

$$X(\underline{\mathbb{N}}, C) = \{x : \mathbb{N} \rightarrow C\}$$

$$(Xx + \beta y)(n) = Xx(n) + \beta y(n)$$

for all $n \in \mathbb{N}$

$$\langle x, y \rangle = \int_{\mathbb{N}} \langle x(n), y(n) \rangle_C d\mu(n)$$

$$\underline{g(\mathbb{N})} \rightarrow x'$$

Symmetry

Transformation that leaves a certain property of said object or system unchanged or invariant.

Group

Set G with a binary operation

$$\circ : G \times G \rightarrow G$$

$$\frac{g \circ h}{\downarrow}$$

Represented henceforth as gh

Axioms

→ Associativity

$$1) (gh)l = g(hl) \quad \forall g, h, l \in G$$

2) Identity $e \in R \rightarrow$ Existence of identity

$$eg = ge = g \quad \forall g \in G$$

3) Inverse — Existence of inverse

$$gg^{-1} = e$$

4) Closure \rightarrow Closure

$$g \in R, h \in R \Rightarrow gh \in R$$

Commutative groups - Abelian

Group action

Group action of G on a set R

$$x \in X(R) \quad u \in R$$

$$(g \cdot x)(u) = x(g^{-1}u) \rightarrow$$

linear group actions - Group representations

Geometric deep learning

- $f : X(\mathbb{R}) \rightarrow Y$ is G -invariant
 $f(g \cdot x) = f(x)$ for all $g \in G$

Example

Translation group

$$G = \left\{ h(-1, -1), (-1, 0), (0, -1), (0, 0) \right. \\ \left. | \quad \quad \quad (1, 1), (0, 1), (1, 0) \right\}$$

$g \cdot x - 2D$ shift of an image

$$f(g \cdot x) = f(x)$$

\Rightarrow Detect the "cat" even if it is shifted.

Similarly, G -equivariant

$x \rightarrow \mathbb{R} \rightarrow C$

$$f: X(\mathbb{R}) \rightarrow X(\mathbb{R})$$

$$\underline{f(g \cdot x) = g \cdot f(x) \quad \forall g \in G}$$

Group-Convolution (Definition)

$$(x * \theta)(g) = \int_{\mathbb{R}} x(u) \theta(g^{-1}u) du$$

\uparrow \mathbb{R}
 G -equivariant

$g \in G, h \in H$

Proof

Refer Geometric deep learning - Bronstein

Too difficult as the group can be very big

e.g

- 1) all rotations, translations, reflections
- 2) all permutations of the graphs

Spectral interpretation of group convolution

$$y_0 = c_0 x_0 + c_1 x_1 + c_2 x_2$$

Facts

- 1) Any circular convolution in 1D represented as a circular convolution

Circulant matrix

$$\rightarrow \boxed{Y = \begin{bmatrix} c_0 & c_1 & c_2 \\ c_2 & c_0 & c_1 \\ c_1 & c_2 & c_0 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix}} \quad \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_0 \\ x_1 \end{bmatrix}$$

- 2) Eigenvectors of ALL CIRCULANT MATRICES

- Fourier basis

$$\Phi = (\varphi_0, \dots, \varphi_{n-1})$$

$$\varphi_k = \frac{1}{\sqrt{n}} \left(1, e^{i \frac{2\pi k}{n}}, e^{i \frac{4\pi k}{n}}, \dots, e^{i \frac{2\pi(n-1)k}{n}} \right)$$

1D convolution in spectral domain

$$x * \theta = \hat{\Phi} \begin{bmatrix} \hat{\theta}_0 \\ \hat{\theta}_1 \\ \vdots \\ \hat{\theta}_{n-1} \end{bmatrix} \hat{\Phi}^* x$$

