Graph Convolutional Neural Networks

Oren Wright
How does AI learn structure?
Graphs Are Everywhere

Grandjean, 2015
Graphs Are Everywhere
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

\[
\begin{bmatrix}
2 & 0 & 0 & 4 & 4 & 0 \\
1 & 1 & 0 & 0 & 2 & 0 \\
1 & 0 & 1 & 2 & 3 & 0 \\
1 & 1 & 2 & 3 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 \\
\end{bmatrix}
\times
\begin{bmatrix}
1 & 0 & 1 \\
0 & 1 & 0 \\
1 & 0 & 1 \\
\end{bmatrix}
=
\begin{bmatrix}
5 & 6 & 8 & 8 \\
4 & 6 & 7 & 8 \\
4 & 4 & 8 & 4 \\
3 & 5 & 4 & 3 \\
\end{bmatrix}
\]
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**

\[
x = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}
\]

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

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

Time-Shifted Signal

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

Graph Convolution

**General Graph**

\[
x = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}
\]

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

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

Graph-Shifted Signal

\[
x^{(\ell+1)} = \sigma(\mathbf{G}x^{(\ell)} + \mathbf{b})
\]

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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GCNNs  graphs