

Graph Convolutional Neural Networks

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How does AI learn structure?

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Graphs Are Everywhere



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Data Structures as Graphs

Regular Data Structures

Irregular Data Structures

Images



Time Series



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

. . .



The Convolutional Kernel



The Convolutional Kernel



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Why Are CNNs So Useful?

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



Redmon & Farhadi, 2018

Building a Graph Convolution

 $\mathbf{x} = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$ $\mathbf{C} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$ $\mathbf{x}' = \mathbf{C}\mathbf{x} = \begin{vmatrix} a \\ b \end{vmatrix}$ **Time Series** Signal Shift Matrix Time-Shifted Signal = Adjacency Matrix $\mathbf{x} = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$ $\mathbf{A} = \begin{vmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{vmatrix}$ $\mathbf{x}' = \mathbf{A}\mathbf{x} = \begin{vmatrix} a \\ a \\ a + d \end{vmatrix}$ **General Graph** 3 Signal Adjacency Matrix **Graph-Shifted Signal** $\mathbf{G} = \sum_{k=0}^{n} g_k \mathbf{A}^k$ $\mathbf{x}^{(\ell+1)} = \sigma \big(\mathbf{G} \mathbf{x}^{(\ell)} + \mathbf{b} \big)$ **Graph Convolution GCNN** layer

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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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How does Al learn structure? GCNNs graphs