

Glossary

Absolute error The absolute value of the difference between the true value and the approximate value; for instance, $|x - \text{fl}(x)|$.

Adaptive algorithm An algorithm that changes its behavior based on the resources available.

Adjoint The transpose of the matrix of cofactors.

Algorithm A sequence of steps that solve a problem in a finite amount of time.

Argand diagram The plane in which the real part of a complex number lies on the real axis, while the imaginary part lies on the imaginary axis.

Arnoldi method A matrix decomposition of the form $AQ_m = Q_{m+1}\overline{H}_m$, where A is $n \times n$, Q_m is $n \times m$, Q_{m+1} is $n \times (m+1)$, and \overline{H}_m is an $(m+1) \times m$ upper Hessenberg matrix. Q_m is orthogonal, and Q_{m+1} has orthonormal columns. The Arnoldi method is used as a portion of the GMRES algorithm. It is also used in the computation of eigenvalues and their corresponding eigenvectors for a large sparse matrix.

Augmented matrix When solving $Ax = b$ using Gaussian elimination, the matrix formed by attaching the right-hand side vector b as column $n+1$.

Back substitution Solve an upper-triangular system in reverse order from x_n to x_1 .

Backward error Roundoff or other errors in the data have produced the result \hat{y} . The *backward error* is the smallest Δx for which $\hat{y} = f(x + \Delta x)$; in other words, backward error tells us what problem we actually solved.

Banded matrix A sparse matrix whose nonzero entries appear in a diagonal band, consisting of the main diagonal and zero or more diagonals on either side.

Basic QR iteration A straightforward method of finding all the eigenvalues of a real matrix whose eigenvalues satisfy the relation $|\lambda_1| > |\lambda_2| > \dots > |\lambda_n|$. There are much better, but more complex, methods of computing the eigenvalues.

Basis A collection of linearly independent vectors. The set of all linear combinations of the basis vectors generates the subspace spanned by the basis. The dimension of the subspace is the number of vectors in the basis.

Bidiagonal matrix A matrix with nonzero entries along the main diagonal and either the diagonal above or the diagonal below.

Big-O A notation that provides an upper bound on the growth rate of a function; for instance, $f(x) = x^3 + x^2 + 5x + 1$ is $O(x^3)$ and also $O(x^4)$, but not $O(x^2)$.

Biharmonic equation The two-dimensional equation takes the form

$$\frac{\partial^4 u}{\partial x^4} + 2 \frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^4} = f(x, y),$$

with specified boundary conditions on a bounded domain. The equation has applications in the theory of elasticity, mechanics of elastic plates and the slow flow of viscous fluids.

Boundary value problem An ordinary or partial differential equation or system of equations with prescribed values on a boundary; for instance $(d^2y/dx^2) + 5(dy/dx) + x = 0$, $y(0) = 1$, $y(2\pi) = 3$ is a boundary value problem.

Cancellation error An error in floating point arithmetic that occurs when two unequal numbers are close enough together that their difference is 0.

Cauchy-Schwartz inequality An important result in numerical linear algebra: $|\langle x, y \rangle| \leq \|x\|_2 \|y\|_2$.

Characteristic equation The equation that defines the eigenvalues of a matrix A : $\det(A - \lambda I) = 0$.

Characteristic polynomial The polynomial whose roots are the eigenvalues of the associated matrix A : $p(\lambda) = \det(A - \lambda I)$.

Cholesky decomposition If A is a real positive definite $n \times n$ matrix, there is exactly one upper-triangular matrix R such that $A = R^T R$.

Coefficient matrix The matrix of coefficients, A , for a linear algebraic system $Ax = b$.

Cofactor $C_{ij} = (-1)^{i+j} M_{ij}$, where M_{ij} is the minor for row i , column j of a square matrix. The 2-norm is commonly used.

Column rank The number of linear independent columns in an $m \times n$ matrix.

Column space The subspace generated by the columns of an $m \times n$ matrix.

Column vector An $n \times 1$ matrix.

Complex conjugate If $z = x + iy$, its conjugate is $\bar{z} = x - iy$.

Complex plane The plane in which the real part of a complex number lies on the real axis, while the imaginary part lies on the imaginary axis.

