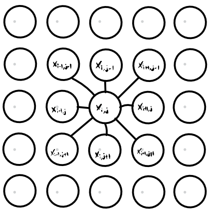
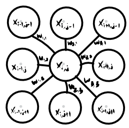
A message Passing View of Convolution

Signal

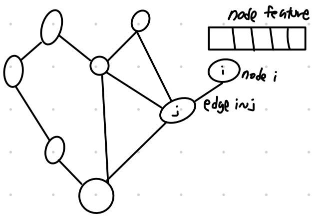




$$x'_{ij} = \underbrace{w_{2,2}x_{i,j}}_{\text{Update Self-Feature}} + \underbrace{\left(w_{1,1}x_{i-1,j-1} + \cdots + w_{3,3}x_{i+1,j+1}\right)}_{\text{Receive Messages from Neighbors}}$$

Graphs = Systems of Relations and Interactions

ex) Molecules, Social Networks, ...



· Permutations and permutation matrices.

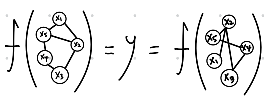
: Within linear algebra, each permutation defines a $|V| \times |V|$ matrix.

- Such matrices are called permutation matrices (group action $P(g)$)
- 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



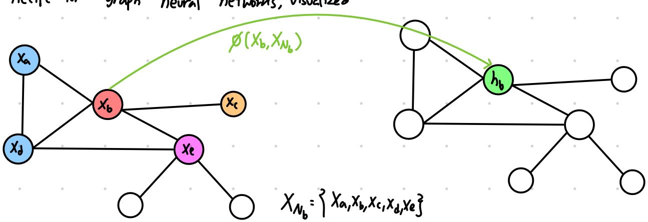
We need to appropriately permute both rows and columns of A. When applying a permutation matrix P, this amounts to PAP^T.

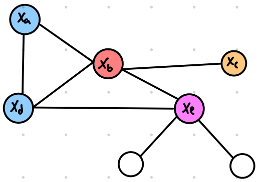
We arrive at updated definitions of suitable functions over graphs:

- Invariance: $f(PX, PAP^T) = f(X, A)$
- Equivariance: $F(PX, PAP^T) = PF(X, A)$

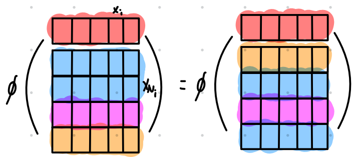
★ Why PAP^T to permute A? : the multiplication of the permutation matrix P and its transpose P^T ensures that both rows and columns are permuted consistently, preserving the connectivity structure of the graph after permuting the nodes.

Recipe for graph neural networks, visualized





local function:



Permutation invariant

Message Passing:

Permutation-invariant aggregation operator, e.g. Sum

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

New feature of node i

ϕ, ψ: Learnable functions, like MLP

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

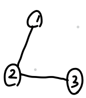
itself

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