Orthogonal Iteration

 A generalization of the power method for computing higher-dimensional invariant subspaces

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Algorithm: Method of Orthogonal Iteration input: \mathbf{A} \in \mathbb{C}^{n \times n}, r \in \{1, \dots, n\}, \mathbf{Q}^{(0)} \in \mathbb{C}^{n \times r} semi-unitary for k = 1, 2, \dots (until a termination criterion is satisfied ) \mathbf{Z}^{(k)} = \mathbf{A}\mathbf{Q}^{(k-1)} Find (thin) QR decomposition of \mathbf{Z}^{(k)}: \mathbf{Q}^{(k)}\mathbf{R}^{(k)} = \mathbf{Z}^{(k)}, \mathbf{Q}^{(k)} \in \mathbb{C}^{n \times r} Find the eigenvalues \lambda_1^{(k)}, \dots, \lambda_r^{(k)} of (\mathbf{Q}^{(k)})^H \mathbf{A} \mathbf{Q}^{(k)} end output: \mathbf{Q}^{(k)}, \lambda_1^{(k)}, \dots, \lambda_r^{(k)}
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- $\mathbf{Q}^{(k)} \dot{\mathbf{e}}_1$ is the vector generated by the power method starting from $\mathbf{v}^{(0)} = \mathbf{Q}^{(0)} \mathbf{e}_1$
- When r = 1, the algorithm reduces to the power method $\mathcal{I}^{(k)}$ is defined by normalizing $\mathcal{I}^{(k)}$

Analysis of Orthogonal Iteration

Recall the Schur decomposition of $\mathbf{A} \in \mathbb{C}^{n \times n}$

$$\mathbf{U}^{H}\mathbf{A}\mathbf{U} = \mathbf{T}, \quad \mathbf{U} = \begin{bmatrix} \mathbf{u}_{1} & \cdots & \mathbf{u}_{n} \end{bmatrix} \text{ unitary, } \mathbf{T} \text{ uppertriangular, } t_{ii} = \lambda_{i}$$

$$\mathbf{Fact}: \text{ Let } \mathbf{U}_{i} = \begin{bmatrix} \mathbf{u}_{1} & \cdots & \mathbf{u}_{i} \end{bmatrix}, i = 1, \dots, n. \text{ Then, } \mathcal{R}(\mathbf{U}_{i}) \text{ is an invariant}$$
subspace for \mathbf{A} and the eigenvalues of $\mathbf{U}_{i}^{H}\mathbf{A}\mathbf{U}_{i}$ are $\lambda_{1}, \dots, \lambda_{i}$

$$\mathbf{U}^{H}\mathbf{A}\mathbf{U} = \mathbf{U}^{T} \iff \mathbf{A}\mathbf{U} = \mathbf{U}^{T} \iff \mathbf{A}\mathbf{U}_{c} = \mathbf{U}^{T}\mathbf{C}$$

$$\mathbf{A}\mathbf{U}_{c} = \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c}$$

$$\mathbf{A}\mathbf{U}_{c} = \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c}$$

$$\mathbf{U}^{T}\mathbf{U}_{c} = \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c}$$

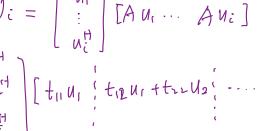
$$\mathbf{U}^{T}\mathbf{U}_{c} = \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c} + \mathbf{U}^{T}\mathbf{U}_{c}$$

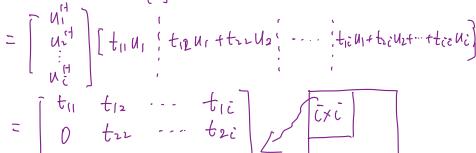
Let
$$g = \alpha_1 u_1 + \cdots + \alpha_i u_i \in \mathbb{R}(U_i)$$

 $Ag = \alpha_1 A u_1 + \cdots + \alpha_i A u_i$
 $= \alpha_1 (t_{ii} u_1) + \cdots + \alpha_i (t_{ii} u_1 + \cdots + t_{ii} u_i)$
 $\in \mathbb{R}(U_i) \subset invariant subspace for A$

Analysis of Orthogonal Iteration (cont'd)

Analysis of Orthogonal Iteration (cont of
$$V_i^{th} \wedge V_i = \begin{bmatrix} u_i^{th} \\ \vdots \\ u_i^{th} \end{bmatrix} [A u_i \cdots A u_i]$$





 $= \begin{bmatrix} t_{11} & t_{12} & \cdots & t_{1\hat{c}} \\ 0 & t_{22} & \cdots & t_{2\hat{c}} \end{bmatrix}$

eigenvalues of Vita Vi: til= Nilisia.