Condition number For an $n \times n$ matrix A , the condition number is $\eta(A) = \|A\| \|A^{-1}\|$ and measures the sensitivity of errors in computing the solutions to problems involving the matrix. The 2-norm is commonly used.

Conjugate gradient method The iterative method of choice for solving a large, sparse, system $Ax = b$, where A is symmetric positive definite.

Cramer's rule A method of solving a square system $Ax = b$. Let B_j be the matrix obtained by replacing column j of A by vector b . Then $x_j = \det(B_j)/\det(A)$. Cramer's rule should not be used, except for very small systems.

Crank-Nicholson method A finite difference scheme for approximating the solution to a partial differential equation over a rectangular grid.

Cross product Given two vectors u, v in \mathbb{R}^3 , $u \times v = \det \begin{bmatrix} i & j & k \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{bmatrix}$, where i, j, k are the standard basis vectors. $u \times v$ is orthogonal to both u and v .

Crout's method An method of performing the LU decomposition of an $n \times n$ matrix. The elements of L and U are determined using formulas that are easily programmed.

Cubic spline interpolation An algorithm that fits a cubic polynomial between every pair of adjacent points $\{[a = x_1, x_2], [x_2, x_3], \dots, [x_n, x_{n+1} = b]\}$. The piecewise polynomial function is twice differentiable. The value of the piecewise polynomial at any $a \leq x \leq b$ provides accurate interpolation.

Data perturbations Small changes in data that may cause large changes in the solution of a problem using that data.

Demmel and Kahan zero-shift QR downward sweep algorithm Finds the SVD of a matrix. The first step is transformation to upper bidiagonal form, followed by bulge chasing to compute U, V , and the singular values.

Determinant A real number defined recursively using expansion by minors. Row elimination techniques provide a practical means of computing a determinant. Note that

$$\det(AB) = \det(A) \det(B), \quad \det(A^T) = \det(A), \quad \text{and} \quad \det(A^{-1}) = 1/\det(A).$$

Diagonal dominance The absolute value of the diagonal element in a square matrix is greater than the sum of the absolute values of the off-diagonal elements. $|a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}|$, $1 \leq i \leq n$.

Diagonal matrix A matrix A whose only nonzero elements are on the diagonal: $a_{ij} = 0$, $i \neq j$.

Diagonalization A matrix A can be diagonalized if there exists an invertible matrix S such that $D = S^{-1}AS$, where D is a diagonal matrix. A and D are similar matrices.

Dimension of a subspace The number of elements in a basis for the subspace.

Digraph A set of vertices and directed edges, with or without weights.

Dominant eigenvalue The eigenvalue of a matrix that is largest in magnitude.

Dominant operations The most expensive operations performed during the execution of an algorithm.

Eigenpair A pair (λ, v) , where v is an eigenvector of matrix A associated with eigenvalue λ .

Eigenproblem Finding the eigenvalues and associated eigenvectors of an $n \times n$ matrix.

Eigenvalue A real or complex number such that $Ax = \lambda x$, where A is an $n \times n$ matrix and x is a vector in \mathbb{R}^n .

Eigenvector A vector associated with an eigenvalue. If λ is an eigenvalue of A , then v is an eigenvector if $Av = \lambda v$.

Elementary row matrix A matrix E such that if A is a square matrix EA performs an elementary row operation.

Elementary row operations In a matrix, adding a multiple of one row to another, multiplying a row by a scalar, and exchanging two rows.

Encryption The process of transforming information using an algorithm to make it unreadable to anyone except those possessing a key.

Euler's identity $e^{i\pi} = -1$.

Euler's formula $e^{ix} = \cos(x) + i \sin(x)$.

Expansion by minors Computing the value of a determinant by adding multiples of the cofactors in any row or column.

Exponent In a floating point representation $\pm (0.d_1d_2 \dots d_p) \times b^n$, n is the exponent, and the d_i are the significant digits.

Extrapolation Taking data in an interval $a \leq x \leq b$ and using them to approximate values outside that interval. Least-squares can be used for this purpose.

Filtering polynomial A polynomial function designed for restarting the implicit Arnoldi or Lanczos methods for computing eigenvalues and eigenvectors of large sparse matrices.

