Graph Convolutional Networks

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ML Reading Group

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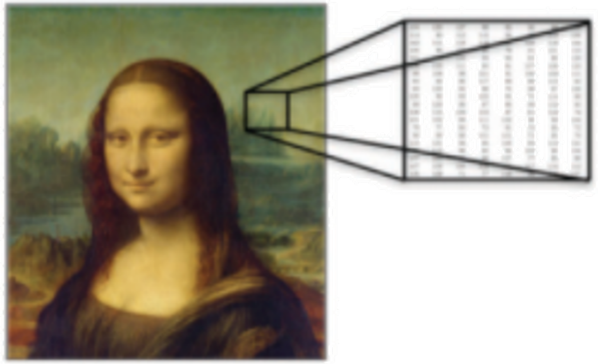
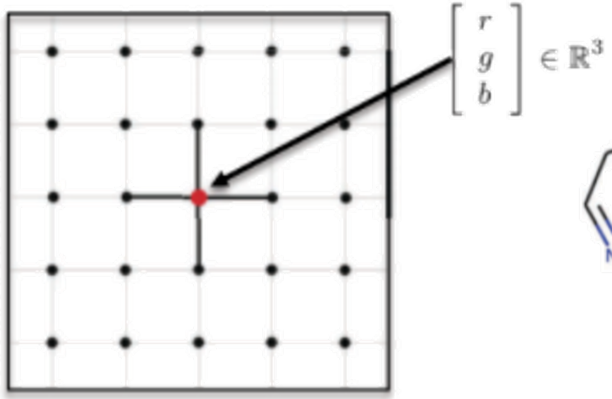
Graph Domains

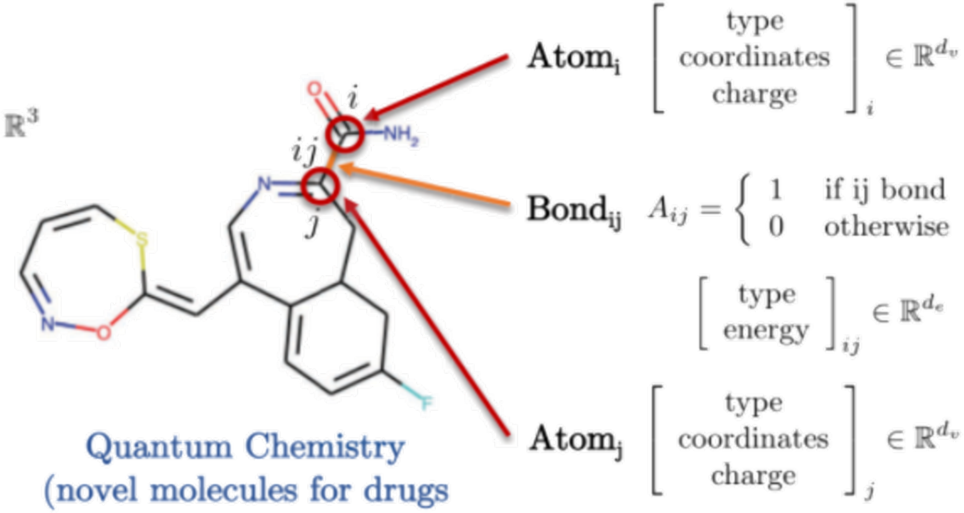
Data Domain

Graph Domain

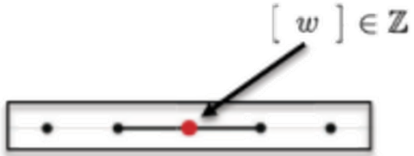




2D grid



Quantum Chemistry
(novel molecules for drugs and materials)