Analysis of Orthogonal Iteration (cont'd)

Suppose the eigenvalues of **A** are ordered as

$$|\lambda_1| \ge \cdots \ge |\lambda_r| > |\lambda_{r+1}| \ge \cdots \ge |\lambda_n|, \quad t_{ii} = \lambda_i$$

Partition **U** and **T** as

$$\begin{aligned} \mathbf{U} &= \begin{bmatrix} \mathbf{U}_r & \mathbf{U}_\beta \end{bmatrix}, \quad \mathbf{U}_r \in \mathbb{C}^{n \times r}, \ \mathbf{U}_\beta \in \mathbb{C}^{n \times (n-r)} \\ \mathbf{T} &= \begin{bmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} \\ \mathbf{0} & \mathbf{T}_{22} \end{bmatrix}, \quad \mathbf{T}_{11} \in \mathbb{C}^{r \times r}, \ \mathbf{T}_{22} \in \mathbb{C}^{(n-r) \times (n-r)} \end{aligned}$$

With $|\lambda_r| > |\lambda_{r+1}|$, $D_r(\mathbf{A}) := \mathcal{R}(\mathbf{U}_r)$ is called the dominant invariant subspace, which is the unique invariant subspace associated with the eigenvalues $\lambda_1, \ldots, \lambda_r$ of **A**

Convergence: With proper assumptions, 1

Orthogonal Iteration (cont'd)

Let $\mathbf{A} \in \mathbb{C}^{n \times n}$ with Schur Decomposition $\mathbf{U}^H \mathbf{A} \mathbf{U} = \mathbf{T}$, where $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_n]$ is unitary and \mathbf{T} is uppertriangular with $t_{ii} = \lambda_i$ s.t.

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|, \quad t_{ii} = \lambda_i$$

Let $\mathbf{Q}^{(k)} = \begin{bmatrix} \mathbf{q}_1^{(k)} & \cdots & \mathbf{q}_n^{(k)} \end{bmatrix}$ be generated by the method of orthogonal iteration with r = n

It can be shown that with a proper $\mathbf{Q}^{(0)}$,

$$\operatorname{dist}(\operatorname{span}\{\mathbf{q}_1^{(k)},\ldots,\mathbf{q}_i^{(k)}\},\operatorname{span}\{\mathbf{u}_1,\ldots,\mathbf{u}_i\})\to 0 \text{ as } k\to\infty, \quad \forall i=1,\ldots,n$$

This implies that $\mathbf{T}^k = (\mathbf{Q}^{(k)})^H \mathbf{A} \mathbf{Q}^{(k)}$ converges to an upper triangular matrix, so that the algorithm leads to a Schur decomposition



Orthogonal Iteration (cont'd)
$$T^{(k)} = \left(Q^{(k)} \right)^{H} A Q^{(k)}$$

Compute \mathbf{T}^k more efficiently via its predecessor $\mathbf{T}^{(k-1)}$

$$\mathbf{T}^{(k-1)} = (\mathbf{Q}^{(k-1)})^{H} \mathbf{A} \mathbf{Q}^{(k-1)} = (\mathbf{Q}^{(k-1)})^{H} \mathbf{Z}^{(k)} = (\mathbf{Q}^{(k-1)})^{H} \mathbf{Q}^{(k)} \mathbf{R}^{(k)}$$

$$\mathbf{T}^{(k)} = (\mathbf{Q}^{(k)})^{H} \mathbf{A} \mathbf{Q}^{(k)} = (\mathbf{Q}^{(k)})^{H} \mathbf{A} \mathbf{Q}^{(k-1)} \cdot (\mathbf{Q}^{(k-1)})^{H} \mathbf{Q}^{(k)}$$

$$= (\mathbf{Q}^{(k)})^{H} \mathbf{Z}^{(k)} \cdot (\mathbf{Q}^{(k-1)})^{H} \mathbf{Q}^{(k)} = \mathbf{R}^{(k)} (\mathbf{Q}^{(k-1)})^{H} \mathbf{Q}^{(k)}$$

