Approximation of eigenvalues

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Some definitions

- Given vector $\mathbf{v} \in \mathbb{C}^n$, with components $v_j = a_j + ib_j$, where a_j and $b_j \in \mathbb{R}$ for all $j = 1, \ldots, n$:
  - $\overline{\mathbf{v}}$ is the complex conjugate of $\mathbf{v}$, with components $\overline{v}_j = a_j - ib_j$ for all $j = 1, \ldots, n$
  - $\mathbf{v}^H := (\overline{\mathbf{v}})^T$ is the transpose complex conjugate vector of $\mathbf{v}$.

- The matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ is Hermitian if $\mathbf{A}^H = \mathbf{A}$ (i.e., $\overline{\mathbf{A}}^T = \mathbf{A}$).

Eigenvalues and Eigenvectors

Definition (7.3)

Let $\mathrm{A} \in \mathbb{C}^{n \times n}$, the eigenvalue problem consists in finding a scalar λ (real or complex) and a non-zero vector $\mathbf{x} \in \mathbb{C}^n$ such that

$$\mathrm{A}\mathbf{x} = \lambda \mathbf{x} \tag{1}$$

λ is called an eigenvalue of A, while $\mathbf{x}$ is the associated eigenvector. The latter is not unique; indeed $\alpha\mathbf{x}$ with $\alpha \neq 0$, are also eigenvectors associated with λ.
The eigenvalues of A are the roots of the characteristic polynomial of A:

$$p_{\mathrm{A}}(\lambda) = \det(\mathrm{A} - \lambda \mathrm{I}).$$

An $n \times n$ matrix has exactly n eigenvalues (real or complex), not necessarily distinct.

Generalized eigenvalue problem

Definition (7.4)

Given a matrix $A \in \mathbf{C}^{n\times n}$ and a nonsingular matrix $B \in \mathbf{C}^{n\times n}$, the generalized eigenvalue problem reads: find $\lambda \in \mathbf{C}$ and $\mathbf{x} \in C^n$ such that $A\mathbf{x} = \lambda B\mathbf{x}$, where λ is a generalized eigenvalue and $\mathbf{x}$ the corresponding eigenvector. The characteristic polynomial of the matrix A with respect to B is

$$p_{A,B}(\lambda) = \det(A - \lambda B),$$

the n eigenvalues $\{\lambda_i(A, B)\}_{i=1}^n$ of A with respect to B are the zeros of $p_{\mathbf{A},\mathbf{B}}(\lambda)$.

Eigenvalues and Eigenvectors

Definition (7.5)

Given $\mathrm{A} \in \mathbb{C}^{n \times n}$ and eigenvector $\mathbf{x}_i \in \mathbb{C}^n$, λ_i can be recovered by using the Rayleigh quotient

$$\lambda_i = \mathbf{x}_i{}^H \mathrm{A} \mathbf{x}_i / \|\mathbf{x}_i\|^2, \text{ for } \mathbf{x_i} \neq 0.$$

If λ_i is known, the corresponding eigenvector x_i can be computed by solving:

$$(A - \lambda_i I) x_i = 0.$$

Eigenvalues and Eigenvectors

- A matrix A$\in \mathbb{C}^{n\times n}$ is said to be diagonalizable if there exists a nonsingular matrix U$\in \mathbb{C}^{n\times n}$ such that $\mathrm{U}^{-1}\mathrm{AU} = \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$.
  - A has n linearly independent eigenvectors
- Real symmetric matrices, $A = A^T$,
  - have real eigenvalues
  - are diagonalizable by orthogonal matrices and eigenvectors can be chosen to be orthogonal
- Generally, matrices are diagonalizable by unitary matrices if and only if they are normal ($A^H A = AA^H$).

