Graph laplacians and graph convolutional network for single-cell data

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Overview

1. GCN Basics
   - Classical Fourier Transform
   - Graph Laplacian
   - Graph Fourier Transform
   - Chebyshev's Approximation

2. GCN application in single-cell RNA-seq

Classical Fourier Transform

The classical Fourier transform

$$\hat{f}(\xi) := \langle f, e^{2\pi i \xi t} \rangle = \int_{\mathbb{R}} f(t) e^{-2\pi i \xi t} dt \tag{1}$$

can be interpreted as a projection of the signal f to the eigenspace spanned by the eigenfunctions of the Laplace operator. The eigenfunctions of the laplace operator is given by

$$-\Delta(e^{2\pi i \xi t}) = -\frac{\partial^2}{\partial t^2} e^{2\pi i \xi t} = (2\pi\xi)^2 e^{2\pi i \xi t} \tag{2}$$

for $-\Delta f = \lambda f$ [Shuman et al., 2013].

Graph Laplacian

The graph Laplacian for an undirected weighted graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is defined as

$$L = D - A, \tag{3}$$

where the adjacency matrix $A \in \mathbb{R}^{n \times n}$ is defined as $A[i,j] = \mathbb{1}\{e_{ij} \in \mathcal{E}\}$ and the diagonal degree matrix $D \in \mathbb{R}^{n \times n}$ is defined as $D[i,i] = \sum_j A[i,j]$. The normalized graph Laplacian is given by

$$\mathcal{L} = I_n - D^{-1/2} A D^{-1/2} = D^{-1/2} L D^{-1/2} \tag{4}$$

Since the normalized graph Laplacian is a real symmetric matrix [Hammond et al., 2011], we can obtain the eigendecomposition of the normalized graph Laplacian

$$\mathcal{L} = U \Lambda U^{\top} \tag{5}$$

Graph Fourier Transform

Theorem (Graph Fourier Transform)

Given $f : \mathcal{V} \to \mathbb{R}$, the graph Fourier transform $\hat{f}$ is the expansion of f in terms of the eigenvectors of the graph Laplacian [Shuman et al., 2013]

$$\hat{f}(\lambda_l) := \langle f, u_l \rangle = \sum_{i=0}^{N-1} f(i) u_l^*(i). \tag{6}$$

Theorem (Inverse Graph Fourier Transform)

The inverse graph Fourier transform is defined as

$$f(i) = \sum_{l=0}^{N-1} \hat{f}(\lambda_l) u_l(i). \tag{7}$$

Chebyshev's Approximation

The spectral convolutions on graph given by the signal $x \in \mathbb{R}^N$ multiplied with a filter $g_\theta = \text{diag}(\theta);\ \theta \in \mathbb{R}^N$ in the Fourier domain is:

$$g_\theta \ \circ \ x = U g_\theta U^\top x \tag{8}$$

with run time complexity $\mathcal{O}(N^2)$. [Kipf et al., 2017].

Theorem (Chebyshev Polynomial Approximations)

The filter $g_\theta(\Lambda)$ can be approximated by the Chebyshev polynomials $T_k(x)$ up to the K^{th} order with complexity $\mathcal{O}(|\mathcal{E}|)$:

$$g_{\theta'}(\Lambda) \approx \sum_{k=0}^{K} \theta'_k T_k(\tilde{\Lambda}), \tag{9}$$

where $\tilde{\Lambda} = \frac{2}{\lambda_{\max}}\mathcal{L} - I_N$, $\lambda_{\max}$ is the largest eigenvalue of $\mathcal{L}$, $T_k(x) := 2xT_{k-1}(x) - T_{k-2}(x)$, $T_0(x) := 1$, $T_1(x) := x$, and $\theta' \in \mathbb{R}^K$ is a vector of Chebyshev coefficients [Hammond et al., 2011].

References

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