DM587

Scientific Programming

Eigenvalues and Page Rank

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Outline

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Eigenvalues and Eigenvectors

Definition

Let A be a square matrix.

- The number λ is said to be an eigenvalue of A if for some non-zero vector $\boldsymbol{x}$,

$$A\boldsymbol{x} = \lambda\boldsymbol{x}$$

- Any non-zero vector $\boldsymbol{x}$ for which this equation holds is called
  eigenvector for eigenvalue λ or
  eigenvector of A corresponding to eigenvalue λ

Diagonalization

Recall: Square matrices are similar if there is an invertible matrix P such that $P^{-1}AP = M$.

Definition (Diagonalizable matrix)

The matrix A is diagonalizable if it is similar to a diagonal matrix; that is,
if there is a diagonal matrix D and an invertible matrix P such that $P^{-1}AP = D$

Example

$$A = \begin{bmatrix} 7 & -15 \\ 2 & -4 \end{bmatrix}$$

$$P = \begin{bmatrix} 5 & 3 \\ 2 & 1 \end{bmatrix} \qquad P^{-1} = \begin{bmatrix} -1 & 3 \\ 2 & -5 \end{bmatrix}$$

$$P^{-1}AP = D = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

How was such a matrix P found?

When is a matrix diagonalizable?

Summary

- Characteristic polynomial and characteristic equation of a matrix
- eigenvalues, eigenvectors, diagonalization
- finding eigenvalues and eigenvectors
- eigenspace
- diagonalize a diagonalizable matrix
- conditions for digonalizability
- diagonalization as a change of basis, similarity
- geometric effect of linear transformation via diagonalization

Uses of Diagonalization

- find powers of matrices
- solving systems of simultaneous linear difference equations
- Markov chains
- PageRank algorithm

Powers of Matrices

$$A^n = \underbrace{AAA\cdots A}_{n \text{ times}}$$

If we can write: $P^{-1}AP = D$ then $A = PDP^{-1}$

$$\begin{aligned} A^n &= \underbrace{AAA\cdots A}_{n \text{ times}} \\ &= \underbrace{(PDP^{-1})(PDP^{-1})(PDP^{-1})\cdots(PDP^{-1})}_{n \text{ times}} \\ &= PD(P^{-1}P)D(P^{-1}P)D(P^{-1}P)\cdots DP^{-1} \\ &= P\underbrace{DDD\cdots D}_{n \text{ times}}P^{-1} \\ &= PD^nP^{-1} \end{aligned}$$

then closed formula to calculate the power of a matrix.

Difference equations

- A difference equation is an equation linking terms of a sequence to previous terms, eg:

  $$x_{t+1} = 5x_t - 1$$

  is a first order difference equation.

- a first order difference equation can be fully determined if we know the first term of the sequence (initial condition)

- a solution is an expression of the terms x_t

  $$x_{t+1} = ax_t \implies x_t = a^t x_0$$

System of Difference equations

Suppose the sequences x_t and y_t are related as follows:
$x_0 = 1, y_0 = 1$ for $t \geq 0$

$$\begin{aligned} x_{t+1} &= 7x_t - 15y_t \\ y_{t+1} &= 2x_t - 4y_t \end{aligned}$$

Coupled system of difference equations.

Let

$$\boldsymbol{x}_t = \begin{bmatrix} x_t \\ y_t \end{bmatrix}$$

then $\boldsymbol{x}_{t+1} = A\boldsymbol{x}_t$ and $\boldsymbol{x}_0 = [1, 1]^T$ and

$$A = \begin{bmatrix} 7 & -15 \\ 2 & -4 \end{bmatrix}$$

Then:

$$\begin{aligned} \boldsymbol{x}_1 &= A\boldsymbol{x}_0 \\ \boldsymbol{x}_2 &= A\boldsymbol{x}_1 = A(A\boldsymbol{x}_0) = A^2\boldsymbol{x}_0 \\ \boldsymbol{x}_3 &= A\boldsymbol{x}_2 = A(A^2\boldsymbol{x}_0) = A^3\boldsymbol{x}_0 \\ &\vdots \\ \boldsymbol{x}_t &= A^t\boldsymbol{x}_0 \end{aligned}$$

