

Graph Convolutional Networks

summary

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Graph Convolutional Networks

- Graph Convolutions
- Empirical Risk Minimization with Graph
 Signals
- Learning with Graph Convolutional
 Filters
- Learning with Graph Perceptrons
- GCN Types
- GCN general architecture

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Two ways to define Convolution:

- 1. Spectral Graph Convolution
 - Simple Spectral GCN, Spline GCN, LapGCN, ChebNet, CayleyNet
- 2. Spatial Graph Convolution
 - Simple Spatial GCN, GraphSage, GIN, MoNet, GAT, GatedGCN
- GCN from scratch with numpy
- Spatio-Temporal GCN



 V_4

 V_2

 V_3

 V_1

Graph definition: $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathcal{W})$

- \mathcal{V} : set of nodes,
- E: set of edges,
- \mathcal{W} : set of edge weights.
- N: number of nodes
- E: number of edges

Graph types:

- Directed / Undirected or Symmetric,
- Weighted / Unweighted.



Graph-Shift Operator (GSO):

$$\mathbf{S} \in \mathbb{R}^{N \times N}$$
, $S_{ij} \neq 0$ if $i = j$ and/or $(i, j) \in \mathcal{E}$.

- It enables matrix representations of graphs.
- It captures the local graph structure.
- If the graph is symmetric, S is also symmetric.



- Various algebraic choices of **S**:
 - Adjacency matrix: S = A,

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• Graph Laplacian matrix (Directed Graphs):

$$\mathbf{S} = \mathbf{L}_{in} = \mathbf{D}_{in} - \mathbf{A}, \qquad \mathbf{S} = \mathbf{L}_{out} = \mathbf{D}_{out} - \mathbf{A}$$
$$[\mathbf{D}_{in}]_{ii} = \sum_{j=1}^{N} \mathbf{A}_{ji}, \qquad [\mathbf{D}_{out}]_{ii} = \sum_{j=1}^{N} \mathbf{A}_{ij}$$

Symmetric Graph Laplacian (Undirected Graphs):

$$S = L = D - A$$
, $D = D_{in} = D_{out}$

The choice matters in practice, however the analysis results hold for any selection.



• Vertex signal:

$$x_i: \mathcal{V} \to \mathbb{R}.$$

Vectorial vertex signal:

$$\mathbf{x}_i: \mathcal{V} \to \mathbb{R}^n$$

• Graph signal:

For notation simplification, it can be described by a vector:

 $\mathbf{x} = [x_1, x_2, \dots, x_N]^T \in \mathbb{R}^N,$





 W_{24}

 $x_{3}W_{23}W_{25}$

 $x_1 W_{12}$

- **Diffusion** of a Graph Signal: y = Sx.
 - Component *i* of **y** is affected by the set of nodes $j \in \mathcal{N}_i$:





 Local operation where components are mixed with components of neighboring nodes.

Graph Signal Diffusion

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• **Diffusion sequence** \rightarrow Recursive application of Diffusion:

$$\mathbf{x}^{(k+1)} = \mathbf{S}\mathbf{x}^{(k)},$$
$$\mathbf{x}^{(0)} = \mathbf{x}.$$

 $\mathbf{x}^{(k)} = \mathbf{S}^{(k)}\mathbf{x}$

• We can also write the diffusion sequence as the power sequence:

 $\mathbf{x}^{(0)} = \mathbf{x} = \mathbf{S}^{(0)}\mathbf{x}$ $\mathbf{x}^{(1)} = \mathbf{S}\mathbf{x}^{(0)} = \mathbf{S}^{(1)}\mathbf{x}$ $\mathbf{x}^{(2)} = \mathbf{S}\mathbf{x}^{(1)} = \mathbf{S}^{(2)}\mathbf{x}$

Always implement the recursive version. Power version only for analysis.