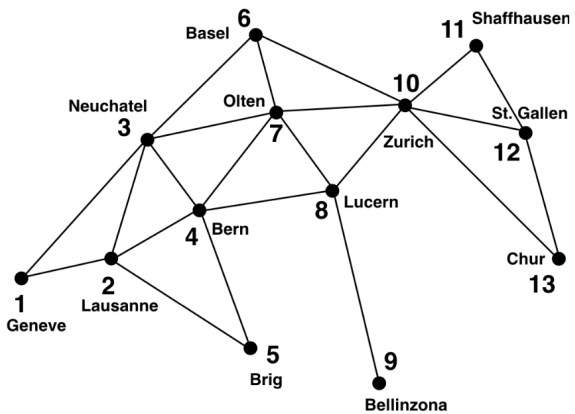
Example

Example (Rail connectivity of some cities in Switzerland)

- Form $A \in \mathbb{R}^{n \times n}$ the connectivity matrix
- $A_{ij} = 1$ if cities i and j connected, 0 otherwise
- Compute largest eigenvalue λ_1 and associated eigenvector x_1, obtain

$$\mathbf{x}_1 = \begin{pmatrix} 0.16 & 0.28 & 0.39 & 0.39 & 0.17 & 0.29 & 0.43 & 0.31 & 0.078 & 0.36 \\ 0.13 & 0.15 & 0.13 \end{pmatrix}^T$$

- Bellinzona ($x_{1,9}$) is the least connected, Olten ($x_{1,7}$) is the most connected



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Definitions and examples

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Power method

Let $A \in \mathbb{C}^{n \times n}$, assume that its eigenvalues are ordered,

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \ldots \geq |\lambda_n|. \tag{2}$$

and eigenvectors are linearly independent, that is $det([\mathbf{x}_1, \ldots, \mathbf{x}_n]) \neq 0$.

The power method approximates the largest eigenvalue of A and corresponding eigenvector.
Let $\mathbf{x}^{(0)} \in \mathbb{C}^n$ be given s.t. $\|\mathbf{x}^{(0)}\| \neq 0$, and set $\mathbf{y}^{(0)} = \mathbf{x}^{(0)}/\|\mathbf{x}^{(0)}\|$, for $k = 1, 2, \ldots$ compute

$$\mathbf{x}^{(k)} = A\mathbf{y}^{(k-1)}, \quad \mathbf{y}^{(k)} = \frac{\mathbf{x}^{(k)}}{\|\mathbf{x}^{(k)}\|}, \quad \lambda^{(k)} = (\mathbf{y}^{(k)})^H A\mathbf{y}^{(k)}$$

Until $\frac{|\lambda^{(k)} - \lambda^{(k-1)}|}{|\lambda^{(k)}|} < tol$, where tol is the desired tolerance.

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$$\mathbf{x}^{(k)} = \mathrm{A}\mathbf{y}^{(k-1)}, \quad \mathbf{y}^{(k)} = \frac{\mathbf{x}^{(k)}}{\|\mathbf{x}^{(k)}\|}, \quad \lambda^{(k)} = (\mathbf{y}^{(k)})^H \mathrm{A}\mathbf{y}^{(k)}$$

Until $\frac{|\lambda^{(k)} - \lambda^{(k-1)}|}{|\lambda^{(k)}|} < tol$, where tol is the desired tolerance.

The power method: algorithm

Algorithm 7.1: Power Method

1: Set $\mathbf{x}^{(0)} \in \mathbb{C}^n$, with $\|\mathbf{x}^{(0)}\| \neq \mathbf{0}$;
2: $\mathbf{y}^{(0)} = \frac{\mathbf{x}^{(0)}}{\|\mathbf{x}^{(0)}\|}$;
3: **for** $k = 1, 2, \ldots,$ until a stopping criterion is satisfied **do**
4: $\quad \mathbf{x}^{(k)} = \mathbf{A}\mathbf{y}^{(k-1)}$;
5: $\quad \mathbf{y}^{(k)} = \frac{\mathbf{x}^{(k)}}{\|\mathbf{x}^{(k)}\|}$;
6: $\quad \lambda^{(k)} = (\mathbf{y}^{(k)})^H \mathbf{A}\mathbf{y}^{(k)}$;
7: **end for**

Convergence

Since we have assumed that the eigenvectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of A are linearly independent, these eigenvectors form a basis for $\mathbb{C}^n$. Thus the vectors $\mathbf{x}^{(0)}$ and $\mathbf{y}^{(0)}$ can be written as

$$\mathbf{x}^{(0)} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i, \quad \mathbf{y}^{(0)} = \beta^{(0)} \sum_{i=1}^{n} \alpha_i \mathbf{x}_i, \quad \text{with } \beta^{(0)} = 1/\|\mathbf{x}^{(0)}\| \text{ and } \alpha_i \in \mathbb{C}.$$