Power sequence generated by A

Markov Chains

- Suppose two supermarkets compete for customers in a region with 20000 shoppers.
- Assume no shopper goes to both supermarkets in a week.
- The table gives the probability that a shopper will change from one to another supermarket:

	From A	From B	From none
To A	0.70	0.15	0.30
To B	0.20	0.80	0.20
To none	0.10	0.05	0.50

  (note that probabilities in the columns add up to 1)
- Suppose that at the end of week 0 it is known that 10000 went to A, 8000 to B and 2000 to none.
- Can we predict the number of shoppers at each supermarket in any future week t? And the long-term distribution?

Formulation as a system of difference equations:

- Let $\boldsymbol{x}_t$ be the percentage of shoppers going in the two supermarkets or none
- then we have the difference equation:

$$\boldsymbol{x}_t = A\boldsymbol{x}_{t-1}$$

$$A = \begin{bmatrix} 0.70 & 0.15 & 0.30 \\ 0.20 & 0.80 & 0.20 \\ 0.10 & 0.05 & 0.50 \end{bmatrix}, \qquad \boldsymbol{x}_t = \begin{bmatrix} x_t \\ y_t \\ z_t \end{bmatrix}$$

- a Markov chain (or process) is a closed system of a fixed population distributed into n different states, transitioning between the states during specific time intervals.
- The transition probabilities are known in a transition matrix A (coefficients all non-negative + sum of entries in the columns is 1)
- state vector $\boldsymbol{x}_t$, entries sum to 1.

- A solution is given by (assuming A is diagonalizable):

$$\boldsymbol{x}_t = A^t \boldsymbol{x}_0 = (PD^tP^{-1})\boldsymbol{x}_0$$

- let $\boldsymbol{x}_0 = P\boldsymbol{z}_0$ and $\boldsymbol{z}_0 = P^{-1}\boldsymbol{x}_0 = \begin{bmatrix} b_1 & b_2 \cdots & b_n \end{bmatrix}^T$ be the representation of $\boldsymbol{x}_0$ in the basis of eigenvectors, then:

$$\boldsymbol{x}_t = PD^tP^{-1}\boldsymbol{x}_0 = b_1\lambda_1^t\boldsymbol{v}_1 + b_2\lambda_2^t\boldsymbol{v}_2 + \cdots + b_n\lambda_n^t\boldsymbol{v}_n$$

- Th.: if A is the transition matrix of a regular Markov chain, then $\lambda = 1$ is an eigenvalue of multiplicity 1 and all other eigenvalues satisfy $|\lambda| < 1$

- $\boldsymbol{x}_t = b_1(1)^t\boldsymbol{v}_1 + b_2(0.6)^t\boldsymbol{v}_2 + \cdots + b_n(0.4)^t\boldsymbol{v}_n$

- $\lim_{t\to\infty} 1^t = 1, \quad \lim_{t\to\infty} 0.6^t = 0$ hence the long-term distribution is

$$\boldsymbol{q} = b_1\boldsymbol{v}_1 = 0.125\begin{bmatrix} 3 \\ 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.375 \\ 0.500 \\ 0.125 \end{bmatrix}$$

Theory

Definition

A stochastic process is any sequence of experiments for which the outcome at any stage depends on chance.
A Markov process is a stochastic process with the following properties:

1. The set of possible outcomes or states is finite
2. The probability of the next outcome depends only on the previous outcome
3. The probabilities are constant over time:

$$\boldsymbol{x}_{t+1} = A\boldsymbol{x}_t \qquad A \text{ transition matrix}$$

Theory

Definitions:

- Non-negative matrices are matrices with exclusively non-negative real numbers as elements.
- Positive matrices are matrices with exclusively positive real numbers as elements.
- The eigenvalues of a real square matrix A are in the general case complex numbers that make up the spectrum of the matrix.
- The exponential growth rate of the matrix powers A^k as $k \to \infty$ is controlled by the eigenvalue of A with the largest absolute value (modulus).
- If the distinct eigenvalues of a matrix A are $\lambda_1, \lambda_2, \ldots, \lambda_k$, and if $|\lambda_1|$ is larger than $|\lambda_2|, \ldots, |\lambda_k|$, then λ_1 is called a dominant eigenvalue of A.
- Any eigenvector corresponding to a dominant eigenvalue is called a dominat eigenvector of A.