This suggests that we may find $\mathbf{T}^{(k)}$ by computing the QR decomposition of $\mathbf{T}^{(k-1)}$ and then multiplying the factors in reverse order

The QR Algorithm/QR Iteration

The above computation of $\mathbf{T}^{(k)}$ motivates the QR algorithm

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Algorithm: QR algorithm input: \mathbf{A} \in \mathbb{C}^{n \times n} \mathbf{A}^{(0)} = \mathbf{A} for k = 1, 2, \dots (until a termination criterion is satisfied) Find QR decomposition of \mathbf{A}^{(k-1)} : \mathbf{Q}^{(k)} \mathbf{R}^{(k)} = \mathbf{A}^{(k-1)} \mathbf{A}^{(k)} = \mathbf{R}^{(k)} \mathbf{Q}^{(k)} end output: \mathbf{A}^{(k)} = \mathbf{A}^{(k)} =
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- $\mathbf{A}^{(k)} \ \forall k$ are similar matrices and thus have the same set of eigenvalues
- If the Schur decomposition of **A** is $\mathbf{A} = \mathbf{U}\mathbf{T}\mathbf{U}^H$, then under some mild assumptions, $\mathbf{A}^{(k)}$ converges to \mathbf{T}
 - The diagonal elements of $\mathbf{A}^{(k)}$ for a sufficiently large k would give all the eigenvalues of \mathbf{A}
- Complexity of each iteration: $O(n^3)$
- Improved algorithms can be found in Sections 7.4 and 7.5 of textbook, including the practical QR algorithm (same main idea)



Matrix Computations Chapter 4: Eigenvalues, Eigenvectors, and Eigendecomposition

Section 4.5 Power method for PageRank

Jie Lu ShanghaiTech University

Case Study: PageRank

An algorithm used by Google to rank the pages of a search result ¹

More important webpages are likely to receive more links from other websites

Determine the importance of each webpage based on the quality and quantity of links pointing to it



Figure: PageRank. Source: Wikipedia

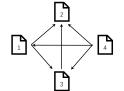
¹K. Bryan and L. Tanya, "The 25,000,000,000 eigenvector: The linear algebra behind Google," SIAM Review, vol. 48, no. 3, pp. 569–581, 2006.

PageRank Model

Let v_i be the importance score of page $i=1,\ldots,n$, \mathcal{L}_i be the set of pages containing a link to page i, and c_j be the number of outgoing links from page j

$$\sum_{j\in\mathcal{L}_i}\frac{v_j}{c_j}=v_i,\quad\forall i=1,\ldots,n$$

Example:



$$\mathcal{L}_1 = \{4\}$$
 $c_1 = 2$ $\mathcal{L}_2 = \{1, 3, 4\}$ $c_2 = 0$ $\mathcal{L}_3 = \{1, 4\}$ $c_3 = 1$ $\mathcal{L}_4 = \emptyset$ $c_4 = 3$

$$\begin{bmatrix} 0 & 0 & 0 & \frac{1}{3} \\ \frac{1}{2} & 0 & 1 & \frac{1}{3} \\ \frac{1}{2} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}$$

Notation and Definitions

Notation: For any $x, y \in \mathbb{R}^n$,

- $\mathbf{x} \ge \mathbf{y}$ means that $x_i \ge y_i$ for all i element wise
- $\mathbf{x} > \mathbf{y}$ means that $x_i > y_i$ for all i
- $x \not\ge y$ means that $x \ge y$ does not hold
- The same notation applies to matrices

Definitions:

- x is said to be non-negative if $x \ge 0$, and non-positive if $-x \ge 0$
- x is said to be positive if x > 0, and negative if -x > 0
- The same definitions apply to matrices
- A square matrix A is said to be column-stochastic if $\textbf{A} \geq \textbf{0}$ and $\textbf{A}^{\mathcal{T}} \textbf{1} = \textbf{1}$
 - Each column \mathbf{a}_i of column-stochastic \mathbf{A} satisfies $\mathbf{a}_i^T \mathbf{1} = \sum_{i=1}^n a_{ji} = 1$

PageRank Problem

A 20

Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a matrix s.t. $a_{ij} = 1/c_j$ if $j \in \mathcal{L}_i$ and $a_{ij} = 0$ if $j \notin \mathcal{L}_i$ **Problem**: Find a non-negative \mathbf{v} s.t. $\mathbf{A}\mathbf{v} = \mathbf{v}$

