Linear Algebra and Graphs Applications

Ulises Tirado Zatarain [1]
(ulises.tirado@cimat.mx)

[1] Algorists Group

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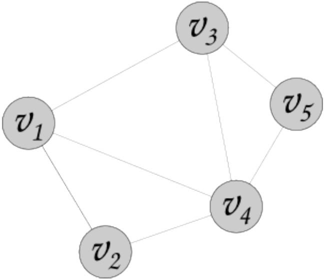
Outline

Basics

Simple graph

Is a pair $G = (V, E)$, where V is a finite set of vertices and $E \subseteq V \times V$ is a symetric and antireflexive relation. In a directed graph E isn't necessarily symetric.



Basics

- The adjacency matrix $\mathbf{A} = [a_{ij}] \in \{0,1\}^{|V|\times|V|}$ is defined as:

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

- The incidence matrix $\mathbf{B} = [b_{ij}] \in \{0,1\}^{|V|\times|E|}$ is defined as:

$$b_{ij} = \begin{cases} 1 & \text{if } i \in V \text{ is incident on } j \in E \\ 0 & \text{otherwise} \end{cases}$$

- We can denote with $\mathbf{1}$ a vector/matrix with all-ones entries such that the operations are defined.

Basics

Degree of a vertex

Let $v \in V$, its degree is the number of edges incident from/to the vertex and is denoted as $\deg(v)$.

- The degree of vertex k is the k-th entry of vector $\mathbf{d} \in \mathbb{R}^{|V|}$:

$$\mathbf{d} = \mathbf{A}\mathbf{1}$$

- In a directed graph, we have two kinds of vertex degrees:

$$\mathbf{d}_{\text{in}}^{\top} = \mathbf{1}^{\top}\mathbf{A}$$

$$\mathbf{d}_{\text{out}} = \mathbf{A}\mathbf{1}$$

- We can write the average degree as:

$$\bar{d} = \frac{1}{|V|}\mathbf{1}^{\top}\mathbf{d} = \frac{1}{|V|}\sum_{v \in V}\deg(v) = 2\frac{|E|}{|V|}$$

Relations

- There is one relation between $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{D} = \operatorname{diag}(\mathbf{d})$:

$$\mathbf{A} = \mathbf{B}\mathbf{B}^\top - \mathbf{D}$$

- The link matrix $\mathbf{E} = \left[e_{ij}\right] \in \{0,1\}^{|E| \times |E|}$ is defined as:

$$e_{ij} = \begin{cases} 1 & \text{if } i,j \in E \text{ have a common vertex} \\ 0 & \text{otherwise} \end{cases}$$

- The relation between $\mathbf{E}$ and $\mathbf{B}$ is:

$$\mathbf{E} = \mathbf{B}^\top \mathbf{B} - \mathbf{I}$$

Relations

- Edges have degree too as vertex:

$$\delta = E\mathbf{1}$$

- It's easy verify that if edge $k = (i, j)$ then:

$$\delta_k = d_i + d_j - 2$$

- Also, if p_2 is the number of 2-paths, then:

$$\mathbf{1}^\top E\mathbf{1} = \mathbf{1}^\top \delta = 2p_2$$

Shapes and structures

- Let $G = (V, E)$ with adjacency matrix $\mathbf{A}$, then entry i, j of $\mathbf{A}^n$ is the number of n-walks from i to j.
- Let $G = (V, E)$ a bipartite simple graph, such that $V = S \cup T$ and $S \cap T = \emptyset$, we can write adjacency matrix of G as:

$$\mathbf{A} = \begin{bmatrix} 0 & \tilde{\mathbf{A}}^\top \\ \tilde{\mathbf{A}} & 0 \end{bmatrix}$$

  where $\tilde{A} \in \{0,1\}^{|S|\times|T|}$ contains adjacency relations betwen vertex in S and T.
- If $K_{|V|}$ is a complete graph of orden $|V|$, then its adjacency matrix is $\mathbf{A} = \mathbf{1} - \mathbf{I}$.