The Perron–Frobenius theorem (next slide) describes the properties of the dominant eigenvalue and of the corresponding eigenvectors when A is a non-negative real square matrix. In the next slide we focus only on a restricted case, the case of positive square martices.

Theory

Theorem (Perron's Theorem)

If A is a positive $n \times n$ matrix, then A has a positive real eigenvalue r with the following properties:

1. *r is simple root of the charachteristic equation*
2. *r has a positive eigenvector $\mathbf{x}$*
3. *If λ is any other eigenvealue of A, then $|\lambda| < r$.*

(The theorem is a special case of a more general theorem due to Frobenius on irreducible non-negative matrices.)

- If A is square stochastic and all its entries are positive, it follows from Perron's theorem that $\lambda_1 = 1$ is an eigenvalue of A and the remaining eigenvalues satisfy $|\lambda_j| \leq 1$ for $j = 2, \ldots, n$.

- Consequences of Perron's theorem on Markov chains (next two slides):

Theory

Definition

A matrix such that all its entries are non-negative and the sum of the entries over the columns is 1 is called a stochastic matrix.

Definition

A stochastic matrix A is said to be regular if A or some positive power of A has all positive entries. A Markov chain whose transition matrix is regular is said to be a regular Markov chain.

Theorem

If A is the transition matrix for a regular Markov chain, then:

1. *There is a unique probability vector $\boldsymbol{q}$ such that $A\boldsymbol{q} = \boldsymbol{q}$.*
2. *For any initial probability vector $\boldsymbol{x}_0$, the sequence of state vectors*

$$\boldsymbol{x}_0, A\boldsymbol{x}_0, \ldots, A^k\boldsymbol{x}_0$$

converges to $\boldsymbol{q}$.

Theory

Theorem

If a Markov chain with an $n \times n$ transition matrix A converges to a steady state vector $\boldsymbol{x}$, then

1. $\boldsymbol{x}$ *is a probability vector*
2. $\lambda_1 = 1$ *is an eigenvalue of* A *and* $\boldsymbol{x}$ *is an eigenvector belonging to* λ_1

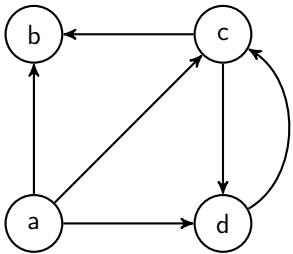
Outline

Page Rank Algorithm

- The PageRank algorithm is one way of ranking the nodes in a graph by importance
- Brin, S.; Page, L. (1998). "The anatomy of a large-scale hypertextual Web search engine". Computer Networks and ISDN Systems. 30: 107–117.
- Currently, PageRank is not the only algorithm used by Google to order search results, but it is the first algorithm that was used by the company, and it is the best-known.

The Model

Let's consider a Tiny-Web: nodes are pages and arcs are hyperlinks.



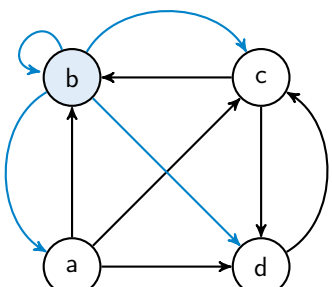
Adiacency matrix for a directed graph

$$A = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

If n users start on random pages in the network and click on a link every 5 minutes, which page in the network will have the most views after an hour?
Which will have the fewest?

The Model

In nodes with no outgoing link (dangling pages), the surfer would stand. Unrealistic. $\rightsquigarrow$ modify each sink in the graph by adding arcs from the sink to every node in the graph (random jumps).