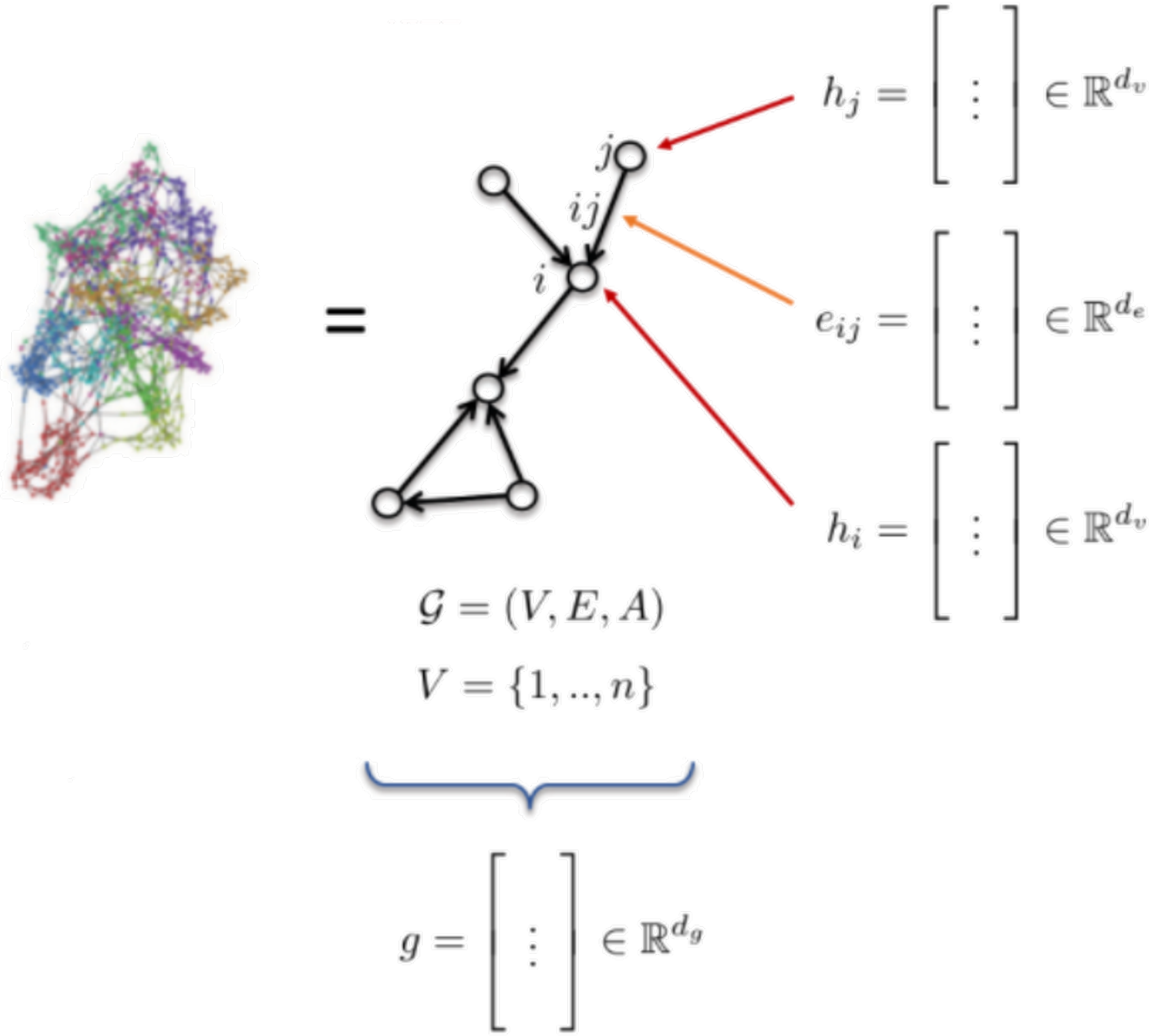


1D grid

Graph Definitions

- Graph G is defined as:
  - Vertices V
  - Edges E
  - Adjacency Matrix A