A is extremely large and sparse, so we choose the power method

Questions:

- Does a solution to $\mathbf{A}\mathbf{v} = \mathbf{v}$ always exist? Or, is $\lambda = 1$ always an eigenvalue of **A**?
- Does Av = v have a non-negative solution? Or, is there a non-negative eigenvector associated with $\lambda = 1$?
- Is the solution to $\mathbf{A}\mathbf{v} = \mathbf{v}$ unique? Or, would there exist more than one eigenvector associated with $\lambda = 1$?
- A unique solution is desired for PageRank

 When the place of N=1 (5)

 Is $\lambda=1$ the only eigenvalue that is the largest in modulus?

 M=1 the only eigenvalue that is the largest in modulus?
 - Required by the power method

PageRank Matrix Properties

Observation: In PageRank, **A** is column-stochastic if all pages have outgoing links

Properties: Let **A** be column-stochastic. Then,

- $\lambda = 1$ is an eigenvalue of **A**
- $|\lambda| \le 1$ for any eigenvalue λ of **A**

Implications: There exists a solution to $\mathbf{A}\mathbf{v} = \mathbf{v}$ and $\lambda = 1$ is an eigenvalue with the largest modulus

Remaining questions: We still don't know

- whether $\mathbf{v} \geq \mathbf{0}$ or not
- whether $\lambda=1$ is the *only* eigenvalue that has the largest modulus (i.e., whether its algebraic multiplicity is 1 and no other distinct eigenvalues have modulus 1)

We resort to non-negative matrix theory to find the answers



Non-Negative Matrix Theory

Theorem (Perron-Frobenius)

Let **A** be a positive square matrix. There exists an eigenvalue ρ of **A** s.t.

- ρ is real and $\rho > 0$
- $|\lambda| < \rho$ for any eigenvalue λ of **A** with $\lambda \neq \rho$
- There exists a positive eigenvector associated with ρ
- The algebraic multiplicity of ρ is 1 (so the geometric multiplicity of ρ is also 1)

Theorem (more general matrix, weaker result)

Let **A** be a non-negative square matrix. There exists an eigenvalue ρ of **A** s.t.

- ρ is real and $\rho \geq 0$
- $|\lambda| \le \rho$ for any eigenvalue λ of **A**
- There exists a non-negative eigenvector associated with ρ

Modified PageRank Model

From the theorem for non-negative matrices, there exists a non-negative solution to $\mathbf{A}\mathbf{v}=\mathbf{v}$, but we don't know whether there exists another solution \mathbf{v}' and whether $\mathbf{v}'\not\geq 0$

For PageRank, we actually consider a modified version of A

$$\tilde{\mathbf{A}} = (1 - \beta)\mathbf{A} + \beta \begin{bmatrix} 1/n & \dots & 1/n \\ \vdots & & \vdots \\ 1/n & \dots & 1/n \end{bmatrix}$$

and column stockestic

where $0<\beta<1$ (typical value is $\beta=0.15$), so that $\tilde{\bf A}$ is positive From the Perron-Frobenius Theorem,

- $\lambda = 1$ is the only eigenvalue that has the largest modulus
- There exists only one eigenvector associated with $\lambda=1$, either positive or negative with the state of the
- Therefore, the power method can work

Matrix Computations Chapter 4: Eigenvalues, Eigenvectors, and Eigendecomposition

Section 4.6 More on Variational Characterizations of Eigenvalues

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Courant-Fischer Min-Max Theorem (Revisit)

For $\mathbf{A} \in \mathbb{H}^{n \times n}$, let $\lambda_k(\mathbf{A})$ denote the kth largest eigenvalue of \mathbf{A} , i.e.,

$$\lambda_{\min}(\mathbf{A}) := \lambda_n(\mathbf{A}) \le \cdots \le \lambda_1(\mathbf{A}) =: \lambda_{\max}(\mathbf{A})$$

For simplicity, we may also write $\lambda_{\min} := \lambda_n \leq \cdots \leq \lambda_1 =: \lambda_{\max}$

