Numerical Calculus

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References

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Symmetries (Meyer, 2000)

Let $A = (a_{ij}) \in \mathcal{M}_n(\mathbb{C})$ be a square matrix. The *conjugate transpose* (or *adjoint*) A^* is defined by $a^*_{ij} = \overline{a}_{ji}$. Moreover, it is

- *symmetric* matrix: $A = A^t \, (a_{ij} = a_{ji})$
- *skew-symmetric* matrix: $A = -A^t \, (a_{ij} = -a_{ji})$
- *hermitian* matrix: $A = A^* \, (a_{ij} = \overline{a}_{ji})$
- *skew-hermitian* matrix: $A = -A^* \, (a_{ij} = -\overline{a}_{ji})$
- *orthogonal* matrix: $A^t A = AA^t = I_n \, (A^{-1} = A^t)$
- *unitary* matrix: $A^* A = AA^* = I_n \, (A^{-1} = A^*)$

Diagonally Dominant Matrices (Burden *et al.*,2022)

A matrix $A \in \mathcal{M}_n(\mathbb{C})$ is said to be *diagonally dominant* when

$$|a_{ii}| \geqslant \sum_{j=1, j \neq i}^{n} |a_{ij}|, \quad i = 1, \ldots, n.$$

A diagonally dominant matrix is said to be *strictly diagonally dominant* when

$$|a_{ii}| > \sum_{j=1, j \neq i}^{n} |a_{ij}|, \quad i = 1, \ldots, n.$$

A strictly diagonally dominant matrix is nonsingular.

Positive Definite Matrices (Burden *et al.*, 2022)

A matrix A is *positive definite* if

$$\boldsymbol{x}^t A \boldsymbol{x} > 0, \quad \forall\, \boldsymbol{x} \in \mathbb{R}^n,\ \boldsymbol{x} \neq \mathbf{0}_{\mathbb{R}^n} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

If A is positive definite matrix then

a) A has an inverse

b) $a_{ii} > 0, \quad i = 1, \ldots, n$

c) $\max\limits_{1 \leqslant k,j \leqslant n} |a_{kj}| \leqslant \max\limits_{1 \leqslant i \leqslant n} |a_{ii}|$

d) $(a_{ij})^2 \leqslant a_{ii} a_{jj}, \quad i \neq j$

Leading principal submatrix (Burden *et al.*, 2022)

A *leading principal submatrix* of a matrix A is a matrix of the form

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1k} \\ a_{21} & a_{22} & \dots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \dots & a_{kk} \end{bmatrix}$$

for some $1 \leqslant k \leqslant n$.

A symmetric matrix A is positive definite if and only if each of its leading principal submatrices has a positive determinant.

Band Matrices (Burden *et al.*,2022)

A matrix $A \in \mathcal{M}_n(\mathbb{R})$ is called *band matrix* if integers p and q with $1 < p, q < n$ exist with the property that $a_{ij} = 0$ whenever $p \leqslant j - i$ or $q \leqslant i - j$.
The *band width* of a band matrix is defined as $l = p + q - 1$.

Lower bidiagonal: $p = 1, q = 0$

Upper bidiagonal: $p = 0, q = 1$

Tridiagonal matrices: $p = q = 2$

Pentadiagonal matrices: $p = q = 4$

Lower Hessenberg matrices: $p = n - 1, q = 1$

Upper Hessenberg matrices: $p = 1, q = n - 1$

Permutation Matrices (Burden *et al.*, 2022)

An $n \times n$ *permutation matrix* $P = (p_{ij})$ is a matrix obtained by rearranging the rows of the identity matrix I_n. This gives a matrix with precisely one nonzero entry in each row and in each column, and each nonzero entry is a 1.

$$P = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

PA permutes the rows of A; AP permutes the columns of A.
$det(P) = \pm 1$, $P^t P = PP^t = I_n$, $P^{-1} = P^t$
P_1, P_2 permutation matrices $\Rightarrow P_1 P_2$ permutation matrix

The algebra of triangular matrices (Golub and Van Loan; 2013)

A *unit* triangular matrix is a triangular matrix with 1's on the diagonal.

- The inverse of an upper (lower) triangular matrix is upper (lower) triangular.
- The product of two upper (lower) triangular matrices is upper (lower) triangular.
- The inverse of a unit upper (lower) triangular matrix is unit upper (lower) triangular.
- The product of two unit upper (lower) triangular matrices is unit upper (lower) triangular.

