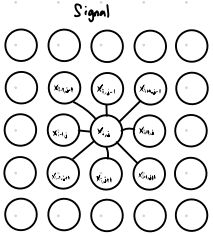
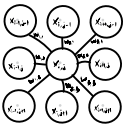
Graph Convolutional Network

A message passing View of Convolution





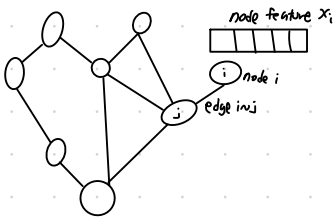
$$x'_{i,j} = w_{2,2}x_{i,j} + (w_{1,1}x_{i-1,j-1} + \cdots + w_{3,3}x_{i+1,j+1})$$

Update Self-Feature

Receive Messages from Neighbors

Graphs = Systems of Relations and Interactions

ex) Molecules, Social Networks, ...



· Permutations and permutation matrices.

: Within linear algebra, each permutation defines a $|V| \times |V|$ matrix.

· Such matrices are called permutation matrices (group action P(4))

· They have exactly one 1 in every row and column, zeroes elsewhere

Ex)

$$P_{(2,4,1,3)}X = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} -X_1- \\ -X_2- \\ -X_3- \\ -X_4- \end{bmatrix} = \begin{bmatrix} -X_2- \\ -X_4- \\ -X_1- \\ -X_3- \end{bmatrix}$$

Permutation Invariance

$$f\left(\text{graph}\right) = y = f\left(\text{graph}\right)$$

We need to appropriately permute both rows and columns of A. When applying a permutation matrix P, this amounts to PAP^T.

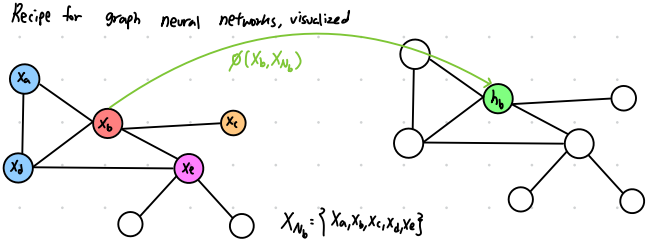
We arrive at updated definitions of suitable functions over graphs:

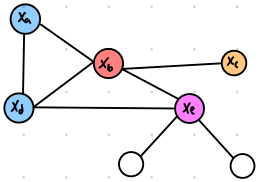
· Invariance: $f(PX, PAP^T) = f(X, A)$

· Equivariance: $F(PX, PAP^T) = PF(X, A)$

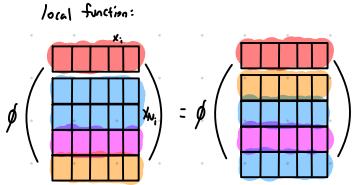
★ Why PAP^T to permute A? : the multiplication of the permutation matrix P and its transpose P^T ensures that both rows and columns are permuted consistently, preserving the connectivity structure of the graph after permuting the nodes.

Recipe for graph neural networks, visualized





local function:



Permutation invariant

Message Passing:

Permutation-invariant aggregation operator, e.g. Sum

$$f(x_i) = \phi\left(x_i, \square_{j \in N_i} \psi(x_i, x_j)\right)$$

$f(x_i)$: New feature of node i

ϕ, ψ: Learnable functions, like MLP

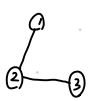
Update rule: $h_i^{(l+1)} = \sigma\left(h_i^{(l)} W_0^{(l)} + \sum_{j \in N_i} \frac{1}{c_{i,j}} h_j^{(l)} W_1^{(l)}\right)$

$W_0^{(l)}$: itself; $W_1^{(l)}$: 1st neighbors

$$H^{(l+1)} = \sigma\left(\hat{A} H^{(l)} W^{(l)}\right)$$

Why PAP^T?

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$



$$P = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$: Swapping nodes 1 and 3.

$$PAP^T = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$: This new matrix corresponds to a graph where nodes 1 and 3 have been swapped, while the edges between them are correctly maintained