

Graph Convolutional Network (GCN)

Xi Chen

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why GCN?

- 1 CNN cannot hold the characteristics of translation invariance on non-euclidean structure data
- 2 but we want to implement machine learning by fetching spatial features from this kind of topology data
- 3 Topology connects is actually one of generalized data structures (i.e spectral clustering)

How to extract spatial feature from non-euclidean structure data?

From the perspective of spectral domain, researches went through Fourier Transformation, and convolution on graph, to Graph Convolutional Network which inspired by deep learning

Note: Spectral graph theory: making use of the eigenvalues and eigenvectors of the Laplace matrix of the graph to explore what the graph brings us

why Laplace matrix plays critical role on GCN?

Since GCN cannot pass Laplace matrix on Graph Fourier Transformation and the definition of Graph Conovolution, we would like to see what is Laplace matrix.

There are mainly 3 versions:

(1)

$$L = D - A$$

: Combinatorial Laplacian

(2)

$$L^{sys} = D^{-\frac{1}{2}} L D^{\frac{1}{2}}$$

: Symmetric normalized Laplacian

(3)

$$L^{rw} = D^{-1} A$$

: Random walk normalized Laplacian

Great nature of Laplacian matrix:

- (1) The Laplace matrix is a symmetric matrix, which can be decomposed by eigenvalues
- (2) The Laplace matrix has only non-zero elements on 1-hop neighbor, and everything else is zero
- (3) Laplacian operator and Laplacian matrix are analogy to each other

Decomposition of Laplace matrix

The decomposition:

$$L = U \begin{bmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_n \end{bmatrix} U^{-1} = U \begin{bmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_n \end{bmatrix} U^T$$

Note we have the orthogonal matrix, i.e $UU^T = E$

Fourier Transformation and convolution on GRAPH

Classical Fourier Transformation:

$$F(\omega) = F[f(t)] = \int f(t)e^{-i\omega t} dt$$

Here, $e^{-i\omega t}$ is the eigenvalue function of Laplace operator, which leads to the relationship between ω and eigenvalue

Generalized eigenvalue equation:

$$AV = \lambda V$$

Here are transformation, eigenvalue vector, and eigenvalue for AV and λ respectively.

We have $e^{-i\omega t}$ satisfied:

$$\Delta e^{-i\omega t} = \frac{\partial^2}{\partial t^2} e^{-i\omega t} = -\omega^2 e^{-i\omega t}$$

$e^{-i\omega t}$ is the eigenvalue function of Transformation Δ , and ω has strong bond with eigenvalue.

Now, when we turn to handle the Graph issue, Laplace matrix naturally brings us to find the eigenvector.

So:

$$LV = \lambda V$$

$$F(\lambda_l) = \hat{f}(\lambda_l) = \sum_{i=1}^N f(i)u_l^*(i)$$

f is N dimension vector on Graph, $f(i)$ connected to vetexes correspondently, $u_l(i)$ is the ith component of lth eigenvector. Under λ_l , the Fourier transformation of f in Graph is the inner product of λ_l and its eigenvector u_l