RESEARCH REVIEW 2019

Graph Convolutional Neural Networks

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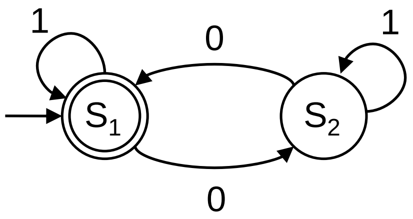
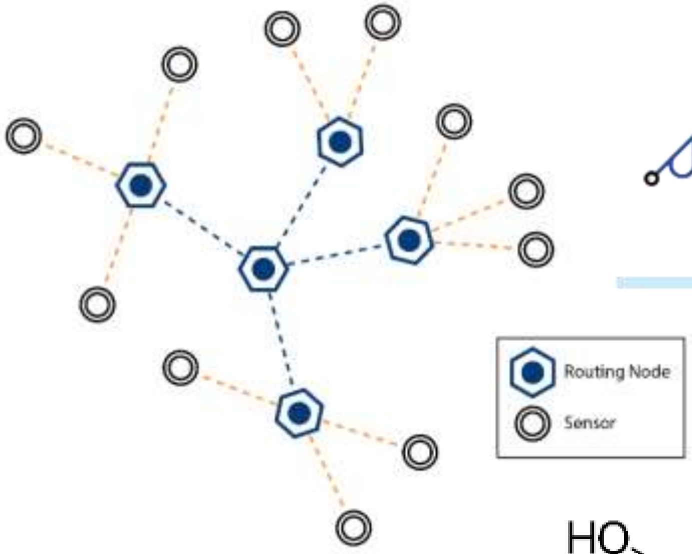
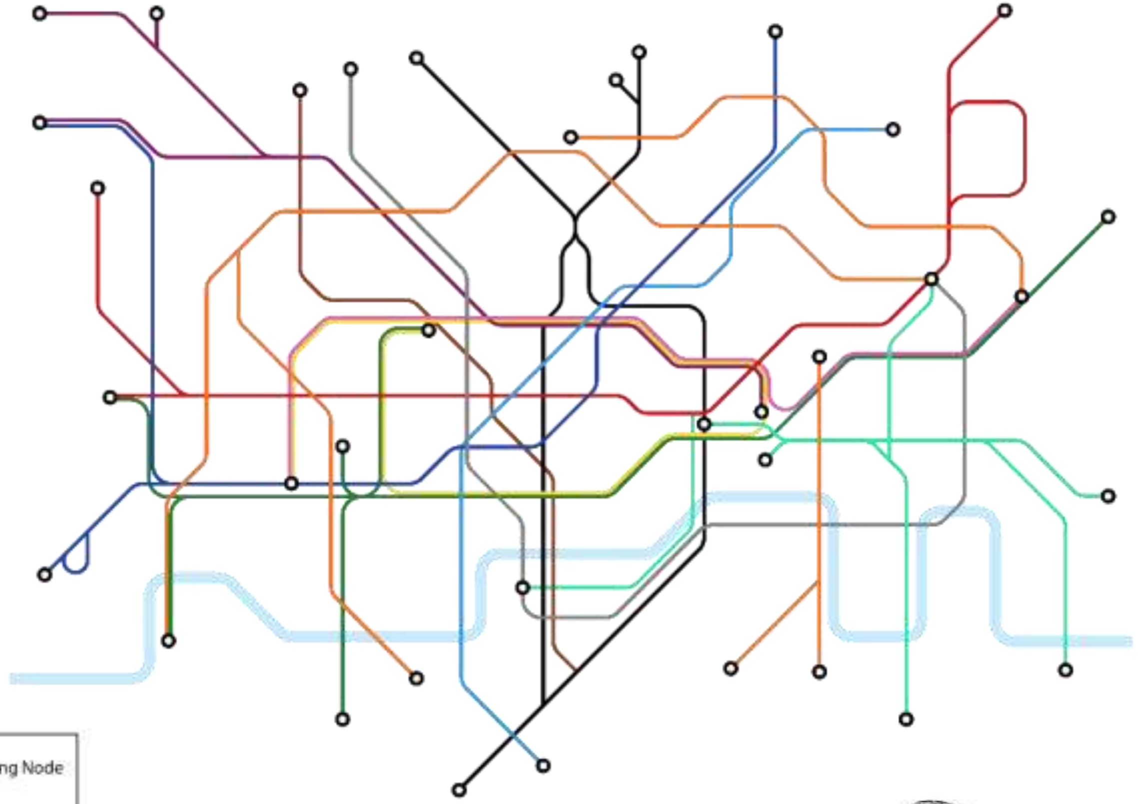
DM19-1108