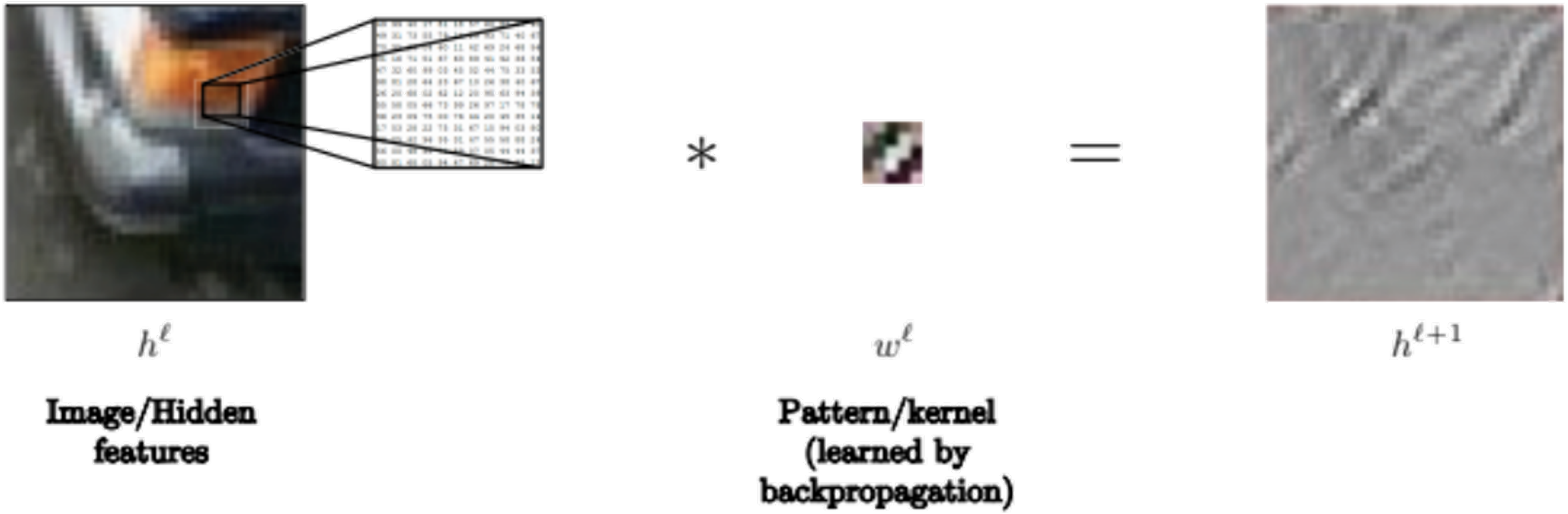
- Graph features are:
  - Node features: h_i, h_j (atom type)
  - Edge features: e_{ij}
  - Graph features: g (molecular energy)



