

$$\mathcal{X}(\Omega, \mathbb{C}) = \{x: \Omega \rightarrow \mathbb{C}\}$$

$$(\alpha x + \beta y)(u) = \alpha x(u) + \beta y(u)$$

for all  $u \in \Omega$

$$\langle x, y \rangle = \int_{\Omega} \langle x(u), y(u) \rangle_{\mathbb{C}} d\mu(u)$$

Symmetry

$$g(\Omega) \rightarrow x'$$

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 hereforth as gh

## Axioms

- 1)  $(gh)l = g(hl) \quad \forall g, h, l \in G$   $\rightarrow$  Associativity
- 2) Identity  $e \in \Omega \rightarrow$  Existence of identity  
 $eg = ge = g \quad \forall g \in G$
- 3) Inverse  $\rightarrow$  Existence of inverse  
 $gg^{-1} = e$
- 4) Closure  $\rightarrow$  Closure  
 $g \in \Omega, h \in \Omega \Rightarrow gh \in G$

Commutative groups - Abelian

## Group action

Group action of  $G$  on a set  $\Omega$

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

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

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

$$G = \left\{ \begin{array}{l} (-1, -1), (-1, 0), (0, -1), (0, 0) \\ (1, 1), (0, 1), (1, 0) \end{array} \right\}$$

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

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

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

Similarly,  $G$ -equivariant  $x \rightarrow \Omega \rightarrow \mathcal{L}$

$$f: \mathcal{X}(\Omega) \rightarrow \mathcal{X}(\mathcal{L})$$

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

Group-convolution (Definition)

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

$\uparrow$   
 $G$ -equivariant

$$g \in G, u \in \Omega$$

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

$$\rightarrow y = \begin{matrix} \text{circulant matrix} \\ \begin{bmatrix} c_0 & c_1 & c_2 \\ c_2 & c_0 & c_1 \\ c_1 & c_2 & c_0 \end{bmatrix} \end{matrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_0 \\ x_1 \end{bmatrix}$$

- 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

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

Finally, graphs - Nodes  $V$  (1 to  $n$ )

$$X = [x_0 \ x_1 \ \dots \ x_n] \quad - \mathbb{R}^{d \times n}$$

$$A = \mathbb{R}^{n \times n}$$

adjacency matrix

D - degree matrix (Diagonal)

$$\frac{D^{-1/2} A D^{-1/2}}{\downarrow}$$

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

$$f(X) = X \underbrace{L}_{n \times n} \quad (\text{permutation equivariant})$$

f will be permutation equivariant

Key idea: Choose eigenvectors  $V$  of  $L$  as spectral basis

L

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

X

$$X' = X P$$

$$P P^T = I$$

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

## Spectral graph convolution

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

---

$\theta$  - 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 convolution)

Somewhat similar to CNN over local neighborhoods

- What Jonathan and Ting-Han presented

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

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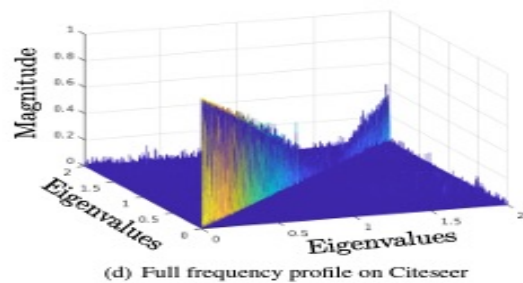
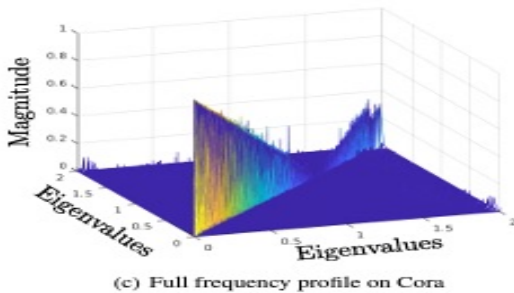
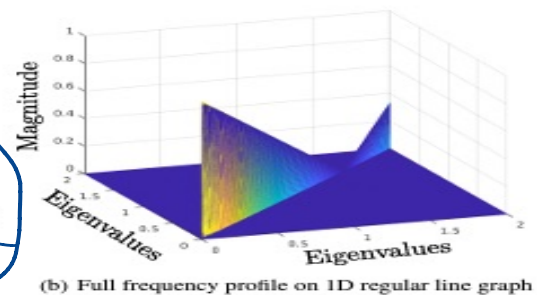
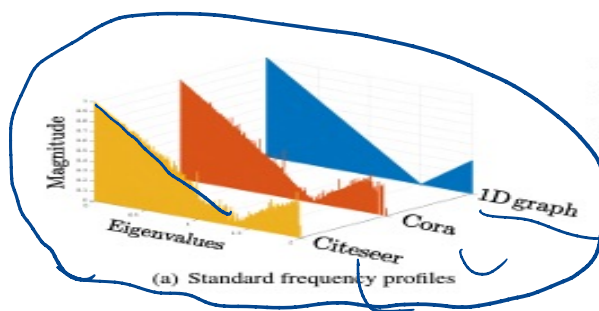


Figure 4: Frequency profiles of GCN on different graphs.

$$f(x) = \sigma(x(I+A))$$
$$= \sigma\left(\sum_s x_s W_s\right)$$

$(I+A)$        $W_s$       learnable weights

## Preceding neural networks

CNN - translation equivariance

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

GNN - permutation equivariance

Transformers - special case of GNN

Creodesins and gauges - ?