lambda U^T)x = U g_\theta(\Lambda) U^T x$$

where a non-parametric filter whose parameters are all free would be defined as $g_\theta(\Lambda) = \text{diag}(\theta)$, with $\theta \in \mathbb{R}^N$ be a vector of Fourier coefficients.

Non-parametric filters are not localized in space and have learning complexity of $O(N)$. Solution: using a polynomial filter:

$$g_\theta(\Lambda) = \sum_{k=0}^{K-1} \theta_k \Lambda^k$$

where $\theta \in \mathbb{R}^K$ is a vector of polynomial coefficients.
Something we skipped in the first paper\textsuperscript{8}:

Kronecker delta function $\delta_i \in \mathbb{R}^N$.

$$\delta_n(i) = \begin{cases} 1 & \text{if } i = n \\ 0 & \text{otherwise} \end{cases}$$

Usage: for localization.

\textsuperscript{8}It is in the \textbf{translation} part.
What is the value of filter $g_{\theta}$, at vertex $j$, centered at vertex $i$?

$$(g_{\theta}(L)\delta_{i})_{j} = (g_{\theta}(L))_{i,j} = \sum_{k} \theta_{k}(L^{k})_{i,j}$$
Let $d_G$ denote the shortest path distance, $d_G(i, j) > K$ means that $(L^K)_{i,j} = 0$.

Spectral filters represented by $K^{th}$-order polynomials of the Laplacian are exactly $K$-localized.

The learning complexity is $O(K)$, the support size of the filter, thus same complexity as classic CNN.
Note that computing \( y = U g_\theta(\Lambda) U^T x \) is still expensive when having to do multiplication with the Fourier basis \( U \).

How to achieve fast filtering?

**Solution**

Parameterize \( g_\theta(L) \) as a polynomial function that can be recursively computed from \( L \), then it costs us \( K \) multiplications of \( L \), time complexity will be reduced from \( O(N^2) \) to \( O(K|\mathcal{E}|) \).

- Existing tools in the field of GSP: Chebyshev expansion and Krylov subspace.
- The reason why Chebyshev and not Krylov: simpler.
- Chebyshev expansion: \( T_0(x) = 0 \), \( T_1(x) = x \),
  \( T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x) \).
Recall the parameterized filter:

\[ g_\theta(\Lambda) = \sum_{k=0}^{K-1} \theta_k \Lambda^k \]

With Chebyshev expansion, we have

\[ g_\theta(\Lambda) \approx \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\Lambda}) \]

where \( \tilde{\Lambda} = 2\Lambda/\lambda_{max} - I_N \) is a diagonal matrix of scaled eigenvalues lie in \([-1, 1]\). Now \( \theta \in \mathbb{R}^K \) becomes a vector of Chebyshev coefficients.

With \( \tilde{L} = 2L/\lambda_{max} - I_N \), we have \( \bar{x}_0 = x, \bar{x}_1 = \tilde{L}x, \bar{x}_k = T_k(\tilde{L})x = 2\tilde{L}\bar{x}_{k-1} - \bar{x}_{k-2} \):

\[ y = g_\theta(L)x \approx \sum_{k=0}^{K-1} \theta_k T_k(\tilde{L})x = [\bar{x}_0, \ldots \bar{x}_{K-1}]\theta \]
\[ y_{s,j} = \sum_{i=1}^{F_{in}} g_{\theta_{i,j}}(L)x_{s,i} \in \mathbb{R}^N \]

**E:** loss energy over a mini-batch of \( S \) samples. Loss energy \( E \) is the cross-entropy with an \( l_2 \) regularization on the weights of all FC\( k \) (Fully-Connected layer with \( k \) hidden units) layers.

**Training:** back propagation using \( E \)'s gradients over \( \theta \) and \( x \).
Pooling: coarsening to create a balanced binary tree (map two unmatched neighbors each time); then the number of vertices is reduced.

Adjacent nodes are hierarchically merged at coarser levels.
Figure 1: Architecture of a CNN on graphs and the four ingredients of a (graph) convolutional layer.
Semi-Supervised Classification with GCN

- Discrete Convolution
- Convolutional Neural Networks (CNN)
- Spectral Graph Convolution (SGC)
- Graph Convolutional Networks (GCN)
- Relational GCN (r-GCN)

Graph Signal Processing (GSP) → Vertex Domain → Spectral Domain

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Problem definition

- Task: semi-supervised entity classification
- Data sets: citation network, knowledge graph, random graph.
- Graph: undirected, weight = 1 if connected otherwise 0.

Contribution

- A layer-wise propagation rule, that is simple and well-behaved, working for NN models.
- Semi-supervised classification, that is fast and scalable, using GCN\(^a\).