What is a Convolution

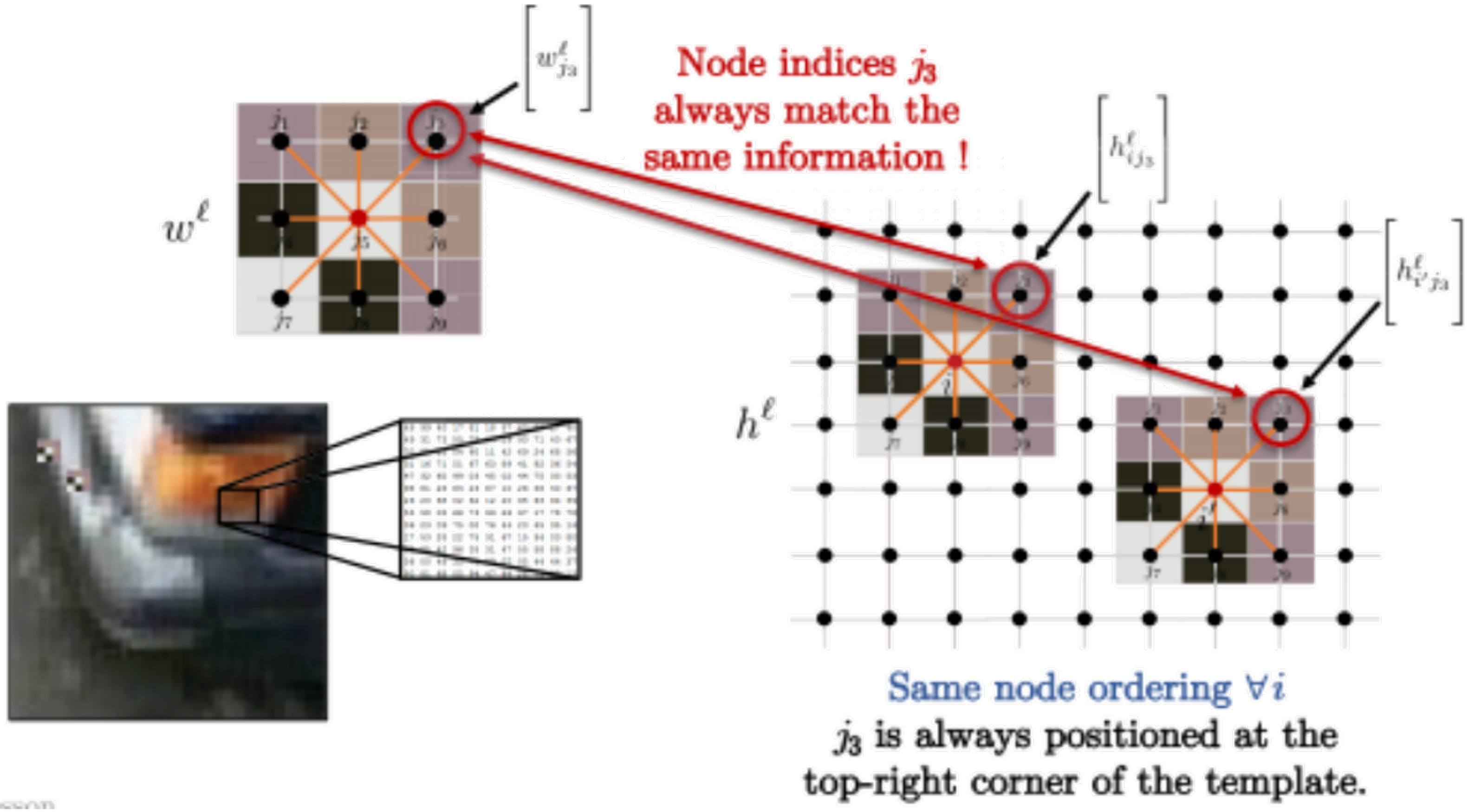
$$h^{l} \times w^{l} = h^{l+1}$$

Features at l^{th} layer	Pattern/Kernel (learned by backpropagation)	Convoluted feature at $(l+1)^{th}$ layer



Convolution as template matching

- The template/kernel w_l is overlayed (as defined by the strides) across the image from top-left to bottom right
- Different kernel convolutions are done to represent an image in terms of kernels/templates
- Kernels might become combination of kernels as we proceed just like ANNs