Finite difference A quotient that approximates a derivative by using a number of nearby points in a grid.

First-row Laplace expansion Evaluation of a determinant using expansion by minors across the first row.

fl The floating-point number associated with the real number x .

Floating point arithmetic Finite-precision arithmetic performed on a computer.

Flop count The number of floating point operations ($\oplus, \ominus, \otimes, \oslash$) required by an algorithm.

Forward error The forward error in computing $f(x)$ is $|\hat{f}(x) - f(x)|$. This measures errors in computation for input x .

Forward substitution Solving a lower-triangular system, $Lx = b$, from x_1 to x_n .

Four fundamental subspaces Let U and V be the orthogonal matrices in the SVD, and r the number of the smallest singular value. The table specifies an orthogonal basis for the range and null space of A and A^T .

| | | |
|-------|--------------------------|--------------------------|
| | $A = U\tilde{\Sigma}V^T$ | |
| | Range | Null space |
| A | $u_i, 1 \leq i \leq r$ | $v_i, r+1 \leq i \leq n$ |
| A^T | $v_i, 1 \leq i \leq r$ | $u_i, r+1 \leq i \leq m$ |

Fourier coefficients The coefficients of the trigonometric functions in a Fourier series expansion of a function.

Fourier series An expansion of a periodic function in terms of an infinite sum of sines and cosines, $f(x) = a_0 \left(\frac{1}{\sqrt{2\pi}} \right) + (1/\sqrt{\pi}) \sum_{i=1}^{\infty} (a_i \cos ix + b_i \sin ix)$

Francis algorithm Often called the implicit QR iteration. Using orthogonal similarity transformations, produce an upper Hessenberg matrix with the same eigenvalues as matrix A . Using bulge chasing, implicitly perform a single or double shift QR step using Givens rotations and Householder reflections, respectively. The end result is an upper triangular matrix whose diagonal contains the eigenvalues of A .

Frobenius norm A matrix norm defined by $\|A\|_F = \sqrt{\text{trace}(A^T A)} = \left(\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2 \right)^{1/2}$. It is not induced by any vector norm.

Function condition number The limiting behavior of $\frac{|f(x) - f(\bar{x})|}{\frac{|f(x)|}{|x - \bar{x}|}}$ as δx becomes small.

Gauss-Seidel iterative method An iterative method for solving a linear system. Starting with an initial approximation x_0 , the iteration produces a new value at each step by using the most recently computed values and the remaining previous values.

Gaussian elimination Use of row elimination operations to solve a linear system or perform some other matrix operation.

Gaussian elimination with partial pivoting During Gaussian elimination, the diagonal element is made largest in magnitude by exchanging rows, if necessary. It is done to help minimize round off error.

Gaussian elimination with complete pivoting In Gaussian elimination, the pivoting strategy exchanges both rows and columns.

Geometric interpretation of the SVD If A is an $m \times n$ matrix, then Ax applied to the unit sphere $\|x\|_2 \leq 1$ in \mathbb{R}^n is a rotated ellipsoid in \mathbb{R}^m with semiaxes σ_i , $1 \leq i \leq r$, where the σ_i are the nonzero singular values of A .

Givens matrix (rotation) An orthogonal matrix, $J(i, j, c, s)$, designed to zero-out a_{ji} when it multiplies another matrix on the left or on the right. c and s must be chosen properly.

GMRES The general minimum residual method for computing the solution to a system $Ax = b$, where A is an $n \times n$ large, sparse, matrix. The method applies to any sparse matrix, but should not be used when A is symmetric positive definite.

Gram-Schmidt algorithm An algorithm that takes a set of n linearly independent column vectors and produces an orthonormal basis for the subspace spanned by the vectors. It also gives rise to a reduced QR decomposition of the matrix formed by the column vectors.

Heat equation A partial differential equation describing heat flow. In one space dimension, the problem is to solve

$$\frac{\partial u}{\partial t} = c \frac{\partial^2 u}{\partial x^2}, \quad 0 \leq x \leq L, \quad u(0, t) = g_1(t), \quad u(L, t) = g_2(t), \quad u(x, 0) = f(x).$$

Hessenberg inverse iteration An algorithm to find an eigenvector of matrix A corresponding to eigenvalue λ . Use an orthogonal similarity transformation to reduce matrix A to upper Hessenberg form, H . Find an eigenvector u of $H = Q^T A Q$ corresponding to eigenvalue λ of A using the inverse iteration. Then Qu is an eigenvector of A corresponding to eigenvalue λ .