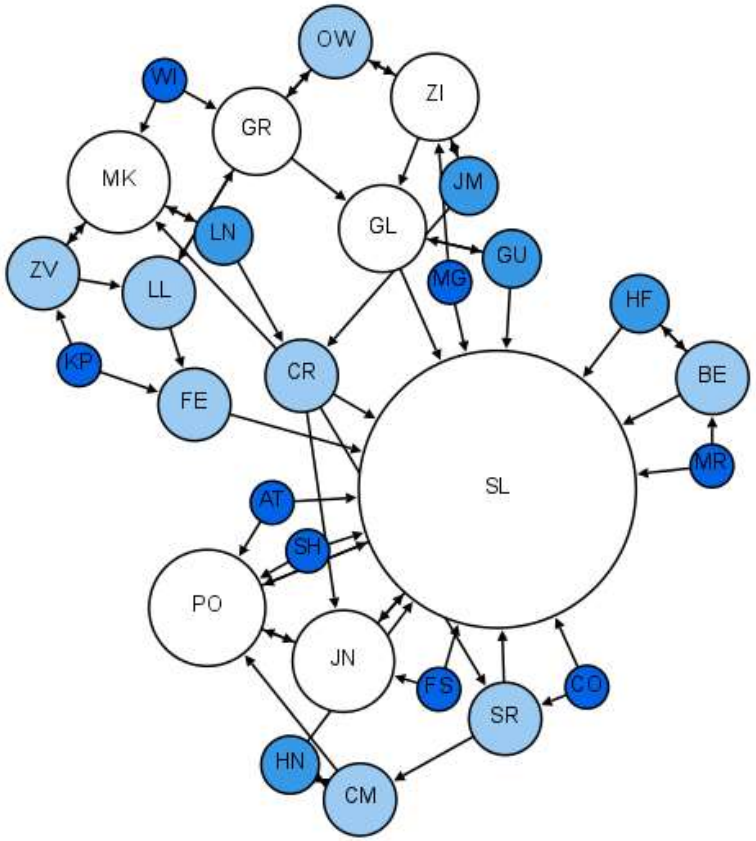
How does AI learn structure?