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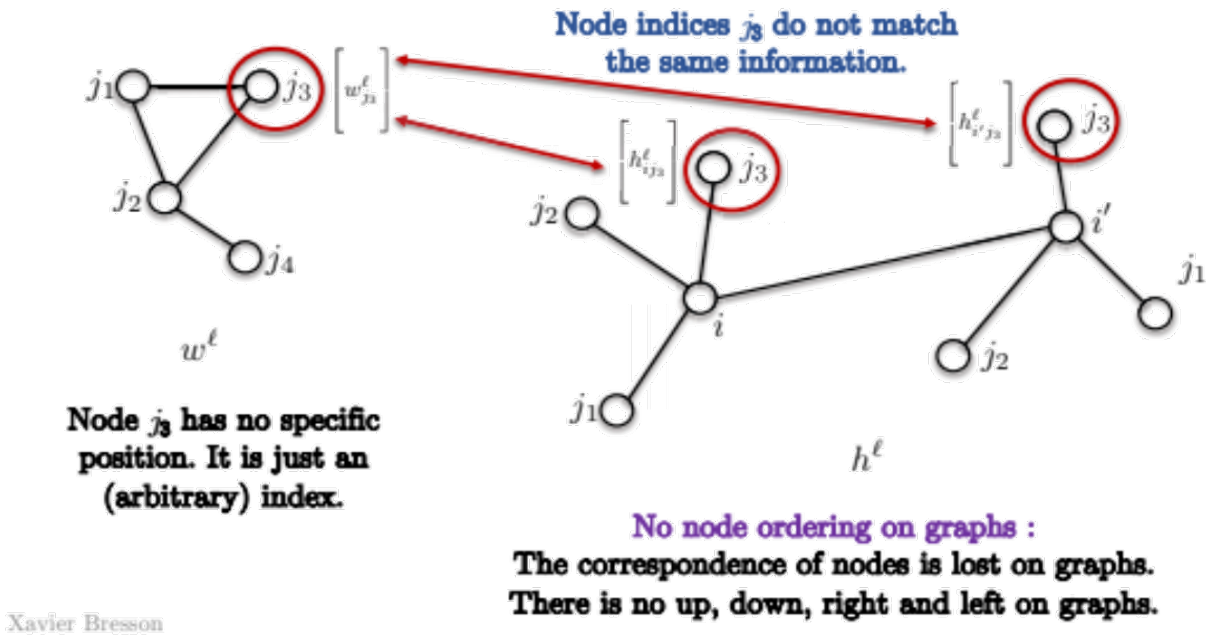
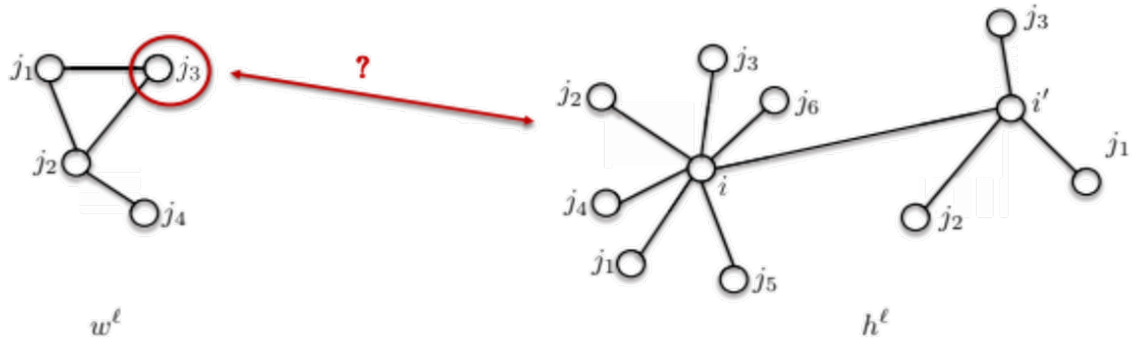
Problems with extending template matching to Graphs

- No ordering of nodes
- Neighborhood sizes are different





Convolution theorem to graphs

$$\mathcal{F}(w * h) = \mathcal{F}\,(w) \odot \mathcal{F}\,(h)$$

- Use convolution theorem for spectral ConvNets

$$
\begin{aligned}
\underset{n\times 1}{w * h} &= \underbrace{\mathcal{F}^{-1}}_{\Phi}\big(\underbrace{\mathcal{F}(w)}_{\Phi^T w = \hat{w}} \odot \underbrace{\mathcal{F}(h)}_{\Phi^T h}\big) \\
&= \underset{n\times n}{\Phi}\left(\underset{n\times 1}{\hat{w}} \odot \underset{n\times 1}{\Phi^T h}\right) \\
&= \Phi\left(\underset{n\times n}{\hat{w}(\Lambda)}\underset{n\times 1}{\Phi^T h}\right) \\
&= \Phi\hat{w}(\Lambda)\Phi^T h \\
&= \hat{w}(\underbrace{\Phi\Lambda\Phi^T}_{\Delta})h \\
&= \underset{n\times n}{\hat{w}(\Delta)}\ \underset{n\times 1}{h}
\end{aligned}
$$