Adiacency matrix

$$\widetilde{A} = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

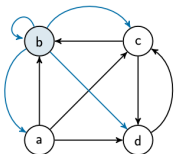
The Model

- Let $x_t(k)$ be the likelihood that a particular internet user is surfing webpage k at time t.
- users reaching i at $t+1$ are those that in t where in an adjacent node and chose the link to i
- we assume outgoing links are chosen with equal likelihood
- thus, $x_{t+1}(i)$ can be computed by counting the number of links pointing to page i, weighted by the total number of outgoing links for each node.

Example:

$$x_{t+1}(a) = \frac{1}{4}x_t(b),$$
$$x_{t+1}(b) = \frac{1}{3}x_t(a) + \frac{1}{4}x_t(b) + \frac{1}{2}x_t(c).$$

$$x_{t+1}(a) = 0x_t(a) + \frac{1}{4}x_t(b) + 0x_t(c) + 0x_t(d),$$
$$x_{t+1}(b) = \frac{1}{3}x_t(a) + \frac{1}{4}x_t(b) + \frac{1}{2}x_t(c) + 0x_t(d).$$



$$x_{t+1}(i) = \sum_{j=1}^{n} \widetilde{A}_{ij} \frac{x_t(j)}{\sum_{k=1}^{n} \widetilde{A}_{kj}}.$$

A More Realistic Model

Let $\epsilon \in [0,1]$ be the probability that a user follows one of the outgoing links at step t (damping factor) and $1-\epsilon$ that he jumps at random.

$$x_{t+1}(i) = \underbrace{\epsilon \sum_{j=1}^{n} \left(\widetilde{A}_{ij} \frac{x_t(j)}{\sum_{k=1}^{n} \widetilde{A}_{kj}} \right)}_{\substack{\text{User stayed interested and} \\ \text{clicked a link on the current page}}} + \underbrace{(1-\epsilon) \sum_{j=1}^{n} \frac{1}{n} x_t(j)}_{\substack{\text{User got bored and} \\ \text{chose a random page}}}$$

In matrix terms:

$$\boldsymbol{x}_{t+1} = \epsilon \widehat{A} \boldsymbol{x}_t + (1-\epsilon) \frac{1}{n} 1 1^{\mathsf{T}} \boldsymbol{x}_t,$$

where $\boldsymbol{x}_t = [x_t(1), x_t(2), \ldots, x_t(n)]^{\mathsf{T}}$, 1 is a vector of n ones, and $\widehat{A}$ is the $n \times n$ matrix with entries

$$\widehat{A}_{ij} = \frac{\widetilde{A}_{ij}}{\sum_{k=1} \widetilde{A}_{kj}}.$$

For our example:

$$\widehat{A} = \begin{array}{c} \\ \mathsf{a} \\ \mathsf{b} \\ \mathsf{c} \\ \mathsf{d} \end{array} \begin{array}{c} \begin{array}{cccc} \mathsf{a} & \mathsf{b} & \mathsf{c} & \mathsf{d} \end{array} \\ \begin{bmatrix} 0 & 1/4 & 0 & 0 \\ 1/3 & 1/4 & 1/2 & 0 \\ 1/3 & 1/4 & 0 & 1 \\ 1/3 & 1/4 & 1/2 & 0 \end{bmatrix} \end{array}$$

$$\frac{1}{n}11^{\mathsf{T}} = \begin{array}{c} \\ \mathsf{a} \\ \mathsf{b} \\ \mathsf{c} \\ \mathsf{d} \end{array} \begin{array}{c} \begin{array}{cccc} \mathsf{a} & \mathsf{b} & \mathsf{c} & \mathsf{d} \end{array} \\ \begin{bmatrix} 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{bmatrix} \end{array}$$

$$\boldsymbol{x}_{t+1} = \left(\epsilon\widehat{A} + (1-\epsilon)\frac{1}{n}11^{\mathsf{T}}\right)\boldsymbol{x}_t$$

$$\bar{A} = \epsilon\widehat{A} + (1-\epsilon)\frac{1}{n}11^{\mathsf{T}}$$

all terms of $\bar{A}$ are nonegative and all its columns sum up to 1, ie, $\bar{A}$ is a positive stochastic matrix

$$\boldsymbol{x}_{t+1} = \bar{A}\boldsymbol{x}_t$$

is a regular Markov chain

Computing the Rankings

- Let's define the page rank of node i as the steady state of the Markov chain:

$$x(i) = \lim_{t \to \infty} x_t(i).$$

1. If $\boldsymbol{x}$ exists, then taking the limit as $t \to \infty$ of both sides of the Markov chain gives the following:

$$\lim_{t \to \infty} \boldsymbol{x}(t+1) = \lim_{t \to \infty} \left[\epsilon \widehat{A} \boldsymbol{x}(t) + (1-\epsilon) \frac{1}{n} 1 1^{\mathsf{T}} \boldsymbol{x}(t) \right]$$

$$\boldsymbol{x} = \epsilon \widehat{A} \boldsymbol{x} + (1-\epsilon) \frac{1}{n} 1 1^{\mathsf{T}} \boldsymbol{x} \qquad \text{because convergent then } \boldsymbol{x}_{t+1} = \boldsymbol{x}_t$$

$$\left(I - \epsilon \widehat{A} - (1-\epsilon) \frac{1}{n} 1 1^{\mathsf{T}} \right) \boldsymbol{x} = 0 \qquad 1^{\mathsf{T}} \boldsymbol{x} = 1 \text{ since } \sum_i x_t(i) = 1$$

$$\left(I - \epsilon \widehat{A} \right) \boldsymbol{x} = \frac{1-\epsilon}{n} 1 \qquad \rightsquigarrow \text{ a system of linear equations!}$$

2. Alternatively, setting $\bar{A} = \epsilon \widehat{A} + \frac{1-\epsilon}{n} 11^{\mathsf{T}}$

$$(I - \bar{A})\, \boldsymbol{x} = 0$$
$$\bar{A}\boldsymbol{x} = \boldsymbol{x}$$

- x is an eigenvector of $\bar{A}$ corresponding to the eigenvalue $\lambda = 1$.
- since the columns of $\bar{A}$ sum to 1, and because the entries of $\bar{A}$ are strictly positive, Perron's theorem guarantees that $\lambda = 1$ is the unique eigenvalue of $\bar{A}$ of largest magnitude, and that the corresponding eigenvector x is unique up to scaling (ie, it can be found negative and rescaled to positive).
- x can be rescaled (for example with L1 $x/\|x\|_1$) so that it represents the desired PageRank probability vector.

An Iterative Method

- Solving the system of linear equations above or finding the eigenvalues/eigenvectors is feasible for small networks, but they are not efficient strategies for very large systems.

3. Iterative technique (Power Method):
   1. Start with $t = 0$ and an initial guess x_0
   2. Compute x_{t+1} with

$$\boldsymbol{x}_{t+1} = \left(\epsilon \widehat{A} + (1-\epsilon)\frac{1}{n} 1 1^{\mathsf{T}}\right) \boldsymbol{x}_t$$

$$\boldsymbol{x}_{t+1} = x_{t+1} / \|x_{t+1}\|_1$$

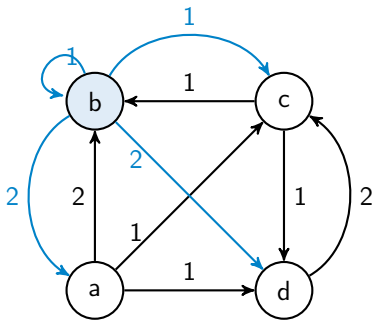
   and set $t \leftarrow t + 1$

   3. if $\| x_t - x_{t-1} \|_2$ is sufficiently small stop, otherwise go to 2.

Finally, one can renormalize with L1 for a probability distribution.