- Implementation of a convolutional filter with coefficients w_k and order K.
- \mathbf{x}_{in} , $\mathbf{x}_{out} \in \mathbb{R}^N$: input, output signals of a convolution filter (each signal value residing on a graph node).
- Linear combination of diffuse versions of the input signal \mathbf{x}_{in} scaled by w_k .





• Graph Convolutional filters perform linear processing of graph signals.



Empirical Risk Minimization with Graph Signals



Machine Learning (*ML*) on graphs is equivalent to *Empirical Risk Minimization* (*ERM*) on graph signals.

- In ERM, we are given:
 - A training set \mathcal{D} with observation graph signal pairs $(\mathbf{x}_i, \mathbf{y}_i) \in \mathcal{D}, i = 1, ..., |\mathcal{D}|$ of equal length: $\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^N$, residing on the nodes of graph $\mathcal{G}(\mathcal{V}, \mathcal{E}, \mathcal{W})$.
 - A loss function $J(\mathbf{y}, \hat{\mathbf{y}})$ to evaluate the similarity between \mathbf{y} and $\hat{\mathbf{y}}$,
 - A function class $f \in C$, $\hat{y} = f(x; \theta)$, the degree of freedom available to the

designer.

Empirical Risk Minimization with Graph Signals



- Learning:
 - find the optimal parameter vector θ of a function f^{*}(x; θ) ∈ C that minimizes J(y, ŷ) averaged over D:

$$\boldsymbol{f}^* = \operatorname*{argmin}_{\boldsymbol{f} \in \mathcal{C}} \sum_{(\mathbf{x}, \mathbf{y}) \in \mathcal{D}} J(\mathbf{y}, \boldsymbol{f}(\mathbf{x}; \boldsymbol{\theta})).$$



Learning with Graph Convolutional Filters



$$\mathbf{x} \longrightarrow \mathbf{z}(\mathbf{x}; \mathbf{\theta}) = \sum_{k=0}^{K-1} w_k \mathbf{S}^k \mathbf{x} \longrightarrow \mathbf{z}(\mathbf{x}; \mathbf{S}, \mathbf{w})$$

• In this case, the learnable parameter vector $\boldsymbol{\theta}$ is the graph convolution kernel coefficient vector $\mathbf{w} = [w_0, ..., w_{K-1}]$:

 $\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{(\mathbf{x}, \mathbf{y}) \in \mathcal{D}} J(\mathbf{y}, \mathbf{f}(\mathbf{x}; \mathbf{S}, \mathbf{w})).$

Learning with Graph Perceptrons (VML

• A GCN composed of several Graph Perceptrons ($\mathbf{W} = [\mathbf{w}_1^T | ... | \mathbf{w}_L^T]^T$):









Plots are generated by Desmos : <u>https://www.desmos.com/calculator</u>

GCN Types

- An isotropic filter treats all neighbors equally, with no particular bias towards certain neighbors.
 - Isotropic GCNs:
 - Use same matrix $\mathbf{W}^{(l)}$, for neighborhood \mathcal{N}_i .
- Anisotropic GCNs:
 - Different neighbors of node *i*, (V_1, V_2, V_3, V_4) are treated differently $(W_{i1}^{(l)}, W_{i2}^{(l)}, W_{i3}^{(l)}, W_{i4}^{(l)})$.





 $V_1, x_1^{(l)}$

 $V_2, x_2^{(l)}$

 $V_1, x_1^{(l)}$

 $W_{i1}^{(l)}$

 $V_2, x_2^{(l)}$

 $W_{i2}^{(l)}$

 $\mathbf{W}^{(l)}$

 $i, x_i^{(l)}$

 $i, x_i^{(l)}$

 $W_{i3}^{(l)}$

 $V_4, x_4^{(l)}$

 $V_{3}, x_{3}^{(l)}$

 $V_4, x_4^{(l)}$

 $V_3, x_3^{(l)}$

16

 $W_{i4}^{(l)}$

GCN Types

- Isotropic GCNs:
 - ChebNet
 - CayleyNet
 - Simple Spatial GCN
 - GraphSage
 - GIN
- Anisotropic GCNs:
 - MoNet
 - GAT
- GatedGCN
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GCN general architecture

1. Input layer:

- Linear embedding of input node features.
- Linear embedding of input edge features.
- 2. GCN layer:
 - Application of a GCN architecture, *L* times.
- 3. Task layer:
 - Graph prediction layer.
 - Node prediction layer.
 - Edge prediction layer.