Convolution Theorem

$$w * h \ = \mathcal{F}^{-1}(\mathcal{F}\,(w) \odot \mathcal{F}\,(h))$$

$$\Delta\,(n \times n) = \ \Phi^T \Lambda\, \Phi$$

- Δ is the graph Laplacian operator
- Φ contains column vectors and those are also called Fourier functions
- Λ is a diagonal matrix with Laplacian Eigenvalues

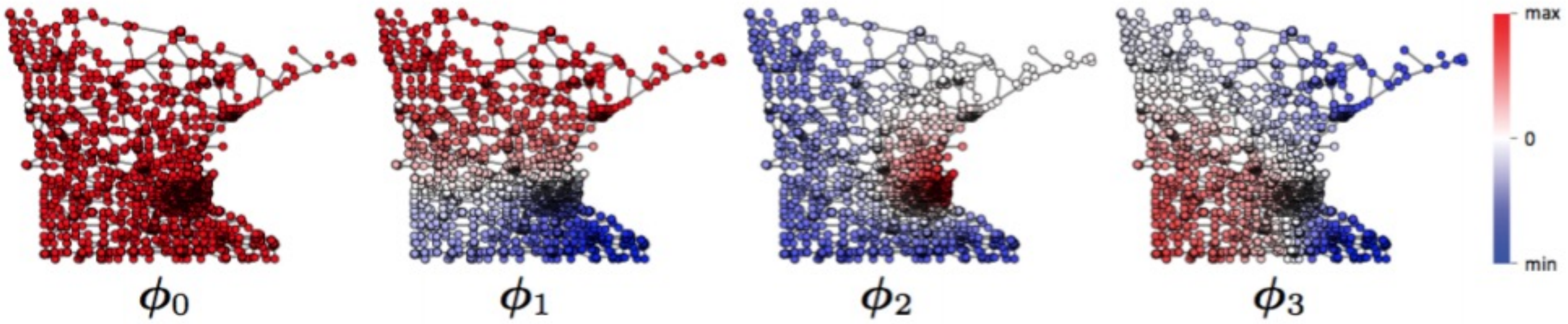
Fourier functions in Graph domain

- Use convolution theorem for spectral ConvNets

Convolution Theorem

$$w * h = \mathcal{F}^{-1}(\mathcal{F}(w) \odot \mathcal{F}(h))$$

$$\Delta\,(n \times n) = \Phi^T \Lambda\, \Phi$$



First Laplacian eigen vectors of a graph

Physical interpretation of terms in the Convolution Theorem

- Use convolution theorem for spectral ConvNets

$$\mathcal{G} = (V, E, A) \rightarrow \underset{n\times n}{\Delta} = \mathrm{I} - D^{-1/2} A D^{-1/2}$$

$$\text{where } \underset{n\times n}{D} = \mathrm{diag}\left(\sum_{j\neq i} A_{ij}\right)$$

- Matrix A is the adjacency matrix.
- I is the identity matrix
- D is the diagonal matrix, and each element on the diagonal is the degree of the node

The Laplacian shows → the measurement of smoothness of graph or the different between local values h_i and its neighborhood values of h_j's.