Hessenberg matrix A square matrix is upper Hessenberg if $a_{ij} = 0$ for $i > j + 1$. The transpose of an upper Hessenberg matrix is a lower Hessenberg matrix ($a_{ij} = 0$ for $j > i + 1$). A Hessenberg matrix is “almost triangular.”

Hilbert matrices Notoriously ill-conditioned matrices defined by $H(i, j) = 1/(i + j - 1)$, $1 \leq i, j \leq n$.

Homogeneous linear system An $n \times n$ system of the form $Ax = 0$. The system has a unique solution $x = 0$ if and only if A is nonsingular.

Householder matrix (reflection) A symmetric orthogonal matrix, H_u , that takes a vector u and reflects it about a plane in \mathbb{R}^n . The transformation has the form

$$H_u = I - \frac{2uu^T}{u^T u}, \quad u \neq 0.$$

Householder matrices are used to compute the QR decomposition, reduction to an upper Hessenberg matrix, and many other things.

Identity matrix An $n \times n$ diagonal matrix whose diagonal consists entirely of ones. If A is an $n \times n$ matrix, $AI = IA = A$.

IEEE arithmetic The standard for 32- and 64-bit hardware-implemented floating point representations.

Ill-conditioned matrix A matrix with a large condition number.

Ill-conditioned problem A problem where small errors in the data may produce large errors in the solution.

Implicit Q theorem If $Q^T A Q = H$ and $Z^T A Z = G$ are both unreduced Hessenberg matrices where Q and Z have the same first column, then Q and Z are essentially the same up to signs.

Implicit QR iteration (see the Francis method).

Implicitly Restarted Arnoldi Method A method for computing eigenvalues and eigenvectors of a large sparse nonsymmetric matrix using the Arnoldi decomposition. Implicit shifts are used to evaluate a filter function that enhances convergence.

Implicitly Restarted Lanczos Method A method for computing eigenvalues and eigenvectors of a large sparse symmetric matrix using the Lanczos decomposition. Implicit shifts are used to evaluate a filter function that enhances convergence.

Inf The MATLAB constant `inf` returns the IEEE arithmetic representation for positive infinity, and in some situations its use is valid. Infinity is also produced by operations like dividing by zero (`1.0/0.0`), or from overflow (`exp(750)`).

Infinity norm A vector norm defined by $\|x\|_{\infty} = \max_{1 \leq i \leq n} |x_i|$. It induces the matrix infinity norm

$$\|A\|_{\infty} = \max_{1 \leq k \leq m} \sum_{j=1}^n |a_{kj}|.$$

Inner product Given two vectors $x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$ and $y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$ in \mathbb{R}^n , we define the *inner product* of x and y , written $\langle x, y \rangle$, to be the real number

$$\langle x, y \rangle = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n = \sum_{i=1}^n x_i y_i. \text{ If } f \text{ and } g \text{ are functions defined on } a \leq x \leq b, \text{ the } L^2 \text{ inner product is } \langle f, g \rangle = \int_a^b f(x)g(x)dx.$$

Interpolation A method of estimating new data points within the range of a discrete set of known data points.

Inverse Iteration An algorithm to compute an eigenvector from its eigenvalue.

Inverse matrix The unique matrix B such that $BA = AB = I$, where A is a square matrix, and I is the identity matrix. It is normally written as A^{-1} .

Inverse power method A method for computing the smallest eigenvalue in magnitude and an associated eigenvector.

Irreducible matrix Beginning at any vertex of the directed graph formed from the nonzero entries of a matrix, edges can be followed to any other vertex.

Iterative refinement An iteration designed to enhance the values obtained from Gaussian elimination.

Jacobi iterative method An iterative method for solving a linear system. Starting with an initial approximation x_0 , the iteration produces a new value at each step by using the previous value.

Jacobi method for computing the eigenvalues of a symmetric matrix Using Jacobi rotations to perform similarity transformations, systematically eliminate a_{ij} and a_{ji} at each step. Even though some zeros may be destroyed, the method converges to a diagonal matrix of eigenvalues.