GCN general architecture

- Input layer:
 - Input node feature vectors $\mathbf{x}_{i,in}$.
 - Input edge features $e_{ij,in}$.
 - Embedding layer of input node/edge features: $\mathbf{x}_{i}^{(l=0)} = \mathbf{x}_{i,in} \in \mathbb{R}^{n}, \quad i = 1, ..., N.$ $\mathbf{e}_{ij}^{(l=0)} = \mathbf{e}_{ij,in} \in \mathbb{R}^{n'}, i = 1, ..., N \text{ and } j = 1, ..., E.$

For notation simplicity, we assume n' = n.

• Output matrix with *n* features for *N* nodes: $\mathbf{X}^{(l=0)} \in \mathbb{R}^{N \times n}$.

• Output matrix with *n* features for *E* edges: $\mathbf{E}^{(l=0)} \in \mathbb{R}^{E \times n}$. Artificial Intelligence & Information Analysis Lab

GCN general architecture



- GCN layer:
 - Input node and edge features embedded into a *n*-dimensional space:

$$\mathbf{X}^{(l=0)} \in \mathbb{R}^{N \times n}.$$
$$\mathbf{E}^{(l=0)} \in \mathbb{R}^{E \times n}.$$

• L GCN layers (l = 1, ..., L). Their structure is defined subsequently.





• *L*-th layer GCN output:

 $\mathbf{X}^{(l=L)} \in \mathbb{R}^{N \times n}.$ $\mathbf{E}^{(l=L)} \in \mathbb{R}^{E \times n}.$





Spatial / Vertex domain:

- A graph is considered as a set of nodes connected by edges.
- Information on one node is aggregated from through its neighbors.
- Spatial Graph Convolution.

Spectral domain:

- A graph is a discrete manifold [GEOM].
- Discretize manifold and do Spectral Convolution using the Laplacian matrix.
- Spectral Graph Convolution.



Simple Spectral GCN

- Proposed by [BRU2013].
- Spectral Graph Convolutional layer:

$$\mathbf{X}^{(l+1)} = f(\widehat{\mathbf{H}}(\mathbf{L})^{(l)}\mathbf{X}^{(l)}) = f(\mathbf{U}\widehat{\mathbf{H}}(\mathbf{\Lambda})^{(l)}\mathbf{U}^{\mathrm{T}}\mathbf{X}^{(l)}),$$

$$\widehat{\mathbf{H}}(\mathbf{\Lambda})^{(l)} = \operatorname{diag}[\widehat{\mathbf{h}}] = \begin{bmatrix} \widehat{h}(\lambda_1) & 0 & 0 \\ 0 & \searrow & 0 \\ 0 & 0 & \widehat{h}(\lambda_N) \end{bmatrix}.$$

• Goal: Learn $\widehat{H}(\Lambda)^{(l)}$ via Backpropagation.