PageRank on Weighted Graphs

If hyperlinks to page b are clicked on more frequently than hyperlinks to page c, the edge to node b should be given more weight than the edge to node c.



$$A = \begin{array}{c} \\ \mathrm{a} \\ \mathrm{b} \\ \mathrm{c} \\ \mathrm{d} \end{array} \begin{array}{c} \begin{array}{cccc} \mathrm{a} & \mathrm{b} & \mathrm{c} & \mathrm{d} \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ 1 & 0 & 0 & 2 \\ 1 & 0 & 2 & 0 \end{bmatrix} \end{array}$$

$$\widehat{A} = \begin{array}{c} \\ \mathrm{a} \\ \mathrm{b} \\ \mathrm{c} \\ \mathrm{d} \end{array} \begin{array}{c} \begin{array}{cccc} \mathrm{a} & \mathrm{b} & \mathrm{c} & \mathrm{d} \end{array} \\ \begin{bmatrix} 0 & 1/4 & 0 & 0 \\ 1/2 & 1/4 & 1/3 & 0 \\ 1/4 & 1/4 & 0 & 1 \\ 1/4 & 1/4 & 2/3 & 0 \end{bmatrix} \end{array}$$

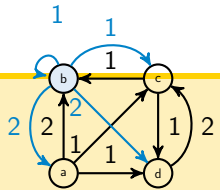
The columns of $\widehat{A}$ still sum to 1. Thus $\bar{A} = \epsilon\widehat{A} + \frac{1-\epsilon}{n}11^{\mathsf{T}}$ is still positive stochastic, so we can expect a unique x to exist.

Python: Networkx

- It represents graphs internally with dictionaries, thus taking full advantage of the sparsity in a graph.
- The base class for directed graphs is called `nx.DiGraph`.
- Nodes and edges are usually added or removed incrementally with the following methods.

Method	Description
`add_node()`	Add a single node.
`add_nodes_from()`	Add a list of nodes.
`add_edge()`	Add an edge between two nodes, adding the nodes if needed.
`add_edges_from()`	Add multiple edges (and corresponding nodes as needed).
`remove_edge()`	Remove a single edge (no nodes are removed).
`remove_edges_from()`	Remove multiple edges (no nodes are removed).
`remove_node()`	Remove a single node and all adjacent edges.
`remove_nodes_from()`	Remove multiple nodes and all adjacent edges.

Example




```
>>> import networkx as nx

# Initialize an empty directed graph.
>>> DG = nx.DiGraph()

# Add the directed edges (nodes are added automatically).
>>> DG.add_edge('a', 'b', weight=2)     # a --> b (adds nodes a and b)
>>> DG.add_edge('a', 'c', weight=1)     # a --> c (adds node c)
>>> DG.add_edge('a', 'd', weight=1)     # a --> d (adds node d)
>>> DG.add_edge('c', 'b', weight=1)     # c --> b
>>> DG.add_edge('c', 'd', weight=2)     # c --> d
>>> DG.add_edge('d', 'c', weight=2)     # d --> c
```

Networkx

- `nx.Digrah` object can be queried for information about the nodes and edges.
- Dictionary-like indexing to access node and edge attributes, such as the weight of an edge.

Method	Description
`has_node(A)`	Return `True` if `A` is a node in the graph.
`has_edge(A,B)`	Return `True` if there is an edge from `A` to `B`.
`edges()`	Iterate through the edges.
`nodes()`	Iterate through the nodes.
`number_of_nodes()`	Return the number of nodes.
`number_of_edges()`	Return the number of edges.

Example

```
# Check the nodes and edges.
>>> DG.has_node('a')
True
>>> DG.has_edge('b', 'a')
False
>>> list(DG.nodes())
['a', 'b', 'c', 'd']
>>> list(DG.edges())
[('a', 'b'), ('a', 'c'), ('a', 'd'), ('c', 'b'), ('c', 'd'), ('d', 'c')]

# Change the weight of the edge (a, b) to 3.
>>> DG['a']['b']["weight"] += 1
>>> DG['a']['b']["weight"]
3
```

PageRank in Networkx

- NetworkX efficiently implements several graph algorithms.
- The function nx.pagerank() computes the PageRank values of each node iteratively with sparse matrix operations.
- This function returns a dictionary mapping nodes to PageRank values

```
# Calculate the PageRank values of the graph.
>>> nx.pagerank(DG, alpha=0.85)     # alpha is the damping factor (epsilon).
{'a': 0.08767781186947843,
 'b': 0.23613138394239835,
 'c': 0.3661321209576019,
 'd': 0.31005868323052127}
```

Summary

1. Eigenvalue Theory Applications

2. Page Rank Algorithm