Graphs Are Everywhere

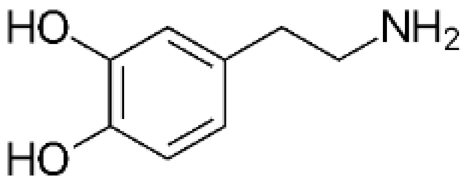


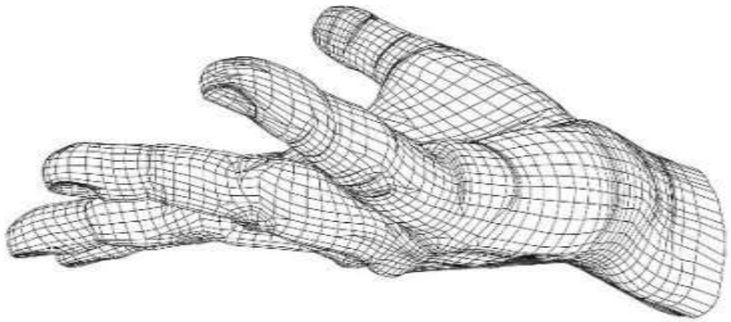






Grandjean, 2015





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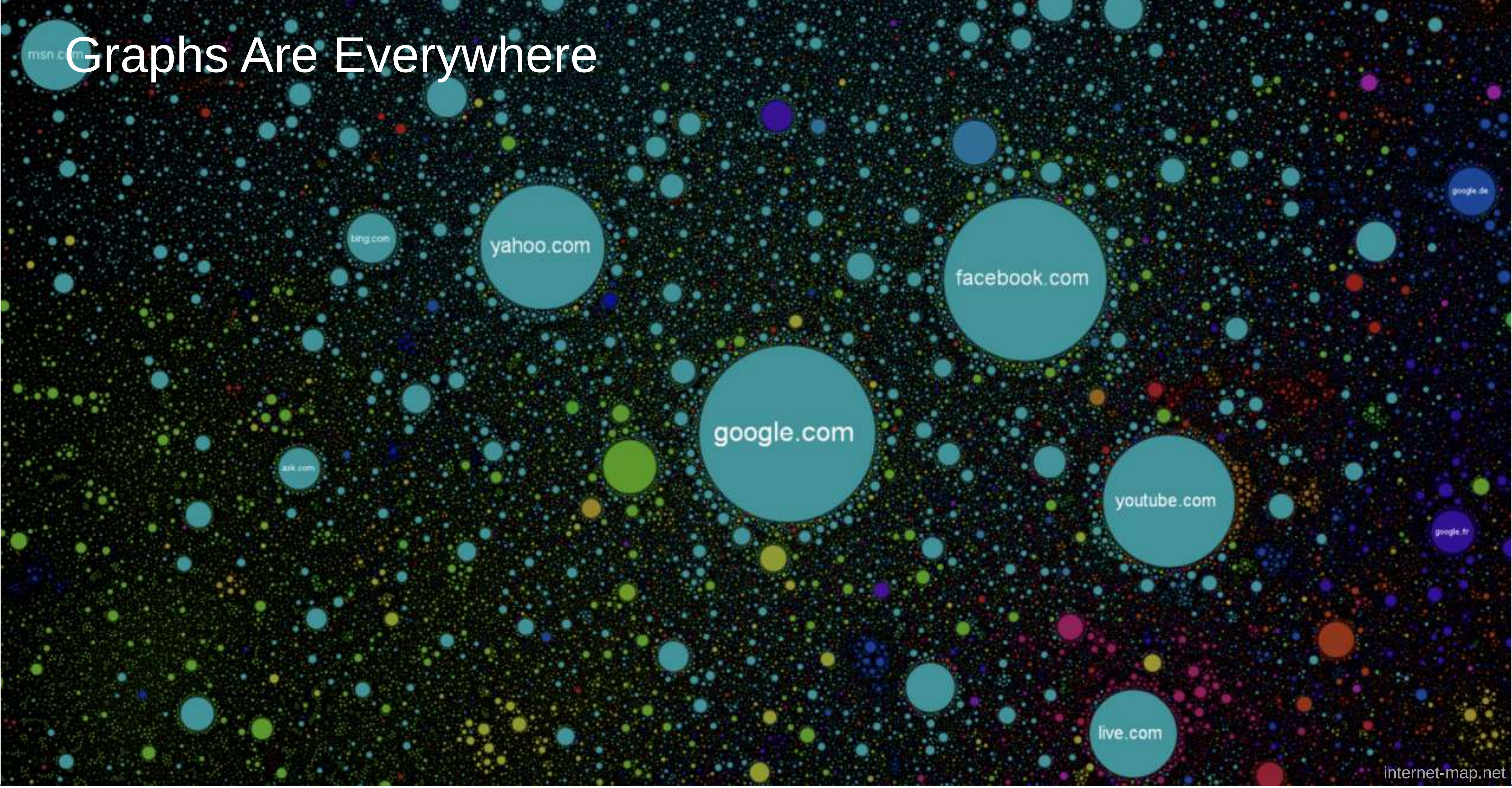
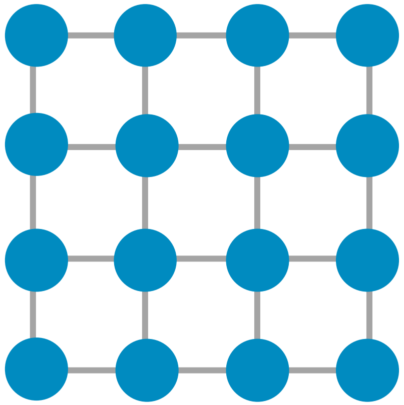


