Numerical Analysis
Calculation of eigenvalues

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Motivations

It is well known that the eigenvalues of the matrix A are the solutions of the **characteristic equation**:

$$\boxed{\det(A - \lambda I) = 0}$$

However, in practice this can be hardly performed.

Numerical approximations are needed!

The simplest localization result is:

$$\boxed{\rho(A) \leq ||A||}$$

with arbitrary induced matrix norm.

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Bounds for the eigenvalues by Gershgorin circles

Let $A = [a_{kj}] \in \mathbf{M}_{N \times N}$ be a square matrix (with possibly complex entries).

Define the numbers $r_k := \sum_{j \neq k} |a_{kj}|$ $(k = 1, 2, ..., N)$, and denote by B_k the closed disk of the complex plane centered at a_{kk} with radius r_k (**Gershgorin disks**).

Gershgorin's theorem

All the eigenvalues of the matrix A are located in the union of the Gershgorin disks.

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Normal matrices

The square matrix $A \in \mathbf{M}_{N\times N}$ is said to be a **normal matrix**, if $AA^* = A^*A$.

Obviously, every self-adjoint matrix is normal.

If $A \in \mathbf{M}_{N\times N}$ is a normal matrix, then A has a system of eigenvectors which form an **orthonormal system** (i.e. the Euclidean norm of any eigenvector is 1, and the different eigenvectors are orthogonal).

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The power iteration

Let $A \in \mathbf{M}_{N \times N}$ be a normal matrix with the eigenvalues: $|\lambda_1| \leq |\lambda_2| \leq ... \leq |\lambda_{N-1}| < |\lambda_N|$, and denote by $s_1, s_2, ..., s_N$ the orthonormal eigenvectors.

The power iteration

Let $x_0 \in \mathbf{R}^N$ be a vector such that $\langle x_0, s_N \rangle \neq 0$, and define:

$$\boxed{x_{n+1} := Ax_n} \qquad (n = 0, 1, 2, ...)$$

Then the sequence of **Rayleigh quotients** $\frac{\langle Ax_n, x_n \rangle}{||x_n||^2} = \frac{\langle x_{n+1}, x_n \rangle}{||x_n||^2}$ converges to λ_N. For the speed of convergence, we have the following estimation:

$$\left| \frac{\langle Ax_n, x_n \rangle}{||x_n||^2} - \lambda_N \right| \leq const. \cdot \left| \frac{\lambda_{N-1}}{\lambda_N} \right|^{2n}$$

The inverse iteration

Let $A \in \mathbf{M}_{N\times N}$ be a normal, regular matrix with the eigenvalues: $0 < |\lambda_1| < |\lambda_2| \le \lambda_3| \le \ldots \le |\lambda_N|$, and denote by $s_1, s_2, \ldots, s_N$ the corresponding othonormal eigenvectors.

The inverse iteration

Apply the power iteration to the matrix A^{-1} (its eigenvalues are $\frac{1}{\lambda_1}$, ..., $\frac{1}{\lambda_N}$).

Let $x_0 \in \mathbf{R}^N$ be a vector such that $\langle x_0, s_1\rangle \ne 0$, and define:

$$\boxed{x_{n+1} := A^{-1}x_n} \qquad (n = 0, 1, 2, \ldots)$$

Then the sequence of the **Rayleigh quotients** $\frac{\langle A^{-1}x_n, x_n\rangle}{||x_n||^2} = \frac{\langle x_{n+1}, x_n\rangle}{||x_n||^2}$ converges to $\frac{1}{\lambda_1}$.

It is worth calculating the vector x_{n+1} by solving the equation $Ax_{n+1} = x_n$ and applying an LU decomposition.

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Shifted inverse power method

Let $A \in \mathbf{M}_{N\times N}$ be a normal matrix with eigenvalues: $\lambda_1, \lambda_2, ...\lambda_N$, and denote by $s_1, s_2, ..., s_N$ the corresponding orthonormal eigenvectors.

Assume that λ_k is a single eigenvalue, and λ_0 is a sufficiently good approximation of λ_k, such that the nearest eigenvalue to λ_0 is λ_k, i.e. for every $j \neq k$, the inequality $|\lambda_j - \lambda_0| > |\lambda_k - \lambda_0|$ holds.

Then the number $\lambda_k - \lambda_0$ is an eigenvalue of the matrix $(A - \lambda_0 I)$ with minimal absolute value, so that the inverse iteration is applicable.

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Shifted inverse iteration

Let $x_0 \in \mathbf{R}^N$ be a vector such that $\langle x_0, s_k \rangle \neq 0$, and define:

$$\boxed{x_{n+1} := (A - \lambda_0 I)^{-1} x_n} \qquad (n = 0, 1, 2, \ldots)$$

Then the sequence of **Rayleigh quotients** $\frac{\langle x_{n+1}, x_n \rangle}{||x_n||^2}$ converges to $\frac{1}{\lambda_k - \lambda_0}$.

Determination of all eigenvalues

Jacobi's method: Let $A \in \mathbf{M}_{N\times N}$ be a self-adjoint matrix. Denote by $A_0 := A$. Define the pair of indices (p,q) $(p<q)$, for which $|A_{pq}|$ is maximal above the main diagonal. Define

$$\cot 2t := \frac{A_{qq}-A_{pp}}{2A_{pq}},$$

and define the (orthogonal) matrix Q_n as follows:

$$Q_n := \begin{pmatrix} 1 &&&&&&&& \\ & 1 &&&&&&& \\ && \cos t & \dots & \dots & \dots & \sin t && \\ && \dots & 1 &&& \dots && \\ && \dots && \dots && \dots && \\ && \dots &&& 1 & \dots && \\ && -\sin t & \dots & \dots & \dots & \cos t && \\ &&&&&&& 1 & \\ &&&&&&&& 1 \end{pmatrix}$$

Determination of all eigenvalues

Method of Jacobi

Define the matrix sequence recursively:

$$\boxed{A_{n+1} := Q_n^* A_n Q_n}$$

If the eigenvalues of A are distinct, then the sequence of matrices (A_n) elementwise converges to a diagonal matrix, the diagonal entries of which are the eigenvalues of the matrix A.

Determination of all eigenvalues

Let $A \in \mathbf{M}_{N\times N}$ be a self-adjoint positive definite matrix.

Method based of the Cholesky decomposition

Denote by $A_0 := A$, and for $n = 0, 1, 2, ...$ define

$$\boxed{A_{n+1} := L_n^* L_n,}$$

where $L_n L_n^*$ is the Cholesky decomposition of A_n. Then the sequence of matrices (A_n) elementwise converges to a diagonal matrix, the diagonal entries of which are the eigenvalues of the matrix A.

Determination of all eigenvalues

Let $A \in \mathbf{M}_{N\times N}$ be a self-adjoint positive definite matrix.

Method based of the QR decomposition

Denote by $A_0 := A$, and for $n = 0, 1, 2, \ldots$ define

$$\boxed{A_{n+1} := R_n Q_n,}$$

where $Q_n R_n$ is the QR decomposition of A_n. Then the sequence of matrices (A_n) elementwise converges to a diagonal matrix, the diagonal entries of which are the eigenvalues of the matrix A.