At the first step the power method gives

$$\mathbf{x}^{(1)} = \mathrm{A}\mathbf{y}^{(0)} = \beta^{(0)} \mathrm{A} \sum_{i=1}^{n} \alpha_i \mathbf{x}_i = \beta^{(0)} \sum_{i=1}^{n} \alpha_i \lambda_i \mathbf{x}_i \qquad \text{and, similarly,}$$

$$\mathbf{y}^{(1)} = \beta^{(1)} \textstyle\sum_{i=1}^{n} \alpha_i \lambda_i \mathbf{x}_i, \qquad \beta^{(1)} = \frac{1}{\|\mathbf{x}^{(0)}\| \ \|\mathbf{x}^{(1)}\|}.$$

At a given step k we will have

$$\mathbf{y}^{(k)} = \beta^{(k)} \textstyle\sum_{i=1}^{n} \alpha_i \lambda_i^k \mathbf{x}_i, \qquad \beta^{(k)} = \frac{1}{\|\mathbf{x}^{(0)}\| \cdots \|\mathbf{x}^{(k)}\|}$$

Convergence

And therefore

$$\mathbf{y}^{(k)} = \lambda_1^k \beta^{(k)} \left(\alpha_1 \mathbf{x}_1 + \sum_{i=2}^{n} \alpha_i \frac{\lambda_i^k}{\lambda_1^k} \mathbf{x}_i \right).$$

Since $|\lambda_i/\lambda_1| < 1$ for $i = 2, \ldots, n$, the vector $\mathbf{y}^{(k)}$ tends to align along the same direction as the eigenvector $\mathbf{x}_1$ when k tends to $+\infty$, provided $\alpha_1 \neq 0$, that is:

$$\lim_{k \to +\infty} \frac{\lambda_i^k}{\lambda_1^k} = 0, \quad \text{since } |\lambda_1| > |\lambda_i| \text{ for all } i = 2, \ldots, n,$$

Convergence: absolute error

The error obtained by the power method (when applicable) reads:

$$e^{(k)} = \frac{\lambda_1 - \lambda^{(k)}}{\lambda_1} \sim \left(\frac{\lambda_2}{\lambda_1}\right)^k \quad \text{for } k \text{ "sufficiently" large.}$$

If the matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$ is Hermitian, i.e., if $\mathbf{A}^H = \mathbf{A}$, then we have:

$$e^{(k)} = \frac{\lambda_1 - \lambda^{(k)}}{\lambda_1} \sim \left(\frac{\lambda_2}{\lambda_1}\right)^{2k} \quad \text{for } k \text{ "sufficiently" large.}$$

Convergence: example

Example

Consider the family of matrices

$$\mathrm{A}(\alpha) = \begin{bmatrix} \alpha & 2 & 3 & 13 \\ 5 & 11 & 10 & 8 \\ 9 & 7 & 6 & 12 \\ 4 & 14 & 15 & 1 \end{bmatrix}, \qquad \alpha \in \mathbb{R}. \tag{3}$$

We want to approximate the eigenvalue with largest modulus by the power method. When $\alpha = 30$, the eigenvalues of the matrix are given by $\lambda_1 = 39.396$, $\lambda_2 = 17.8208$, $\lambda_3 = -9.5022$ and $\lambda_4 = 0.2854$.
The method approximates λ_1 in 22 iterations with a tolerance $tol = 10^{-10}$ and $\mathbf{x}^{(0)} = \mathbf{1}^T$.

If $\alpha = -30$ the iterations are 708. The reasone is that $|\lambda_2|/|\lambda_1| = 0.9704$ is close to unity: $\lambda_1 = -30.643$, $\lambda_2 = 29.7359$, $\lambda_3 = -11.6806$ and $\lambda_4 = 0.5878$.

Plan

How to approximate the smallest eigenvalue ?

If A is nonsingular, then

$$\lambda_i(A^{-1}) = \frac{1}{\lambda_{n+1-i}(A)} \text{ for } i = 1, \ldots, n.$$

- Power method can be used to approximate the largest eigenvalue of A^{-1}; then, obtain the smallest eigenvalue of A as

$$\lambda_n(A) = \frac{1}{\lambda_1(A^{-1})}.$$

- But too expensive to compute A^{-1}

Inverse power method

The inverse power method can be used to find the smallest eigenvalue of a non-singular matrix A.