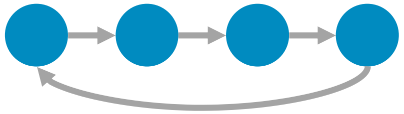
Data Structures as Graphs

Regular Data Structures

Images

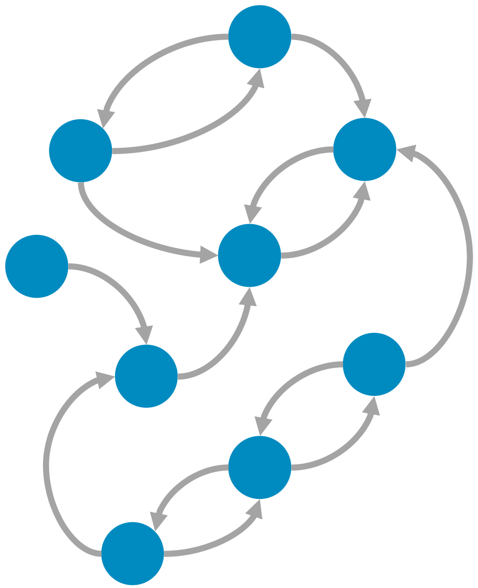


Time Series



Irregular Data Structures

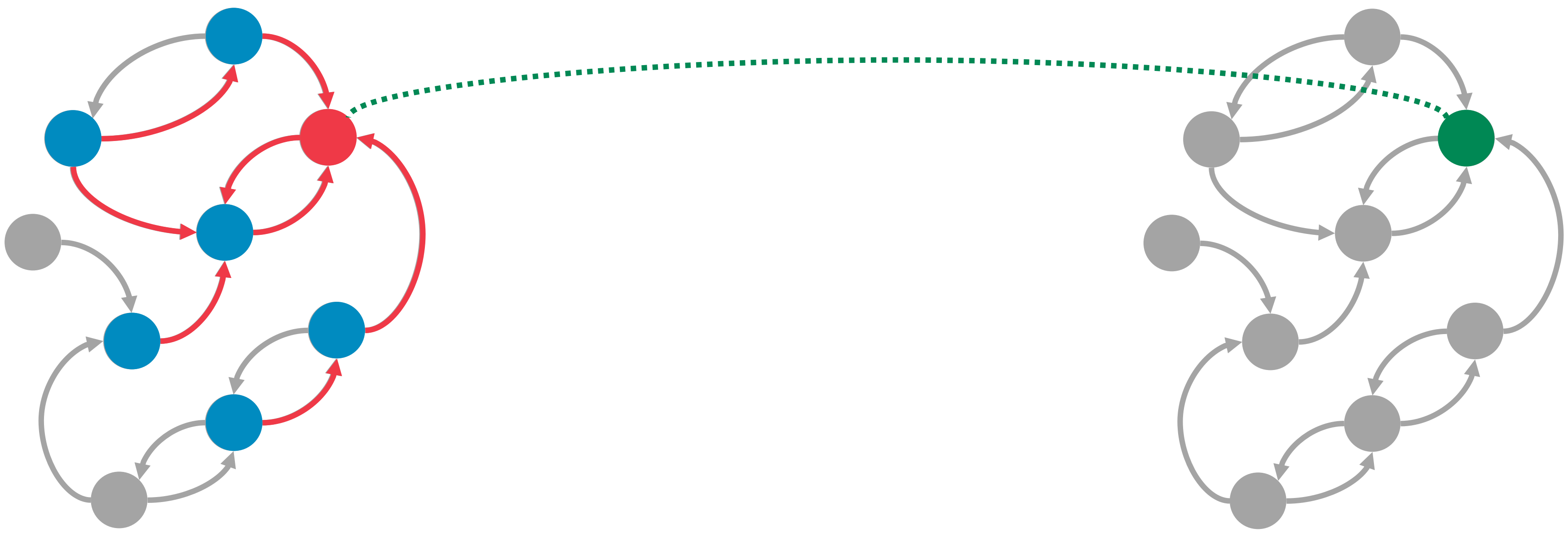
Social Networks
World Wide Web
Telecom Networks
Supply Chains
Biological Systems
Semantic Lexicons
Chemical Models
State Machines
Call Graphs
...