Finally, graphs - Nodes \mathcal{N} (1 to n)

$$\begin{aligned} x &= [x_0 \ x_1 \ \dots \ x_n] \in \mathbb{R}^{d \times n} \\ A &= \text{adjacency matrix} \quad \frac{A}{\mathbb{R}^{n \times n}} \\ D &= \text{degree matrix (Diagonal)} \quad \frac{D^{-1/2} \ A \ D^{-1/2}}{\mathbb{R}^{n \times n}} \end{aligned}$$

$$L = (D - A) \text{ Laplacian matrix}$$

$$f(x) = \underbrace{x^T L^{-1}}_{d \times n} \underbrace{(permutation \ equi)}_{n \times n} \underbrace{(invariant)}_{\mathbb{R}}$$

f will be permutation invariant

Key idea: Choose eigenvectors of L as spatial basis

L

$$L' = P^T L P$$

 X

$$X' = X P$$

$$P P^T = I$$

$$X' L' = (X L) P$$

Spectral graph convolution

$$f_\theta(X) = U \begin{bmatrix} \hat{\theta}_0 & & & \\ & \hat{\theta}_1 & & \\ & & \ddots & \\ & & & \hat{\theta}_2 \end{bmatrix} U^T X$$

θ - learnable parameters
can have additional non-linearities

✗ This was initially called a
graph convolution but is
uncommon now

Reasons

- 1) Cannot generalize to different graph structures
- 2) Very difficult to scale

MORE COMMON (Spatial graph convolutions)

Somewhat similar to CNN over local neighborhoods

- What Jonathan and Ting-Han presented

Bridging the Gap Between Spectral and Spatial Domains in Graph Neural Networks

Muhammet Balciar *, Guillaume Renton, Pierre Héroux, Benoit Gaüzère, Sébastien Adam, Paul Honeine

LITIS Lab, University of Rouen Normandy
Rouen, FRANCE

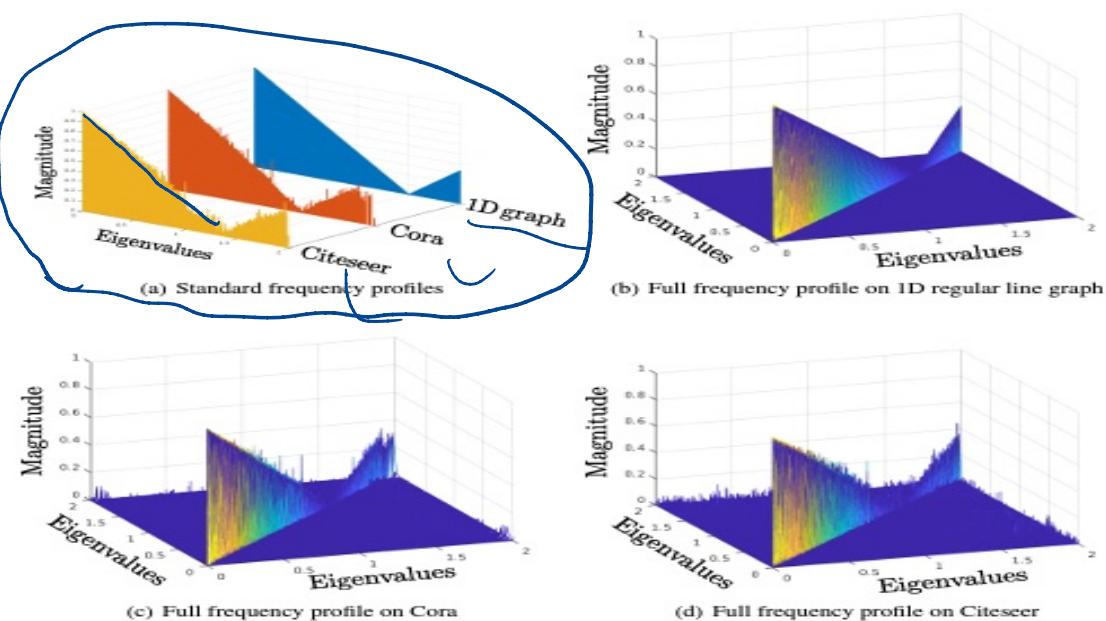


Figure 4: Frequency profiles of GCN on different graphs.

$$\begin{aligned}f(x) &= \sigma\left(\underline{x} \underline{\left(I + A\right)}\right) \\&= \sigma\left(\sum_s x_s w_s\right)\end{aligned}$$

$\left(I + A\right)$

↓
learnable
weights

Preceding neural networks

CNN - translation equivariance

Spherical CNN - equivariance on $SO(3)$
rotation

GNN - permutation equivariance

Transformers - special case of GNN

Grids and gauges - ?