Jacobi rotation A form of Givens rotation, $J(i, j, c, s)$, such that $J(i, j, c, s)^T A J(i, j, c, s)$ zeros-out a_{ij} and a_{ji} , $i \neq j$. c and s must be chosen properly.

Kirchhoff's rules Rules governing an electrical circuit which state that

- At any junction point in a circuit where the current can divide, the sum of the currents into the junction must equal the sum of the currents out of the junction.
- When any closed loop in the circuit is traversed, the sum of the changes in voltage must equal zero.

Krylov subspace methods The Krylov subspace \mathcal{K}_k generated by A and u is $\text{span}\{u, Au, A^2u, \dots, A^{k-1}u\}$. It is of dimension k if the vectors are linearly independent. CG is a Krylov subspace method, as are GMRES and MINRES. For GMRES and MINRES, the idea is to find the solution to $Ax = b$ by solving a least-squares problem in a k -dimensional Krylov subspace, where $k < n$. Hopefully k is much smaller than n .

norm (1-norm) A vector norm defined by $\|x\|_1 = \sum_{i=1}^n |x_i|$. It induces the matrix 1-norm $\|A\|_1 = \max_{1 \leq k \leq n} \sum_{i=1}^m |a_{ik}|$.

norm (2-norm) The vector norm defined by $\|x\|_2 = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$. It induces the matrix 2-norm $\|A\|_2$, that is the square root of the largest eigenvalue of $A^T A$.

Lagrange's identity If u and v are vectors in \mathbb{R}^3 , then $\|u \times v\|_2^2 = \|u\|_2^2 \|v\|_2^2 - \langle u, v \rangle^2$.

Least-squares Given a real $m \times n$ matrix A of rank $k \leq \min(m, n)$ and a real vector b , find a real vector $x \in \mathbb{R}^n$ such that the residual function $r(x) = \|Ax - b\|_2$ is minimized. Among other applications, the method can be used to fit a polynomial of a specified degree to data.

Lanczos method The Arnoldi method applied to a symmetric matrix. The result is

$$AQ_m = Q_m T_m + t_{m+1, m} q_{m+1} e_m^T,$$

where $A^{n \times n}$, $Q_m^{n \times m}$, $T_m^{m \times m}$, and $t_{m+1, m} q_{m+1} e_m^T$ is an $n \times m$ matrix. T_m is symmetric tridiagonal, and Q_m is orthogonal. The Lanczos method is used as a portion of the MINRES algorithm. It is also used to compute some eigenvalues and eigenvectors of a large sparse symmetric matrix.

Left eigenvector If λ is an eigenvalue of matrix A , a left eigenvector associated with λ is a vector x such that $x^T A = \lambda x^T$.

Leslie model A heavily used model in population ecology. It is a model of an age-structured population which predicts how distinct populations change over time.

Linear combination Given a collection of k vectors v_1, v_2, \dots, v_k , a linear combination is the set of all vectors of the form $c_1 v_1 + c_2 v_2 + \dots + c_k v_k$, where the c_i are scalars.

Linear transformation If A is an $m \times n$ matrix and x is an $n \times 1$ vector, Ax is a linear transformation from \mathbb{R}^n to \mathbb{R}^m .

Linearly dependent A set of vectors is linearly dependent if one vector can be written as a linear combination of the others.

Linearly independent A set of vectors is linearly independent if no vector can be written as a linear combination of the others. Equivalently, v_1, v_2, \dots, v_k are linearly independent when $c_1 v_1 + c_2 v_2 + \dots + c_k v_k = 0$ if and only if $c_1 = c_2 = \dots = c_k = 0$.

Lower-triangular matrix An $n \times n$ matrix having zeros above its diagonal; in other words, $a_{ij} = 0$, $j \geq i$.

LU decomposition Using Gaussian elimination to find a lower-triangular matrix, L , an upper-triangular matrix, U , and a permutation matrix, P , such that $PA = LU$.

Machine precision The expression $\text{eps} = \frac{1}{2}b^{1-p}$, where b is the base of the number system used, and p is the number of significant digits. It is the distance from 1 to the next largest floating point number.