The Convolutional Kernel

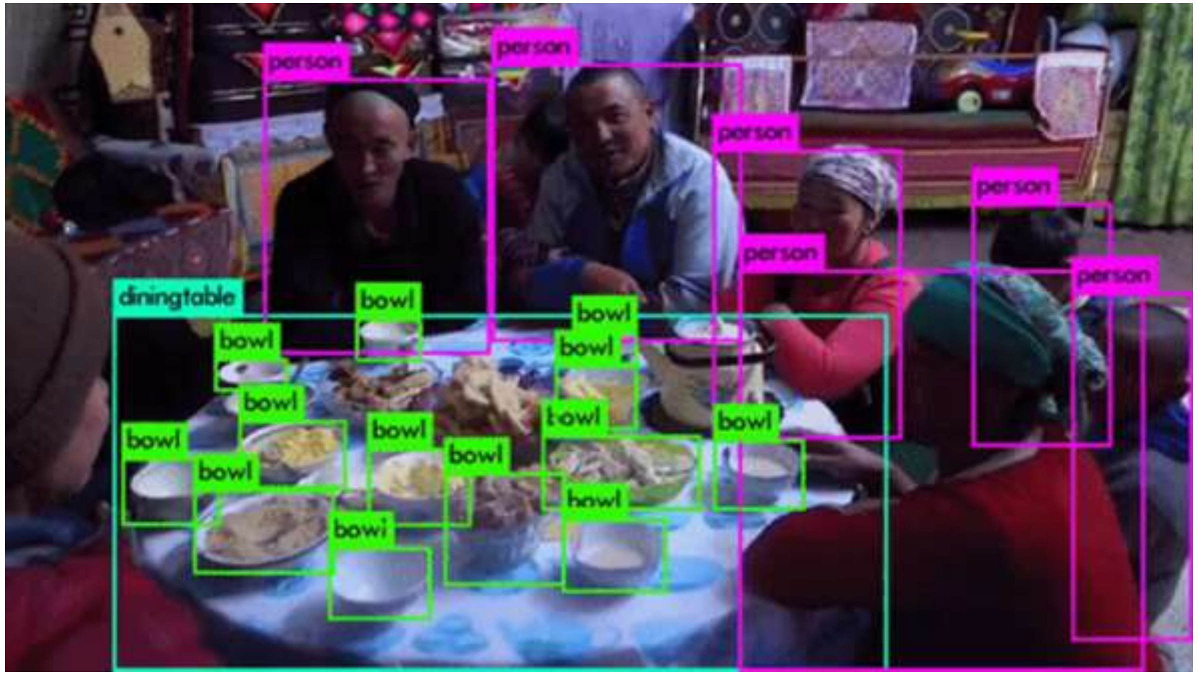
$$\underset{\mathbf{K}}{\begin{bmatrix} 2 & 0 & 0 & 4 & 4 & 0 \\ 1 & 1 & 0 & 0 & 2 & 0 \\ 1 & 0 & 1 & 2 & 3 & 0 \\ 1 & 1 & 2 & 3 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}} * \underset{\mathbf{I}}{\begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}} = \underset{\mathbf{K} * \mathbf{I}}{\begin{bmatrix} 5 & 6 & 8 & 8 \\ 4 & 6 & 7 & 8 \\ 4 & 4 & 8 & 4 \\ 3 & 5 & 4 & 3 \end{bmatrix}}$$

The Convolutional Kernel



Why Are CNNs So Useful?

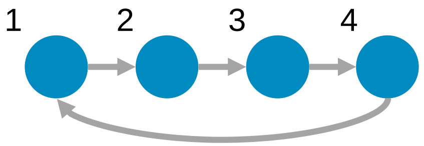
- **Fixed** number of parameters
- **Local** kernel
- **Spatial invariance** properties



Redmon & Farhadi, 2018

Building a Graph Convolution

Time Series



$$\mathbf{x} = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

Signal

$$\mathbf{C} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

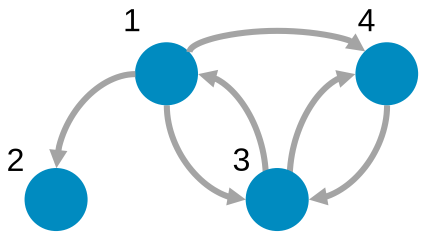
Shift Matrix

= Adjacency Matrix

$$\mathbf{x}' = \mathbf{C}\mathbf{x} = \begin{bmatrix} d \\ a \\ b \\ c \end{bmatrix}$$