Suppose nonsingular matrix $A \in \mathbb{C}^{n\times n}$ admits n linearly independent eigenvectors, and its eigenvalue λ_n of minimum modulus is distinct from the others,

$$|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_{n-1}| > |\lambda_n|. \tag{4}$$

Inverse power method

Let $\mathbf{x}^{(0)} \in \mathbb{C}^n$ be given and set $\mathbf{y}^{(0)} = \mathbf{x}^{(0)}/\|\mathbf{x}^{(0)}\|$, for $k = 1, 2, \ldots$ compute

$$\mathbf{x}^{(k)} = \mathrm{A}^{-1}\mathbf{y}^{(k-1)}, \quad \mathbf{y}^{(k)} = \frac{\mathbf{x}^{(k)}}{\|\mathbf{x}^{(k)}\|}, \quad \mu^{(k)} = (\mathbf{y}^{(k)})^H \mathrm{A}^{-1}\mathbf{y}^{(k)}$$

Until $\frac{|\mu^{(k)} - \mu^{(k-1)}|}{|\mu^{(k)}|} < tol$, where tol is the desired tolerance.

Suppose A admits n linearly independent eigenvectors, and the smallest eigenvalue λ_n is distinct from the others, then

$$\lim_{k \to \infty} \mu^{(k)} = \frac{1}{\lambda_n}.$$

At each step k we have to solve a linear system of the form $\mathrm{A}\mathbf{x}^{(k)} = \mathbf{y}^{(k-1)}$.

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Inverse power method: algorithm

Algorithm 7.2: Inverse Power Method

1: Set $\mathbf{x}^{(0)} \in \mathbb{C}^n$, with $\|\mathbf{x}^{(0)}\| \neq \mathbf{0}$;
2: $\mathbf{y}^{(0)} = \frac{\mathbf{x}^{(0)}}{\|\mathbf{x}^{(0)}\|}$;
3: **for** $k = 1, 2, \ldots,$ until a stopping criterion is satisfied **do**
4: Solve $A\mathbf{x}^{(k)} = \mathbf{y}^{(k-1)}$;
5: $\mathbf{y}^{(k)} = \frac{\mathbf{x}^{(k)}}{\|\mathbf{x}^{(k)}\|}$;
6: $\mu^{(k)} = (\mathbf{y}^{(k)})^H \mathbf{A}^{-1} \mathbf{y}^{(k)}$;
7: **end for**
8: $\lambda = \frac{1}{\mu^{(k)}}$

Remark: Convenient to compute the LU factorization of A to solve the linear systems.

Inverse power method: algorithm

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8: $\lambda = \frac{1}{\mu^{(k)}}$

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Plan

Power method with shift

Power method with shift can find the eigenvalue of A, $\lambda_s(A)$, near a given number s:

- Define $A_s = A - sI$, whose eigenvalues are

$$\lambda_j(\mathrm{A}_s) = \lambda_i(\mathrm{A}) - s, \text{ for some } i, j = 1, \ldots, n$$

- In order to approximate $\lambda_s(A)$, use first inverse power method to approximate the smallest eigenvalue of A_s
  Let $\mathbf{x}^{(0)} \in \mathbb{C}^n$ be given and set $\mathbf{y}^{(0)} = \mathbf{x}^{(0)}/\|\mathbf{x}^{(0)}\|$, for $k = 1, 2, \ldots$ compute

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  Until $|\lambda_s^{(k)} - \lambda_s^{(k-1)}| < tol|\lambda_s^{(k)}|$, where tol is the desired tolerance.
- The searched eigenvalue of A is approximated by $\lambda_s(A) = \lambda_{min}(A_s) + s$.

Power method with shift

Power method with shift can find the eigenvalue of A, $\lambda_s(A)$, near a given number s:

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- The searched eigenvalue of A is approximated by $\lambda_s(A) = \lambda_{min}(A_s) + s$.

Example

For the matrix A(30) of (3) we seek the eigenvalue closest to the value 17. We set $s = 17$ and apply the power method with shift with a tolerance $tol = 10^{-10}$ and initial guess $x^{(0)} = (1, 1, 1, 1)^T$. After 8 iterations the algorithm returns the value $\lambda = 17.82079703055703$. A less accurate knowledge of the *shift* would involve more iterations. For instance, if we set $s = 13$ the program returns the value $\lambda = 17.82079703064106$ after 19 iterations.