\(^a\)Previous methods always use graph Laplacian regularization term in the loss function to smooth the graph and make up for the absence of labels. But they have an assumption of obvious similarity of neighbor, which leads to restriction in model capacity.
Staring from graph signal processing again:

- Using normalized graph Laplacian:
  \[
  \tilde{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I_N - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}
  \]
  
  \(W\) is simplified to be \(A\).

- Using the same approximation used in the previous paper (parameterize using Chebyshev polynomials).

- Further limit \(K = 1\) (only the direct neighbor is reachable at each layer), and stack multiple layers.

- Add self-connection to each vertices.
Recall that, previously, with Chebyshev expansion, we have:

\[ g_\theta(\Lambda) \approx \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\Lambda}) \]

where \( \tilde{\Lambda} = 2\Lambda/\lambda_{max} - I_N \) is a diagonal matrix of scaled eigenvalues lie in \([-1, 1]\). With \( \tilde{L} = 2L/\lambda_{max} - I_N \), we have \( \tilde{x}_0 = x \), \( \tilde{x}_1 = \tilde{L}x \), \( \tilde{x}_k = T_k(\tilde{L})x = 2\tilde{L}\tilde{x}_{k-1} - \tilde{x}_{k-2} \):

\[ y = g_\theta(L)x \approx \sum_{k=0}^{K-1} \theta_k T_k(\tilde{L})x = [\tilde{x}_0, \ldots, \tilde{x}_{K-1}]\theta \]

Now we have layer-wise linear model by limit \( K = 1 \), and further approximate \( \lambda_{max} \approx 2 \). We are expecting that by stacking multiple such layers the model should perform well.
Semi-Supervised Classification with GCN

\[ y = g_\theta(L)x \approx \sum_{k=0}^{K-1} \theta_k T_k(\tilde{L})x = [\bar{x}_0, \ldots, \bar{x}_{K-1}]\theta \]

becomes:

\[ y = g_\theta(L)x \approx \theta_0 x + \theta_1 (L - I_N)x = \theta_0 x - \theta_1 \tilde{L}x \]

where \( \tilde{L} \) is the normalized Laplacian \( (\tilde{L} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}) \) in this case. With \( \theta^* = \theta_0 - \theta_1 \), we have:

\[ y = g_\theta(L)x \approx \theta^* \left( I_N + D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \right)x \]

With \( \tilde{A} = A + I_N \) and \( \tilde{D}_{ii} = \sum_j \tilde{A}_{ij}, \Theta \in \mathbb{R}^{C \times F} \) is the filter parameters, \( Z \in \mathbb{R}^{N \times F} \) be the convolved signal matrix, we have:

\[ Z = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} X\Theta \]
Semi-Supervised Classification with GCN

\[ Z = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} X \Theta \]

Adding an activation function, we get the form of:

\[ H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right) \]

which is the well-known form of GCN. In practice they used ReLU as the non-linear activation function.

In details\(^9\) \((c_{i,j} = \sqrt{d_i d_j}, d_i = |N_i|)\):

\[ h_i^{(l+1)} = \sigma \left( \sum_{j \in N_i} \frac{1}{c_{i,j}} h_j^{(l)} W^{(l)} \right) \]

All the expressions could be generalized as\(^{10}\):

\[ h_i^{(l+1)} = \sigma \left( \sum_{m \in M_i} g_m(h_i^{(l)}, h_j^{(l)}) \right) \]

---

\(^9\)See the Weisfeiler-Lehman algorithm in appendix

\(^{10}\)Will be seen in r-GCN part.
Semi-Supervised Classification with GCN
Semi-Supervised Classification with GCN

Downstream task: **semi-supervised classification**

Loss function:

\[ \mathcal{L} = - \sum_{l \in \mathcal{Y}_L} \sum_{f=1}^{F} Y_{lf} \ln Z_{lf} \]

1. \( \mathcal{Y}_L \): set of labeled nodes (indices)
2. \( F \): number of labels of the nodes
3. \( Z \): predicted outcome, softmax of the output of the network.
Modeling Relational Data with GCN (r-GCN)

- Graph Signal Processing (GSP)
- Vertex Domain
- Spectral Domain
- Convolutional Neural Networks (CNN)
- Spectral Graph Convolution (SGC)
- Graph Convolutional Networks (GCN)
- Relational GCN (r-GCN)
Problem Settings
- Tasks: entity classification and link prediction.
- Data sets: knowledge graph.
- Relations are directed, but the adjacent matrices we use contains each relation and its reverse.

Motivation
Tasks on more general (heterogeneous) graphic structure: knowledge graph completion.