Time-Shifted Signal

General Graph



$$\mathbf{x} = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

Signal

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

Adjacency Matrix

$$\mathbf{x}' = \mathbf{A}\mathbf{x} = \begin{bmatrix} c \\ a \\ a + d \\ a + c \end{bmatrix}$$

Graph-Shifted Signal

$$\mathbf{G} = \sum_{k=0}^{K} g_k \mathbf{A}^k$$

Graph Convolution

$$\mathbf{x}^{(\ell+1)} = \sigma\left(\mathbf{G}\mathbf{x}^{(\ell)} + \mathbf{b}\right)$$

GCNN layer

Learning on Graphs

- **Node classification:** Predict information about unlabeled nodes in a graph, based on labeled nodes.
- **Graph classification:** Predict information about new graphs, based on labeled graphs.

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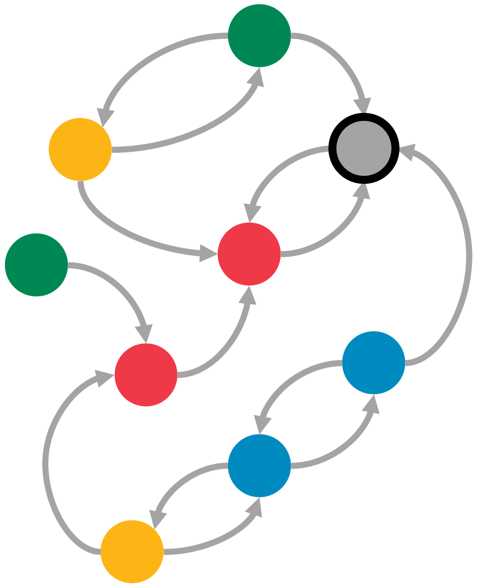

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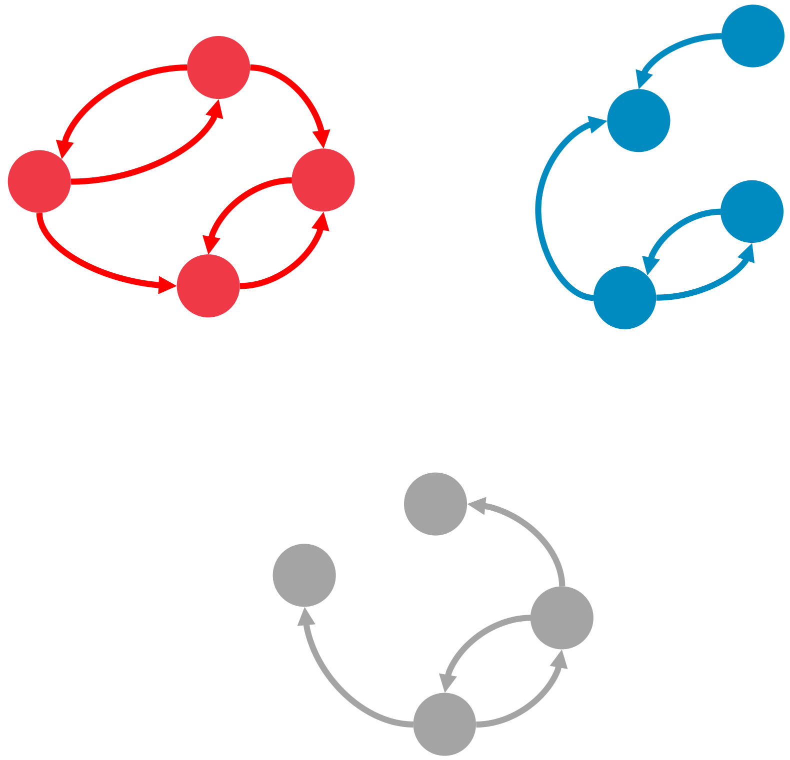

How does AI $\underbrace{\text{learn}}_{\text{GCNNs}}$ $\underbrace{\text{structure}}_{\text{graphs}}$?