SplineGCN

VML

- Proposed by [HEN2015].
- Spectral Graph Convolutional layer:

$$\mathbf{X}^{(l+1)} = f(\widehat{\mathbf{H}}(\mathbf{L})^{(l)}\mathbf{X}^{(l)}) = f(\mathbf{U}\widehat{\mathbf{H}}(\mathbf{\Lambda})^{(l)}\mathbf{U}^{\mathrm{T}}\mathbf{X}^{(l)}),$$

 $\widehat{\mathbf{H}}(\mathbf{\Lambda})^{(l)} = \operatorname{diag}[\mathbf{B}\widehat{\mathbf{h}}^{(l)}],$

 $\widehat{\mathbf{H}}(\boldsymbol{\Lambda})^{(l)} \in \mathbb{R}^{N \times N} \qquad \mathbf{B} \in \mathbb{R}^{N \times S} \qquad \widehat{\mathbf{h}}^{(l)} \in \mathbb{R}^{S}.$



SplineGCN

• If smooth in Spectral domain:



• Then localized in Spatial domain:

Related publication [SHU2016].

(VML



• Obtain exactly localized filters with *k*-hop support:

$$\widehat{\mathbf{H}}(\mathbf{L}) \triangleq \sum_{k=0}^{K-1} w_k \mathbf{L}^k$$





1-hop neighborhood (L^1) 2-hop neighborhood (L^2)





ChebNets

• A filter can be parametrized as the truncated expansion:

$$\widehat{\mathbf{H}}(\widetilde{\mathbf{L}}) = \sum_{k=0}^{K-1} w_k T_k(\widetilde{\mathbf{L}}).$$

- Where w_k are the Chebyshev coefficients and
- $T_k(\mathbf{\tilde{L}}) \in \mathbb{R}^{N \times N}$ is the Chebyshev polynomial evaluated at the scaled Laplacian matrix:

$$\tilde{\mathbf{L}} \triangleq 2\lambda_{max}^{-1}\mathbf{L} - \mathbf{I}.$$





CayleyNets

- Proposed by [LEV2018].
- Choose an orthonormal basis like the Cayley rationals:
- Benefits:
 - Same properties like ChebNets.
 - Localized in frequency (with spectral zoom).
 - Provide a richer class of filters for the same order K.
- Limitations:
 - Isotropic model.

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Template matching in graphs

Limitations:

- Lack of node ordering:
 - Can not match the template features with the data features.
 - The nodes do not have a well-defined position, but only an arbitrary index.
- Heterogeneous neighborhoods:
 - Can not deal with nodes that have a different number of neighbors.





Spatial Graph Convolution

Absence of node ordering solution:

• Use the same template matrix for all neighbors.

Heterogeneous neighborhoods solution:

Compute the average value of all neighbors.



Simple Spatial GCN





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Simple Spatial GCN

Matrix representation: $\mathbf{X}^{(l+1)} = f(\mathbf{D}^{-1}\mathbf{A}\mathbf{X}^{(l)}\mathbf{W}^{(l)})$

 $V_1, \mathbf{x}_1^{(l)}$ $V_1, \mathbf{x}_1^{(l)}$ Layer *l*+1 Layer *l* $i, \mathbf{x}_{i}^{(l+1)}$ $V_{4}, \mathbf{x}_{4}^{(l)}$ $V_4, \mathbf{x}_4^{(l)}$ $i, \mathbf{x}_{i}^{(l)}$ $V_2, \mathbf{x}_2^{(l)}$ $V_2, \mathbf{x}_2^{(l)}$ $V_{3}, \mathbf{x}_{3}^{(l)}$ $V_{3}, \mathbf{x}_{2}^{(l)}$ $\mathbf{W}^{(l)}$ $\mathbf{x}_i^{(l+1)} = f_{GCN}(\mathbf{x}_i^{(l)}, \{\mathbf{x}_j^{(l)}: j \to i\})$ Artificial Intelligence & **Different families of NNs** 31 Information Analysis Lab





GraphSage

- Proposed by [HAM2017].
- A modification of Simple Spatial GCN:

$$\mathbf{x}_{i}^{(l+1)} = f\left(\frac{1}{d_{i}}\sum_{j\in\mathcal{N}_{i}}A_{ij}\mathbf{W}^{(l)}\mathbf{x}_{ij}^{(l)}\right)$$

For connected nodes: A_{ij} values are equal to 1.