Theorem

For any $\mathbf{A} \in \mathbb{H}^{n \times n}$ and k = 1, ..., n,

$$\lambda_{k}(\mathbf{A}) = \max_{\substack{S \subseteq \mathbb{C}^{n}: \\ \dim(S) = k}} \min_{\substack{\mathbf{y} \in S, \\ \mathbf{y} \neq \mathbf{0}}} \frac{\mathbf{y}^{H} \mathbf{A} \mathbf{y}}{\mathbf{y}^{H} \mathbf{y}}$$
$$= \min_{\substack{S \subseteq \mathbb{C}^{n}: \\ \dim(S) = n - k + 1}} \max_{\substack{\mathbf{y} \in S, \\ \mathbf{y} \neq \mathbf{0}}} \frac{\mathbf{y}^{H} \mathbf{A} \mathbf{y}}{\mathbf{y}^{H} \mathbf{y}}$$

 $R_{\mathbf{A}}(\mathbf{y}) = \frac{\mathbf{y}^H \mathbf{A} \mathbf{y}}{\mathbf{y}^H \mathbf{y}}$, $\mathbf{y} \neq \mathbf{0}$ is the Rayleigh-Ritz quotient, or Rayleigh quotient

This section focuses on variational characterizations of eigenvalues of real symmetric matrices (\mathbb{S}^n)



Rayleigh-Ritz Theorem

A special case of Courant-Fischer Min-Max Theorem (let k= | and k=1) Theorem (Rayleigh-Ritz)

For any $\mathbf{A} \in \mathbb{S}^n$,

$$\lambda_{\min} \| \boldsymbol{x} \|_2^2 \leq \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \leq \lambda_{\max} \| \boldsymbol{x} \|_2^2$$

where the equalities can be attained when x is an eigenvector associated with λ_{\min} and λ_{\max} , respectively

• Even without Courant-Fischer Min-Max Theorem, we may prove this using eigendecomposition $\mathbf{A} = \mathbf{V} \Lambda \mathbf{V}^T$, \mathbf{V} real orthogonal

$$x^{T}A = x^{T} \sqrt{\Lambda \sqrt{X}} = (\sqrt{X})^{T} \Lambda (\sqrt{X}) = y^{T} \Lambda y$$

$$= \sum_{i=1}^{n} \lambda_{i} y_{i}^{2} \leq \lambda_{max} \|y\|_{L^{\infty}} = \lambda_{max} \|\sqrt{X}\|_{L^{\infty}}^{2} \leq \lambda_{max} \|x\|_{L^{\infty}}^{2}$$
Let $x = \sqrt{1}, \sqrt{2} \lambda_{max} = x^{T}Ax = \sqrt{1} Ax = \lambda_{max} \|x\|_{L^{\infty}}^{2}$

More Results from Courant-Fischer

Let $\mathbf{A}, \mathbf{B} \in \mathbb{S}^n$, $\mathbf{z} \in \mathbb{R}^n$

• (Weyl)
$$\lambda_k(\mathbf{A}) + \lambda_n(\mathbf{B}) \le \lambda_k(\mathbf{A} + \mathbf{B}) \le \lambda_k(\mathbf{A}) + \lambda_1(\mathbf{B}), k = 1, \dots, n$$

$$= \min_{\substack{C \subseteq |R| \\ \text{obs}(S) = n-k+1}} \max_{\substack{X \in S \\ |K||_{2}=1}} \chi^{7}A\chi + \min_{\substack{S \subseteq |R| \\ \text{obs}(S) = n-k+1}} \mathcal{N}_{1}CB)$$



More Results from Courant-Fischer (cont'd)

Let
$$\mathbf{A}, \mathbf{B} \in \mathbb{S}^n$$
, $\mathbf{z} \in \mathbb{R}^n$

• (Interlacing) $\lambda_{k+1}(\mathbf{A}) \leq \lambda_k(\mathbf{A} \pm \mathbf{z}\mathbf{z}^T) \leq \lambda_{k-1}(\mathbf{A})$ for proper k

($\mathbf{A} + \mathbf{z} \mathbf{z}^T$) = $\mathcal{M}(\mathbf{A})$
 \mathcal

1/2 (A+ZZT) = min max xES dn(s)=n-kf1 11x/12=1

max > min SEIR XESA Span {Z} (XTAX ± XZZTX) din(s)=n-kfl

Note that dim (S 1) span { 2} \(\) = dm (S) + dlm(span { 2}\) - dm (S+ spen {= 31) zn-k

It follows that nr (A = 22T) = min red dim(S)=r wax r xxx 11/1/2=1 retn-k, n] r= n- k 1 m) /k (A) (=) (=) (=)