Mantissa In a floating point representation $\pm (0.d_1 d_2 \dots d_p) \times b^n$, $m = .d_1 d_2 \dots d_p$ is the mantissa.

Matrix A rectangular array of rows and columns.

Matrix diagonalization The process of taking a square matrix, A , and finding an invertible matrix, X , such that $D = X^{-1}AX$. Diagonalizing a matrix is also equivalent to finding the eigenvalues and eigenvectors of A . The eigenvalues are on the diagonal of D , and the corresponding eigenvectors are the columns of X .

Matrix inverse The unique matrix B such that $BA = AB = I$, where A is a square matrix. It is normally written as A^{-1} .

Matrix norm A function $\|\cdot\|: \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is a *matrix norm* provided:

- $\|A\| \geq 0$ for all $A \in \mathbb{R}^{m \times n}$, and $\|A\| = 0$ if and only if $A = 0$;
- $\|\alpha A\| = |\alpha| \|A\|$ for all scalars α .
- $\|A + B\| \leq \|A\| + \|B\|$ for all $A, B \in \mathbb{R}^{m \times n}$.

Matrix product If A is an $m \times k$ matrix, and B is an $k \times n$ matrix, then the product $C = AB$ is the $m \times n$ matrix such that

$$c_{ij} = \sum_{k=1}^n a_{ik} b_{kj} = a_{i1} b_{1j} + \cdots + a_{in} b_{nj}.$$

In general, matrix multiplication is not commutative.

Minor The minor $M_{ij}(A)$ of an $n \times n$ matrix A is the determinant of the $(n-1) \times (n-1)$ submatrix of A formed by deleting the i th row and j th column of A .

MINRES The minimum residual method for computing the solution to a system $Ax = b$, where A is an $n \times n$ large, sparse, symmetric, matrix.

The method applies to any symmetric matrix, but should not be used when A is symmetric positive definite.

Modified Gram-Schmidt A modification of the Gram-Schmidt method that helps minimize round-off errors.

Modified Gram-Schmidt for QR decomposition A modification of the Gram-Schmidt QR decomposition method that helps minimize round-off errors.

Modulus The absolute value of real number and the magnitude $|z| = |x + iy| = \sqrt{x^2 + y^2}$ of a complex number.

NaN Stands for “not a number.” Occurs when an illegal operation such as $0/0$ occurs during floating point computation. It is a sure sign that something is wrong with the algorithm.

Nonsingular matrix A matrix having an inverse. An $n \times n$ matrix whose rank is n is nonsingular. A nonsingular matrix cannot have an eigenvalue $\lambda = 0$.

Normal equations If A is an $m \times n$ matrix, the $n \times n$ system $A^T A x = A^T b$.

Normal matrix A real matrix A is normal if $A^T A = A A^T$. All symmetric matrices are normal, and any normal matrix can be diagonalized.

Null space The set of all vectors for which $Ax = 0$. If A is nonsingular, the null space is empty.

One norm A vector norm defined by $\|x\|_1 = \sum_{i=1}^n |x_i|$. It induces the matrix 1-norm

$$\|A\|_1 = \max_{1 \leq k \leq m} \sum_{i=1}^n |a_{ik}|.$$

One-sided Jacobi iteration An algorithm involving Jacobi rotations that computes the singular value decomposition of a matrix.

Orthogonal invariance For any orthogonal matrices U and V , $\|UAV\|_2 = \|A\|_2$.

Orthogonal matrix A square matrix P such that $PP^T = P^T P = I$. The columns of P are an orthonormal basis for \mathbb{R}^n .

Orthogonal projection An orthogonal projection of v onto u is defined by $\text{proj}_u(v) = \left(\frac{\langle v, u \rangle}{\|u\|_2^2} \right) u$. See Figure 14.1 for a graphical depiction.

Orthogonal vectors Two vectors u and v for which $\langle u, v \rangle = u^T v = v^T u = 0$.

Orthonormal A set of vectors v_1, v_2, \dots, v_k are orthonormal if they are orthogonal and each has unit length.

Orthonormal basis A basis for a subspace in which the basis vectors are orthonormal.

Orthonormalization The process of converting a set of linearly independent vectors into an orthonormal basis for the same subspace.