$$\mathbf{x}_{i}^{(l+1)} = f\left(\frac{1}{d_{i}}\sum_{j\in\mathcal{N}_{i}}\mathbf{W}^{(l)}\,\mathbf{x}_{ij}^{(l)}\right)$$



Graph Isomorphism Networks

VML

- Proposed by [XU2018].
- The architecture of GINs can discriminate Graphs that are not isomorphic:

$$\mathbf{x}_{i}^{(l+1)} = f\left(\mathbf{W}_{2}^{(l)}f\left(BN\left(\mathbf{W}_{1}^{(l)}\tilde{\mathbf{x}}_{i}^{(l)}\right)\right)\right)$$
$$\tilde{\mathbf{x}}_{i}^{(l)} = (1+\varepsilon)\mathbf{x}_{i}^{(l)} + \sum_{j\in\mathcal{N}_{i}}\mathbf{x}_{i}^{(l)}$$

- $\mathbf{W}_1^{(l)} \in \mathbb{R}^{n \times n}$, $\mathbf{W}_2^{(l)} \in \mathbb{R}^{n \times n}$.
- *f* : *ReLU* activation function.
- BN: Batch Normalization.
- ε : can be either a learnable parameter or a fixed scalar.



Graph Isomorphism Networks

• Graph isomorphism example:



- Limitations:
 - Isotropic model.



GNN Types

- How can we can get back anisotropy? •
 - Natural edge features (if available).
 - Anisotropic mechanism independent of node parametrization.
 - Proposed methods:
 - **Edge degrees: MoNets**
 - Edge gates: GatedGCNs
 - Attention mechanism: GATs







MoNet

- Proposed by [MON2017].
- MoNets exploit the Graph degree to learn a Bayesian Gaussian Mixture Model (GMM):

$$\mathbf{x}_{i}^{(l+1)} = f\left(\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_{i}}e_{ij}^{(k,l)}\mathbf{W}_{1}^{(k,l)}\mathbf{x}_{j}^{(l)}\right)$$



- Where:
 - *f* : *ReLU* activation function,
- $\mathbf{W}_{1}^{(k,l)} \in \mathbb{R}^{n \times n}$.

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Graph Attention Networks



 V_4 , $\mathbf{x}_4^{(l)}$

 $V_{3}, \mathbf{x}_{2}^{(l)}$

 $e_{i4}^{(k,l)}$

 $e_{i2}^{(k,l)}e_{i3}^{(k,l)}$

 $V_2, \mathbf{x}_2^{(l)}$

- Proposed by [VEL2017].
- GATs exploit the attention mechanism to increase the impact of some neighbors in the Graph neighborhoods with a multi-headed architecture: $V_1, \mathbf{x}_1^{(l)}$

$$\mathbf{x}_{i}^{(l+1)} = Concat _{k=1}^{K} (f\left(\sum_{j \in \mathcal{N}_{i}} e_{ij}^{(k,l)} \mathbf{W}_{1}^{(k,l)} \mathbf{x}_{j}^{(l)}\right)$$

- Where:
 - *f*: *ELU* activation function.
 - Concat $_{k=1}^{K}$: K independent attention mechanisms, whose features are concatenated.

Gated Graph ConvNets



- Proposed by [BRE2017].
- GatedGCNs employ a gating mechanism on the edges (soft attention):

$$\mathbf{x}_{i}^{(l+1)} = \mathbf{x}_{i}^{(l)} + f\left(BN\left(\mathbf{W}_{1}^{(l)}\mathbf{x}_{i}^{(l)} + \sum_{j \in \mathcal{N}_{i}} \mathbf{e}_{ij}^{(l)} \otimes \mathbf{W}_{2}^{(l)}\mathbf{x}_{j}^{(l)}\right)\right)$$



- Where:
 - *f* : *ReLU* activation function.
 - BN: Batch Normalization.