Cauchy matrices. Hilbert matrices (Demmel, 1997)

Cauchy matrix $C = (c_{ij})$ have entries

$$c_{ij} = \frac{\alpha_i - \beta_j}{\xi_i - \eta_j}$$

where $\alpha = [\alpha_1, \ldots, \alpha_n]$, $\beta = [\beta_1, \ldots, \beta_n]$, $\xi = [\xi_1, \ldots, \xi_n]$ and $\eta = [\eta_1, \ldots, \eta_n]$ are given vectors. The best-known example is notorious ill-conditioned *Hilbert matrix* $H = (h_{ij})$ with

$$h_{ij} = \frac{1}{i + j - 1}.$$

Eigenvalues and eigenvectors (Quarteroni *et al.*, 2000)

Let $A \in \mathcal{M}_n(\mathbb{R})$ or$A \in \mathcal{M}_n(\mathbb{C})$; the number $\lambda \in \mathbb{C}^*$ is an *eigenvalue* of A if there exists a nonnull vector $\boldsymbol{x} \in \mathbb{C}^n$, called *eigenvector*, s.t.

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

The set of the eigenvalues of A is called the *spectrum* of A, denoted by

$$\sigma(A) = \{\lambda \big| \lambda \text{ is eigenvalue of } A\}.$$

The number λ is the solution of the *characteristic equation*

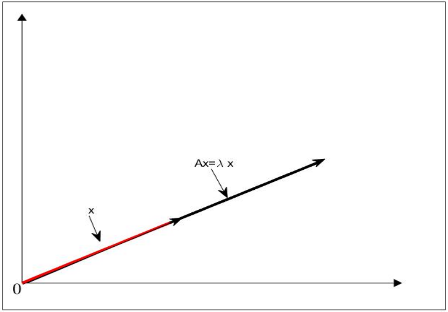
$$det(A - \lambda I_n) = 0$$

or the root of *charactersitic polynomial*

$$p_A(\lambda) = det(A - \lambda I_n).$$

Eigenvalues and eigenvectors (Meyer, 2000)

Geometrically, $A\boldsymbol{x} = \lambda\boldsymbol{x}$ says that under transformation by A, eigenvectors experience only changes in magnitude or sign—the orientation of $A\boldsymbol{x}$ in $\mathbb{R}^n$ is the same as that of $\boldsymbol{x}$. The eigenvalue λ is simply the amount of *stretch* or *shrink* to which the eigenvector $\boldsymbol{x}$ is subjected when transformed by A.



Eigenvalues and eigenvectors (Heath, 2002)

For any matrix there is an associated polynomial (characteristic polynomial) whose roots are the eigenvalues of the matrix. The reverse is also true: for any polynomial is an associated matrix whose eigenvalues are the roots of the polynomial. The *monic polynomial*

$$p_A(\lambda) = \lambda^n + c_{n-1}\lambda^{n-1} + \ldots + c_1\lambda + c_0$$

is the characteristic polynomial of the *companion matrix*

$$C = \begin{pmatrix} 0 & 0 & \ldots & 0 & -c_0 \\ 1 & 0 & \ldots & 0 & -c_1 \\ 0 & 1 & \ldots & 0 & -c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & -c_{n-1} \end{pmatrix}$$

(Dividing a polynomial of positive degree n by the coefficient of its nth-degree term yields a monic polynomial having the same roots as the original polynomial)

Eigenvalues and eigenvectors (Meyer, 2000)

Altogether, A has n eigenvalues, but some may be complex numbers (even if the entries of A are real numbers) and some eigenvalues may be repeated.
If $\lambda^n + c_{n-1}\lambda^{n-1} + \ldots + c_1\lambda + c_0 = 0$ is the characteristic equation ($\det(A - \lambda I_n) = 0$) then

$$tr(A) = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \lambda_i = -c_{n-1}$$

$$det(A) = \prod_{i=1}^{n} \lambda_i = (-1)^n c_0$$

Matlab: $eig(A)$
Properties: $\sigma(A) = \sigma(A^t)$, $\sigma(AB) = \sigma(BA)$

Spectral radius (Quarteroni *et al.*, 2000)

The maximum module of the eigenvalues of A is called the *spectral radius* of A and is denoted by

$$\rho(A) = \max_{\lambda \in \sigma(A)} |\lambda|$$

Properties:

1. $\rho(\alpha A) = |\alpha| \rho(A)$
2. $\rho(A^k) = (\rho(A))^k$
3. $\rho(AB) = \rho(BA)$

The spectral radius is not a norm. We have

$$\rho(A) = 0 \not\Leftrightarrow A = O_n$$

For example, $n = 2$, $A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \neq O_2$, but $\rho(A) = 0$.