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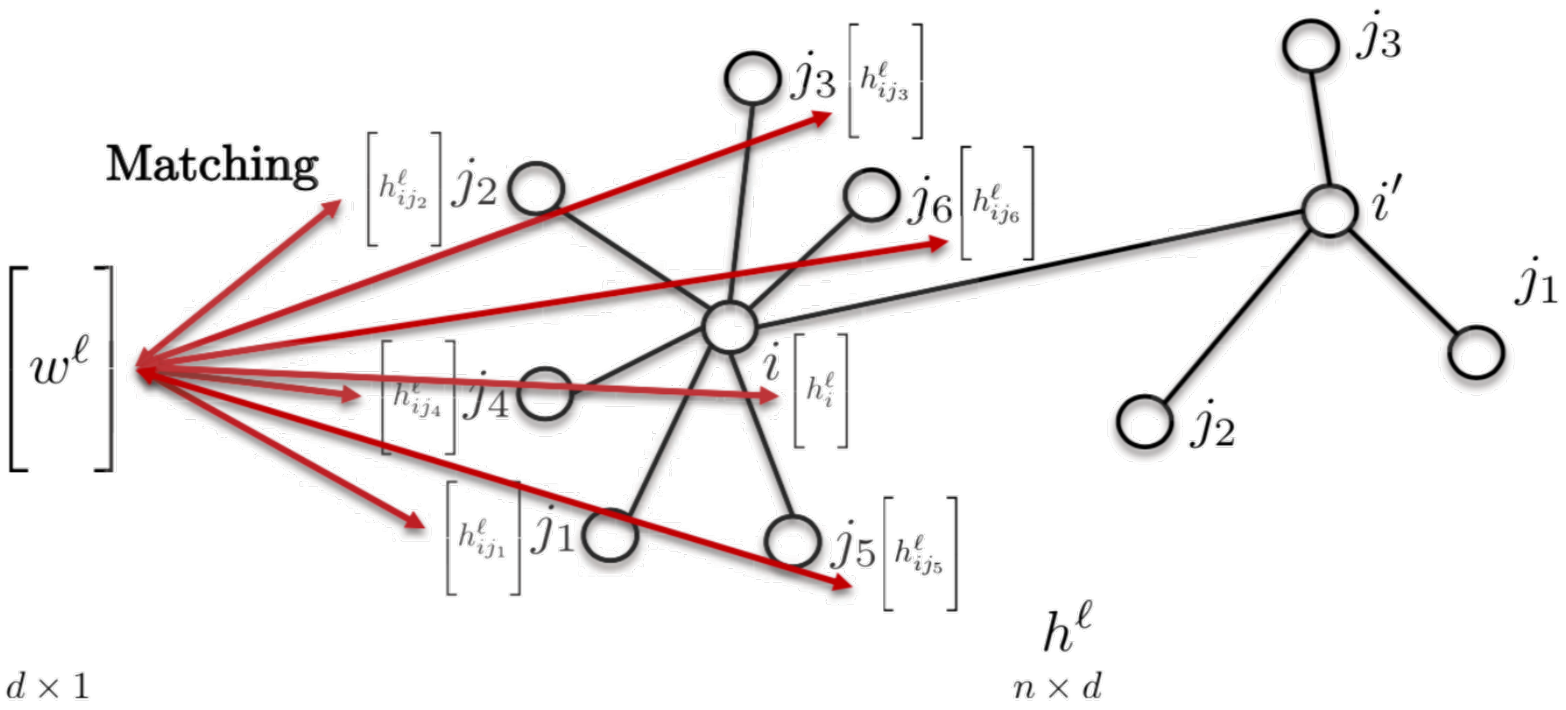
Template matching for Spatial Graph ConvNets

- Using one template vector w_l instead of matrix (like 3 x 3)
- For each feature (in d) we would have a vector/template w



$$\underset{\text{scalar}}{h_i^{\ell+1}} = \eta\Big(\sum_{j \in \mathcal{N}_i} \underbrace{\langle \overset{d\times 1}{w^\ell}, \overset{d\times 1}{h_{ij}^\ell} \rangle}_{(h_{ij}^\ell)^T w^\ell} \Big)$$