The value of the shift can be modified during the iterations, by setting $s = \lambda^{(k)}$. This yields a faster convergence; however the computational cost grows substantially since now at each iteration the matrix A_s does change and the LU factorization has to be performed at each iteration.

How to compute the shift

We need to locate (more or less accurately) the eigenvalues of A in the complex plane.

Let A be a square matrix of dimension n. The Gershgorin circles $C_i^{(r)}$ and $C_i^{(c)}$ associated with its i-th row and i-th column are respectively defined as

$$C_i^{(r)} = \{z \in \mathbb{C} : \ |z - a_{ii}| \leq \sum_{j=1, j\neq i}^{n} |a_{ij}|\},$$

$$C_i^{(c)} = \{z \in \mathbb{C} : \ |z - a_{ii}| \leq \sum_{j=1, j\neq i}^{n} |a_{ji}|\}.$$

$C_i^{(r)}$ is called the i-th row circle and $C_i^{(c)}$ the i-th column circle.

All the eigenvalues of a given matrix $A \in \mathbb{C}^{n \times n}$ belong to the region of the complex plane which is the intersection of the two regions formed respectively by the union of the row circles and column circles.

Moreover, should m row circles (or column circles), with $1 \leq m \leq n$, be disconnected from the union of the remaining $n - m$ circles, then their union contains exactly m eigenvalues.

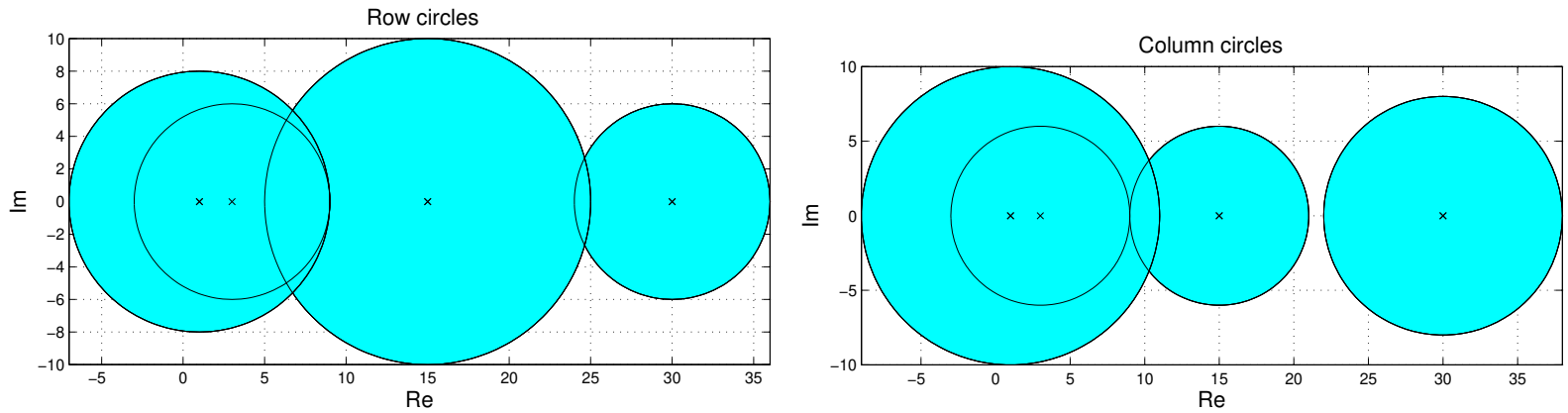
There is no guarantee that a circle should contain eigenvalues, unless it is isolated from the others. The information provided by Ghersghorin circles are in general quite coarse, thus the previous result can provide only a preliminary guess of the shift.

Example

Below we have plotted the Gershgorin circles associated with the matrix

$$\mathrm{A} = \begin{bmatrix} 30 & 1 & 2 & 3 \\ 4 & 15 & -4 & -2 \\ -1 & 0 & 3 & 5 \\ -3 & 5 & 0 & -1 \end{bmatrix}.$$

The centers of the circles have been identified by a cross.



Row circles (*left*) and column circles (*right*) for the matrix of Example