Solution
GCN + weighed sum of neighbors from different relations; regularization applied to weights so as to reduce overfitting problem.
### GCN model

\[
h_i^{(l+1)} = \sigma \left( \sum_{m \in M_i} g_m(h_i^{(l)}, h_j^{(l)}) \right)
\]

- \(h_i^{(l)}\): Hidden state of node \(v_i\) in the \(l^{th}\) layer. size: \(\mathbb{R}^{d(l)}\).
- \(d(l)\): \(l^{th}\) layer’s representation’s dimension.
- \(\sigma(\cdot)\): Nonlinear activation function (e.g. ReLU).
- \(M_i\): Incoming messages for node \(v_i\), always (chosen to be) identical to the incoming edges.
- \(g_m(\cdot, \cdot)\): A message-specific NN-like function, or simply a linear transformation \((g(h_i, h_j) = Wh_j)\). Kipf and Welling did it the weight matrix way.

### r-GCN model

\[
h_i^{(l+1)} = \sigma \left( \left( \sum_{r \in \mathcal{R}} \sum_{j \in \mathcal{N}_{i}^r} \frac{1}{c_{i,r}} W_r^{(l)} h_j^{(l)} + W_0^{(l)} h_i^{(l)} \right) \right)
\]

- \(\mathcal{R}\): Set of all relations.
- \(\mathcal{N}_{i}^r\): Set of neighbor (indices) of node \(v_i\) under relation \(r\).
- \(c_{i,r}\): Problem-specific normalization constant, could be learned or chosen in advance (in their paper, chosen to be \(|\mathcal{N}_{i}^r|\)).
- \(W_0^{(l)} h_i^{(l)}\): A single self-connection of a special relation type to ensure that representation at layer \(l\) is passed to corresponding part of layer \(l + 1\). (In practice, an identity matrix is added when representing the adjacent matrices.)
- \(W_r^{(l)}\): The weight to be regularized (next slide) and learned (next next slide).
r-GCN: ways of regularizing $W_r^{(l)}$

### Basis decomposition

$$W_r^{(l)} = \sum_{b=1}^{B} a_{rb} V_b^{(l)}$$

- **$V_b^{(l)}$**: Basis transformations to be learned, similar with traditional weights. $\in \mathbb{R}^{d(l+1)} \times \mathbb{R}^{d(l)}$.
- **$a_{rb}$**: Coefficients, the only parameter that depends on $r$, dimension related with support and number of basis ($B$), it is a parameter that is assigned individually to each adjacent matrix (|2R + 1| matrices in total, also called support).
- **$B$**: Number of base, user-specified parameter, sometimes called “number of coefficients” in their expression.

### Block-diagonal-decomposition

$$W_r^{(l)} = \bigoplus_{b=1}^{B} Q_{rb}^{(l)}$$

- **$W_r^{(l)}$**: Are block-diagonal matrices: $(Q_{1r}^{(l)}, Q_{2r}^{(l)} \ldots Q_{Br}^{(l)})$.
- **note**: Actually not implemented for node classification task.
- **note**: can be viewed as sparsity constraints (whereas basis decomposition can be viewed as weight sharing).
r-GCN: downstream tasks (Knowledge Graph Completion)

(a) Entity classification

(b) Link prediction
**Entity Classification**

\[ \mathcal{L} = - \sum_{i \in \mathcal{Y}} \sum_{k=1}^{K} t_{ik} \ln h^{(L)}_{ik} \]

- **\mathcal{L}**: Categorical cross-entropy loss.
- **\mathcal{Y}**: Nodes that have labels.
- **t_{ik}**: Ground truth labels.
- **h^{(L)}_{ik}**: \(k\)th entry of node \(i\) at layer \(L\) (Layer \(L\) is the output layer.)

**Link Prediction**

\[ \mathcal{L} = - \frac{1}{|\hat{E}|} \sum_{(s, r, o, y) \in \tau} y \log l(f(s, r, o)) \]

\[ + (1-y) \log (1-l(f(s, r, o))) \]

- \(e_i\) = \(h^{(L)}_i\), use r-GCN as encoder.
- \(f(s, r, o)\): DistMult factorization is used, \(f(s, r, o) = e_s^T R_r e_o\).
- \((s, r, o)\): \(s, o\) are node (indices), \(r\) is the relation between them.
- \(y\): \(y = 1\) for positive triples, \(0\) for negative triples. Negative sampling is used.
- \(\tau\): All triples (real + corrupted).
- \(R\): \(R_r\) is a d*d diagonal matrix to be learned.
- \(l\): Logistic sigmoid function.
Yunsheng’s Slides on GCN

Ferenc Huszar’s comment on GCN (+ followup discussion by Thomas Kipf)

Thomas Kipf (the author)’s comment on GCN (+ replying Ferenc Huszar)
The End