Spectrum (Eigenvalues & Eigenvectors)

- Let a simple graph $G = (V, E)$ with adjacency matrix $\boldsymbol{A}$ and let$\boldsymbol{\Lambda} = \operatorname{diag}\left(\begin{bmatrix} \lambda_1 & \cdots & \lambda_{|V|} \end{bmatrix}\right)$ such that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{|V|}$ are the eigenvalues of $\boldsymbol{A}$, then:

$$\sum_{i=1}^{|V|} \lambda_i = \mathbf{1}^\top \boldsymbol{\Lambda} \mathbf{1} = \operatorname{tr}(A) = \sum_{i=1}^{|V|} a_{ii} = 0$$

- Moreover, the dominant eigenvalue λ_1 is bounded as follow:

$$\delta \leqslant \bar{d} \leqslant \lambda_1 \leqslant \Delta$$

where δ and Δ are the minimun and the maximun vertex degree respectively.

Spectrum (Eigenvalues & Eigenvectors)

- Since $\mathbf{A}$ is symetric, we can write $\mathbf{A} = \mathbf{\Phi}\mathbf{\Lambda}\mathbf{\Phi}^\top$ where $\mathbf{\Phi}$ is an orthonormal matrix its columns are the eigenvectors of $\mathbf{A}$ and then $\mathbf{A}^n = \mathbf{\Phi}\mathbf{\Lambda}^n\mathbf{\Phi}^\top$, we mean:

$$[\mathbf{A}^n]_{ij} = \sum_{k=1}^{|V|} \left[\varphi_{ki}\varphi_{kj}\lambda_k^n\right]$$

- Suppose two graphs G_1 and G_2 with adjacency matrices $\mathbf{A}_1$ and $\mathbf{A}_2$, then there exists a permutation matrix $\mathbf{P}$ such that:

$$\mathbf{A}_1 = \mathbf{P}\mathbf{A}_2\mathbf{P}^{-1}$$

  if and only if G_1 and G_2 are isomorphic and $\mathbf{A}_1$ and $\mathbf{A}_2$ have the same spectrum.

Spectrum (Eigenvalues & Eigenvectors)

- If G is a bipartite graph, then its spectrum is symetric about 0, we mean:

$$\lambda_k = -\lambda_{|V|-k+1}$$

- If $K_{|V|}$ is a complete graph of orden $|V|$, then its adjacency matrix $\mathbf{A} = \mathbf{1} - \mathbf{I}$ has the spectrum is:

$$\lambda_1 = |V| - 1, \lambda_2 = \cdots = \lambda_{|V|} = -1$$

Also, the eigenvalue λ_1 has $\mathbf{1}$ as its respective eigenvector.

Structures

- To work with large and sparse graphs we need an structure to represent adjacency matrix:

  class `matrix`(*int V*) **begin**

      struct `matrix::entry` **rows[V];*

      struct `matrix::entry` **columns[V];*

      int verteces = V;

  end

  static const struct `matrix::entry` z;

Structures

- And the entries are defined as follow:

```
struct matrix::entry(int i,int j,float info) begin
    struct matrix::entry *up = &z;
    struct matrix::entry *left = &z;
    struct matrix::entry *right = &z;
    struct matrix::entry *down = &z;
    int row = i, column = j;
    float data = info;
end
```

- With these structures when we need to compute the product of two sparce matrices we can get this in $\mathcal{O}(|E|)$.

Laplacian operator

- The laplacian matrix $\boldsymbol{\nabla} = [\nabla_{ij}] \in \mathbb{R}^{|V|\times|V|}$ of a simple graph $G = (V, E)$ is defined as:

$$\nabla_{ij} = \begin{cases} -1 & \text{if } (i,j) \in E \\ d_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- We can write this matrix simply as:

$$\boldsymbol{\nabla} = \mathbf{D} - \mathbf{A}$$

- This matrix is always semi+def, then $\lambda_{|V|} = 0$ and its eigenvector is $\boldsymbol{\varphi}_{|V|} = \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}^\top$.