1. Message passing:

- Matrix multiplication of the Adjacency matrix and the feature vector:
 - Mask out all the values, except the ones that the examined node has a connection with.
 - Final result:
 - new feature vector (same shape as the original),
 - each value now represents the sum of the connected neighborhoods of each node.





1. Message passing:

- Matrix multiplication of the Adjacency matrix and the feature vector:
 - Message: Feature vectors,
 - Aggregation function : *Summation*.
- Alternative aggregation function (Average):

 $\mathbf{D}^{-1}\mathbf{A} = \mathbf{A}_{avg}$





• Self connections – modified Adjacency matrix:

$$\widetilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$$

• Normalized Adjacency matrix (scale with each node's degree):

 $\widehat{\mathbf{A}} = \widetilde{\mathbf{D}}^{-1/2} \widetilde{\mathbf{A}} \widetilde{\mathbf{D}}^{-1/2}$



Diffusion mechanism visualized with an animation.



2. GCN from scratch:

• Message passing (multiplication with the Adjacency matrix of the Graph):

GCNLayer forward: self._X = (A @ X).T

• Computation of a linear projection with W followed by an activation function:

 $\mathbf{X}^{(l+1)} = f\left(\mathbf{A}\mathbf{X}^{(l)}\mathbf{W}^{(l)}\right)$

Backpropagation : independent of the Graph (same as in other NNs).





- Proposed by [YAN2018].
- Applied in skeleton-based *Human Action Recognition* from video frames:
 - Important topic in Computer Vision,
 - Identification of *actions* that take place in a video:
 - Primitive action, elementary body part motion (e.g., Hand raising).
 - Action, incorporates multiple temporally organized primitive actions (e.g., Running).
 - Activity, high-level motion that includes several actions (e.g., Playing tennis).
 - Other applications: Robotics, Medicine, Supervised physical training, Human-computer interaction.



- Human skeleton:
 - Keypoints: Nodes in the Graph,
 - Connections: Edges in the Graph.
- Representation with graphs:
 - Invariant to view point and appearance.

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25 keypoints

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17 keypoints

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16 keypoints 15 keypoints 20 keypoints

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- Human skeleton as **ST-GCN input**:
 - 1. Data: Skeleton Spatial Coordinates,
 - 2. Graphical connections: Adjacency matrix.
- Input data tensor: $[B \times C \times T \times V \times M]$.
 - B = batch size,
 - C = number of channels,
 - *T* = number of video frames,
 - V = number of nodes,
 - *M* = number of skeletons in a frame.



- Feed the input data tensor into a PyTorch Conv2d module:
 - Need to rearrange axis : $[(B \times M) \times C \times T \times V]$, with batch size $[B \times M]$.
 - Every batch consists of *C* channels.
 - Each channel is a matrix with T rows and V columns.





- Spatial Convolution block:
 - Uses [1 × 1] kernel, that ensures that features from a frame do not overlap with other frames.



 Sums all the values from the C channels and returns a single value for each node.

The spatial convolution output is then *multiplied with the Adjacency matrix*.





- The multiplication output is fed into a *Temporal Convolution block*.
- The Temporal Convolution uses a $[t_1 \times 1]$ kernel:

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- Deal with absence of node ordering, introduced by [NIE2016]:
 - Partition Strategies to create subsets:

(a)

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- Uni-labeling, all nodes in a neighborhood are treated the same.
- *Distance based*, 1st subset: root node, 2nd subset: 1-hop neighborhood.
- Spatial location based, 1st subset: root node, 2nd subset: centripetal nodes (closer to center than root), 3rd subset: centrifugal nodes (further away).

(C)

(d)





• A sub-graph example of 4 joints and 3 frames:





- The ST-GCN layer is also equipped with:
 - A Residual mechanism,
 - Dropout,





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Thank you very much for your attention!

More material in http://icarus.csd.auth.gr/cvml-web-lecture-series/

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