One feature

$$\underset{d\times 1}{h_i^{\ell+1}} = \eta\Big(\sum_{j \in \mathcal{N}_i} \underset{d\times d}{W^\ell} \underset{d\times 1}{h_{ij}^\ell} \Big)$$

d features

$$\underset{n\times d}{h^{\ell+1}} = \eta\big(A h^\ell W^\ell \big)$$

$d \times d$
$n \times d$
$n \times n$

Vectorial representation

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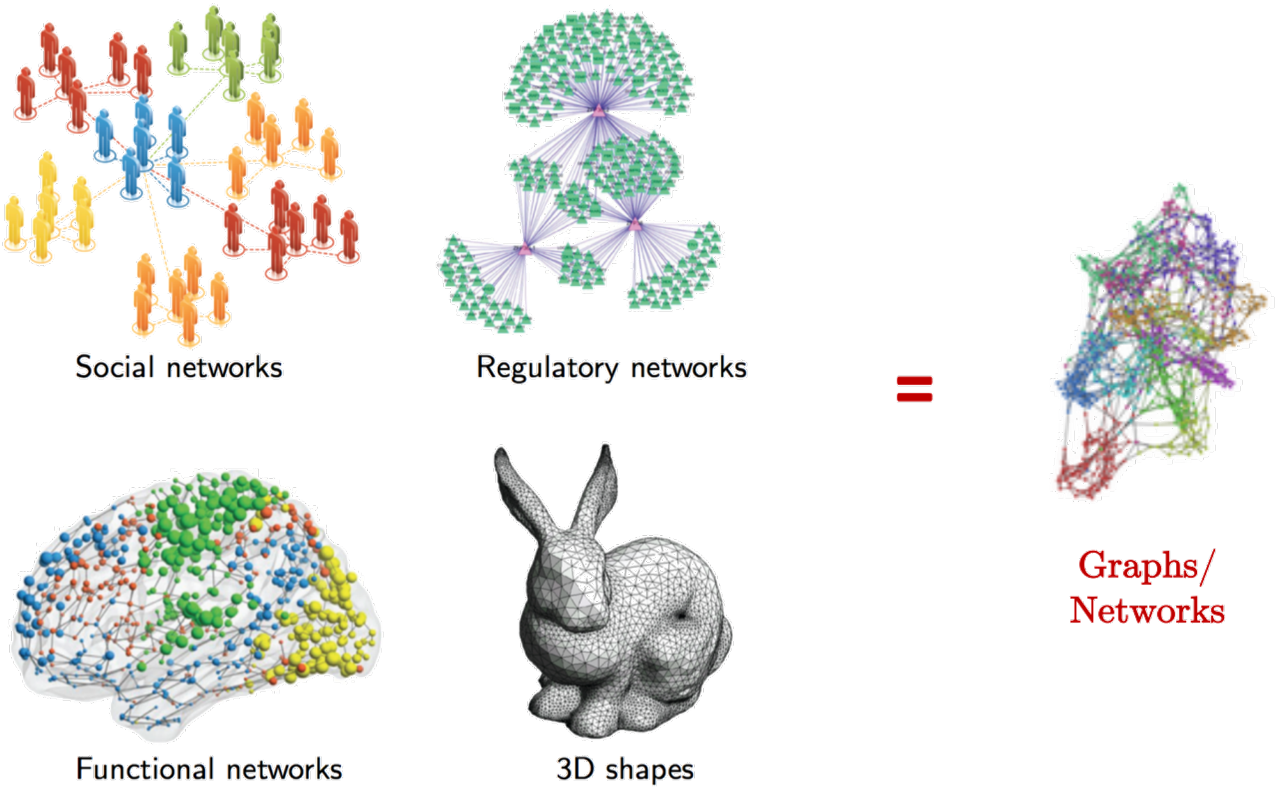
Conclusion

- GCNs generalize CNNs to data on graphs
- The convolution operator needs to be redesigned for graphs → 2 ways, spectral GCNs (Convolution theorem) (cheaper) and Spatial GCNs (expensive)



THANKS FOR YOUR ATTENTION

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ANY QUESTIONS?

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