Spectral radius (Quarteroni *et al.*, 2000)

$$\forall\, A \in \mathcal{M}_n(\mathbb{R}) :\ \rho(A) \leqslant |||A|||,\ \forall\, |||\cdot|||.$$

$$\forall\, A \in \mathcal{M}_n(\mathbb{R}),\ \forall\, \varepsilon > 0 :\ \exists\ \text{ a consistent matrix norm } \|\cdot\|_{A,\varepsilon} \text{ s.t.}$$

$$\|A\|_{A,\varepsilon} \leqslant \rho(A) + \varepsilon.$$

$$\rho(A) = \inf_{|||\cdot|||} |||A|||$$

The infimum being taken on the set of all the consistent norms.
For any consistent matrix norm $\|\cdot\|$

$$\lim_{m\to\infty} |||A^m|||^{1/m} = \rho(A)$$

Algebraic and geometric multiplicity (Quarteroni *et al.*, 2000)

The *algebraic multiplicity* of the eigenvalue λ is the multiplicity of λ as a root of the characteristic polynomial $p_A(\lambda)$.

For each eigenvalue λ of a matrix A the set of the eigenvectors associated with λ, together with the null vector, identifies a subspace of $\mathbb{C}^n$ which is called the *eigenspace* associated with λ. It corresponds by definition to $ker(A - \lambda I_n)$.
The dimension of the eigenspace is

$$dim(ker(A - \lambda I_n)) = n - rank(A - \lambda I_n)$$

and is called *geometric multiplicity* of the eigenvalue λ.
Geometric multiplicity $\leqslant$ Algebraic multiplicity. Eigenvalues having geometric multiplicity strictly less than the algebraic one are called *defective*.

Gerschgorin Circles (Meyer, 2000)

The eigenvalues of A are contained in the union

$$\mathcal{G}_r = \bigcup_{i=1}^{n} \mathcal{R}_i$$

of the n Gerschgorin circles defined by

$$\mathcal{R}_i = \{z \in \mathbb{C} \big| |z - a_{ii}| \leqslant r_i, \text{ where } r_i = \sum_{j=1, j \neq i}^{n} |a_{ij}|\}$$

$\sigma(A^t) = \sigma(A) \Rightarrow$ the eigenvalues of A are also contained in

$$\mathcal{G}_c = \bigcup_{j=1}^{n} \mathcal{C}_j$$

$$\mathcal{C}_j = \{z \in \mathbb{C} \big| |z - a_{jj}| \leqslant c_j, \text{ where } c_j = \sum_{i=1, i \neq j}^{n} |a_{ij}|\}$$

Similarity Transformations (Burden *et al. 2022*, Quarteroni *et al. 2000*)

Two matrices A and B are said to be *similar* if a nonsingular matrix S exists with $A = S^{-1}BS$. The transformation from B to $S^{-1}BS$ is called *similarity transformation*

Suppose A and B are similar matrices with $A = S^{-1}BS$ and λ is an eigenvalue of A with associated eigenvector $\boldsymbol{x}$. Then λ is an eigenvalue of B with associated eigenvector $S\boldsymbol{x}$.

We notice in particular that the product matrices AB and BA, with $A \in \mathcal{M}_{nm}(\mathbb{C})$ and $B \in \mathcal{M}_{mn}(\mathbb{C})$, are not similar but satisfy the following property

$$\sigma(AB)\backslash\{0\} = \sigma(BA)\backslash\{0\}$$

that is, AB and BA share the same spectrum apart from null eigenvalues.

Similarity Transformations (Burden *et al.*, 2022)

If $A \in \mathcal{M}_n(\mathbb{R})$ is a matrix and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are distinct eigenvalues of A with associated eigenvectors $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$. Then $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$ is a linearly independent set.
The matrix A is similar to a diagonal matrix if and only if A has n linearly independent eigenvectors. In this case, $D = S^{-1}AS$, where the columns of S consist of eigenvectors and the ith diagonal element of D is the eigenvalue of A that corresponds to the ith column of S. The pair of matrices S and D is not unique.
The matrix A that has n distinct eigenvalues is similar to a diagonal matrix.

Similarity Transformations (Burden *et al.*, 2022)

Schur's Theorem: Let A be an arbitrary matrix. A nonsingular matrix U exists with the property that

$$T = U^{-1}AU$$

where T is an upper triangular matrix whose diagonal entries consist of the eigenvalues of A.

The matrix A is symmetric if and only if there exists a diagonal matrix D and an orthogonal matrix Q with $A = QDQ^t$.

Suppose that A is a symmetric matrix. There exist n eigenvectors of A that form an orthonormal set, and the eigenvalues of A are real numbers.

A symmetric matrix A is positive definite if and only if all the eigenvalues of A are positive.

Triangle family of polynomials (Dahlquist and Björk, 2008)

By a *triangle family of polynomials* we mean a sequence of polynomials

$$q_1(x) = s_{11}$$

$$q_2(x) = s_{12} + s_{22}x$$

$$q_3(x) = s_{13} + s_{23}x + s_{33}x^2$$

$$\vdots$$

$$q_n(x) = s_{1n} + s_{2n}x + s_{3n}x^3 \ldots + s_{nn}x^{n-1}$$

where $s_{ij} \neq 0$ for all j . Note that the coefficients form a lower triangular matrix S.

