“Graph CNNs”

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Convolution Neural Networks (CNNs) are awesome - they have transformed the pattern recognition community!

LeNet-5, LeCun 1989

AlexNet, Krizhevsky 2012

VGGNet, Simonyan 2014

GoogLeNet (Inception), Szegedy 2014

ResNet, He 2015

DenseNet, Huang 2017

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But, the vast majority of the world’s problems can’t be described by gridded structures such as images. Have you ever tried to do a CNN on a graph?

- **Images**
  - Convolution
  - Pooling
  - Classification

- **Graphs**

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GraphCNN affords the wonderful CNN benefits to non-gridded problems such as trade, security, protein structures, weather, brain scans, etc.

Gridded  Non-Gridded  Homogeneous  Heterogeneous

Graph CNNs introduced by Lab:

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Can have multiple connection types (A can be a tensor) and can have multiple features (V can be a tensor)
Graph-CNN - Convolution

Replace each vertex with $2 \times$ itself + $1 \times$ incoming purple - $1 \times$ incoming orange

No sense of direction in a graph!
In Graph CNN, we will learn many such filters (like the $[2 \ 1 \ -1]$) per adjacency matrix.

Replace each vertex with $2 \times$ itself + $1 \times$ incoming purple - $1 \times$ incoming orange.
Graph-CNN - Convolution

Update V’s for incoming A’s

\[ N_{i,a}^{l} = A_{i,a,j} V_{j,b}^{l} \]

Matrix Multiplication

\[ V_{i,k}^{l} = f \left( N_{i,d}^{l-1} W_{d,k} \right) \]

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Graph-CNN - Convolution

- We are learning the weights of the filters.
- We don’t care how many vertices!
- Can learn several sets of weights, one for each filter.

Update V’s for incoming A’s

\[ N_{i,a,c+b}^{l} = A_{i,a,j}V_{j,b}^{l} \]

Matrix Multiplication

\[ V_{i,k}^{l} = f\left(N_{i,d}^{l-1}W_{d,k}\right) \]
CNN – Fully Connected Layer

- Matrix multiplication.
  - Parameters are learned.
- Requires fixed input shape, size, and order.
- Obtains representation vector.
Graph-CNN — Graph Representation Vector

Turn arbitrary # vertices into a single vertex

- Graphs can have varying vertices, but we often need fixed nodes for say a final classification task.
- Define a soft attention applied to vertices of graph- learn $M$, a linear combination of all vertices.
- This reduces all vertices to a single vertex.
- A softmax is applied to $M$ before computing linear combination, this ensures the sum of the weights=1.

\[
x = [2 \ 1 \ -2 \ 1]
M^* = \text{softmax}(M)
V^T M^* = [0.2 \ 1.3 \ 0.7 \ 1.8] * M^*
\]
Graph-CNN – Embed Pooling

• Instead of generating a single vertex, generate many vertices.
• The number of output vertices is controlled, and can simplify the model.

We now have three $M^*$ row vectors.

If FC layer has ten connections, learn ten $M^*$ row vectors!
Graph-CNN – Embed Pooling

- Many Graph Representation Vectors combined.
- Output Adjacency matrix calculated accordingly.
- Fixed number of output vertices.
- Independent of number of input vertices.
- Results in fully connected graph, including self connections.

\[
V_i^l = M^{*}_{i,j} V_{j,d}^{l-1}
\]

\[
A_i^l_{i,j} = M^{*}_{i,x} A_{x,a,y}^{l-1} M^{*}_{j,y}
\]
Graph-CNN – Applications

• Used for protein and chemical structures.
• Used for (LiDAR) point cloud object identification and point labeling.
• Used for document citation.
• Used for fMRI brain scan processing.
• Currently modifying for cardiac electrophysiology.

• Have extended TensorFlow sparse library for large graphs.
• Have built neuroevolution machine for metalearning.
Latest news: Miguel Dominguez spent several days at Argonne Leadership Computing, Chicago

• Using GraphCNN to estimate energy signatures in their 5-story tall 3D particle detector, part of the ATLAS experiment at CERN’s Large Hadron Collider.

• Due to the heterogeneity of their detectors, gridded CNNs don’t work but graph CNNs do!
Thank you!!

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