Normalized laplacian

- The laplacian matrix $\tilde{\boldsymbol{\nabla}} = \left[\tilde{\nabla}_{ij}\right] \in \mathbb{R}^{|V|\times|V|}$ of a simple graph $G = (V, E)$ is defined as:

$$\tilde{\nabla}_{ij} = \begin{cases} 1 & \text{if } i = j \\ -\frac{1}{\sqrt{d_i d_j}} & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$

- We can write this matrix simply as:

$$\tilde{\boldsymbol{\nabla}} = \mathbf{D}^{-\frac{1}{2}} \boldsymbol{\nabla} \mathbf{D}^{-\frac{1}{2}}$$

- Multiplicity of eigenvalue $\lambda_{|V|} = 0$ indicates the number of connected components in G.

Exponential and sociability matrices

- Exponential matrix:

$$e^{\mathbf{A}} = \sum_{k=1}^{\infty} \frac{1}{k!} \mathbf{A}^k$$

- Sociability matrix of degree r:

$$\boldsymbol{S}^r = \left[\tilde{\mathbf{A}}\mathbf{1} | \tilde{\mathbf{A}}^2 \mathbf{1} | \cdots | \tilde{\mathbf{A}}^r \mathbf{1} \right]$$

where $\tilde{\mathbf{A}}^j = \left[\operatorname{diag}\left(\mathbf{1}^\top \mathbf{A}^j \right) \right]^{-1} \mathbf{A}^j$ with $j \in [r]$.

Spectral Clustering

function `spectral-clustering`($A \in \{0,1\}^{n\times n}$) **begin**

Parameters: $m \in [n]$, $K \in \{2,\ldots,n\}$

1. Compute the singular value decomposition $A = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\top$.
2. Let $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ be the first m columns of $\mathbf{U}$ and $\mathbf{V}$ respectively and let $\tilde{\boldsymbol{\Sigma}}$ be the submatrix of $\boldsymbol{\Sigma}$ given by the first m rows and columns.
3. Define $\tilde{\mathbf{Z}} = [\tilde{\mathbf{U}}\tilde{\boldsymbol{\Sigma}}^{\frac{1}{2}}|\tilde{\mathbf{V}}\tilde{\boldsymbol{\Sigma}}^{\frac{1}{2}}] \in \mathbb{R}^{n\times 2m}$ to be the concatenation of the coordinate-scaled singular vector matrices.
4. Let $(\hat{\psi},\hat{\tau}) = \arg\min_{\psi,\tau}\sum_{i=1}^{n}\|\tilde{z}_i - \psi\|_2^2$ give the centroids and block assignments, where $\tilde{z}_i$ is the i-th row of $\tilde{\mathbf{Z}}$, $\hat{\psi} \in \mathbb{R}^{2m}$ are the centroids and $\hat{\tau} : [n] \mapsto [K]$.
5. **return** $\hat{\tau}$, *the block assignment function.*

end

Image segmentation

function `image-segmentation`($\mathbf{I} : \mathbb{Z}^2 \mapsto \mathbb{Z}^3$) **begin**

Parameters: $w, h \in \mathbb{Z}$, $\beta \in \mathbb{R}$

1. Define a simple graph with the pixels of image $\mathbf{I}$, where the adjacency matrix $\boldsymbol{A}$ defines relations between the pixel $(i,j) \in [w] \times [h]$ and the pixel $(u,v) = (i,j) + \mathbf{s}$ as follow:

$$A_{(i,j),(u,v)} = \begin{cases} 1 & \|\mathbf{I}(i,j) - \mathbf{I}(u,v)\|_2 \leqslant \beta \\ 0 & \text{otherwise} \end{cases}$$

   where $\mathbf{s} \in \{(0,1),(1,0),(-1,0),(0,-1)\}$.

2. `spectral-clustering`($\boldsymbol{A}$; m, K);

end

More applications

- Page rank
- Visualizations
- Random walk modelign
- Biometrics
- Stable matching
- Social networks
- Trading analysis

References I

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