Triangle family of polynomials (Dahlquist and Björk, 2008)

Conversely, for any j, x^{j-1} can be expressed recursively and uniquely as linear combinations of $q_1, \ldots, q_n$. We obtain a triangular scheme also for the inverse transformation:

$$
\begin{aligned}
1 &= t_{11} q_1(x) \\
x &= t_{12} q_1(x) + t_{22} q_2(x) \\
x^2 &= t_{13} q_1(x) + t_{23} q_2(x) + t_{33} q_3(x) \\
&\vdots \\
x^{n-1} &= t_{1n} q_1(x) + t_{2n} q_2(x) + t_{3n} q_3(x) \ldots + t_{nn} q_n(x)
\end{aligned}
$$

where $t_{ij} \neq 0$ for all j, and the coefficients form a lower triangular matrix $T = S^{-1}$. *Thus every triangle family is a basis for Π_n.*

Initial-Value Problems for Ordinary Differential Equations (I.V.P.-O.D.E.) (Burden *et al.*, 2022)

Initial-Value Problem (O.D.E.): first-order differential equation

$$y'(t) = f(t, y(t)), \quad a \leqslant t \leqslant b$$

subject to initial condition

$$y(a) = \alpha.$$

System of first-order differential equations:

$$\begin{cases} y_1'(t) = f_1(t, y_1, y_2, \ldots, y_n) \\ y_2'(t) = f_2(t, y_1, y_2, \ldots, y_n) \\ \ldots \quad \ldots \quad \ldots \\ y_n'(t) = f_n(t, y_1, y_2, \ldots, y_n) \end{cases}, \; a \leqslant t \leqslant b$$

subject to initial conditions

$$y_1(a) = \alpha_1, \; y_2(a) = \alpha_2, \ldots, y_n(a) = \alpha_n.$$

I.V.P.-O.D.E. (Burden *et al.*, 2022)

The *n*th order initial value problem:

$$y^{(n)}(t) = f(t, y, y', \ldots, y^{(n-1)}),\ a \leqslant t \leqslant b$$

subject to initial conditions

$$y(a) = \alpha_1,\ y'(a) = \alpha_2, \ldots, y^{(n-1)}(a) = \alpha_n.$$

Notation: $y_1 = y,\ y_2 = y', \ldots, y_n = y^{(n-1)}$

$$\begin{cases} y_1' = y_2 \\ y_2' = y_3 \\ \ldots \quad \ldots \quad \ldots \\ y_{n-1}' = y_n \\ y_n' = f(t, y_1, y_2, \ldots, y_n). \end{cases}$$

I.V.P.-O.D.E. (Burden *et al.*, 2022)

A function $f(t, y)$ is said to satisfy a *Lipschitz condition* in the variable y on a set $D \subset \mathbb{R}^2$ if a constant $L > 0$ exists with

$$|f(t, y_1) - f(t, y_2)| \leqslant L|y_1 - y_2|, \quad \forall\,(t, y_1), (t, y_2) \in D.$$

The constant L is called a *Lipschitz constant* for f.
Suppose $f(t, y)$ is defined on a convex set $D \subset \mathbb{R}^2$. If a constant $L > 0$ exists with

$$\left|\frac{\partial f}{\partial y}(t, y)\right| \leqslant L, \quad \forall\,(t, y) \in D$$

then f satisfies a Lipschitz condition on D in the variable y with Lipschitz constant L.

I.V.P.-O.D.E. (Burden *et al.*, 2022)

$$D = \{(t, y) | a \leqslant t \leqslant b, \quad -\infty < y < \infty\}$$

Suppose that $f(t, y)$ is continuous on D. If f satisfies a Lipschitz condition on D in the variable y, then the initial-value problem

$$\begin{cases} y'(t) = f(t, y(t)), & a \leqslant t \leqslant b \\ y(a) = \alpha \end{cases}$$

has a unique solution $y : [a, b] \to \mathbb{R}$.

I.V.P.-O.D.E. (Burden *et al.*, 2022)

The initial value problem is said be a *well-posed problem* if

1. A unique solution y to the problem exists.
2. $\exists\, \varepsilon_0 > 0$ and $k > 0$ s.t. $\forall\, \varepsilon \in (0, \varepsilon_0)$, $\forall\, \delta \in C[a, b]$ with $|\delta(t)| < \varepsilon$, $\forall\, t \in [a, b]$ and $\forall\, \delta_0 < \varepsilon$ the initial value problem

$$\begin{cases} z'(t) = f(t, z(t)) + \delta(t) \\ z(a) = \alpha + \delta_0 \end{cases}$$

has a unique solution that satisfies

$$|y(t) - z(t)| \leqslant k\varepsilon, \quad \forall t \in [a, b].$$

The problem specified is called a *perturbed problem* associated with the original problem.