Overdetermined system An $m \times n$ linear system in which $m > n$; in other words, there are more equations than unknowns. Overdetermined systems occur in least-squares problems.

Overflow Occurs when a computer operation generates a number having a magnitude too large to represent; for instance, integer overflow occurs when two positive integers m and n are added and the result is negative. Floating point overflow occurs when an operation produces a result that cannot be represented by the fixed number of bits used to represent a floating point number.

p -norm $\|x\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{1/p} = (\sum_{i=1}^n |x_i|^p)^{1/p}$. The most commonly used p -norms are $p = 2$ and $p = 1$. The infinity norm $\|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$ is also considered a p -norm with $p = \infty$.

Pentadiagonal matrix A matrix with five diagonals, all other entries being zero. There are two sub-subdiagonals, the main diagonal, and two super diagonals. These matrices often appear in finite difference methods for the solution of partial differential equations.

Permutation matrix A matrix whose rows are permutations of the identity matrix. If A is an $n \times n$ matrix PA permutes rows of A .

Perturbation analysis A mathematical study of how small changes in the data of a problem affect the solution.

Pivot The element in row i , column i that is used during Gaussian elimination to zero-out all the elements in column i , rows $i + 1$ to n .

Poisson's equation One of the most important equations in applied mathematics with applications in such fields as astronomy, heat flow, fluid dynamics, and electromagnetism. In two dimensions, let R be a bounded region in the plane with boundary ∂R , $f(x, y)$ be a function defined in R , and $g(x, y)$ be defined on ∂R . Find a function $u(x, y)$ such that

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = f(x, y),$$

$$u(x, y) = g(x, y) \quad \text{on } \partial R.$$

The equation can be defined similarly in n -dimensions.

Positive definite An $n \times n$ symmetric matrix A such that $x^T A x > 0$ for all $x \neq 0$. If A is a positive definite matrix, then there exists an upper-triangular matrix R such that $A = R^T R$, $r_{ii} > 0$, (the Cholesky decomposition), and all the eigenvalues of A are real and greater than zero.

Positive semidefinite An $n \times n$ matrix A such that $x^T A x \geq 0$ for all $x \neq 0$.

Power method An algorithm for computing the largest eigenvalue in magnitude and an associated eigenvector by computing successive matrix powers.

Preconditioning A technique designed to solve a linear system whose matrix is ill-conditioned. Choose a preconditioner, P , whose inverse is close enough to A^{-1} so that the system

$$P^{-1}Ax = P^{-1}b$$

is not as ill-conditioned. Preconditioning can be used effectively with the conjugate gradient and GMRES methods.

Pseudocode An informal language for describing algorithms.

Pseudoinverse If A is an $m \times n$ matrix, the pseudoinverse $A^\dagger = (A^T A)^{-1} A^T$. The pseudoinverse generalizes the concept of an inverse. When $m = n$, $A^\dagger = A^{-1}$.

QR decomposition A matrix decomposition of an $m \times n$ matrix A such that $A = QR$, where Q is an $m \times m$ orthogonal matrix and R is an $m \times n$ upper-triangular matrix.

QR iteration An iterative algorithm that computes the eigenvalues of a real matrix A with distinct eigenvalues using the QR decomposition. If A_i is the current matrix in the iteration, compute $A_i = Q_i R_i$, and then set $A_{i+1} = R_i Q_i$. The sequence of matrices converges to an upper-triangular matrix with all the eigenvalues of A on the diagonal. Convergence tends to be slow, so a shift, σ_i , is normally applied as follows: $A_i - \sigma_i I = Q_i R_i$ and $A_{i+1} = R_i Q_i + \sigma_i I$. Choose σ_i to better isolate eigenvalue λ_i .

Quadratic form An expression in real variables x and y of the form $ax^2 + 2hxy + by^2$. If $X = \begin{bmatrix} x \\ y \end{bmatrix}$, the expression can be written as

$$ax^2 + 2hxy + by^2 = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a & h \\ h & b \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = X^T A X.$$

There is a more general definition of a quadratic form, but general quadratic forms are not discussed in the book.

Rank deficient An $m \times n$ matrix that has a zero singular value. Equivalently, the rank is less than $\min(m, n)$.

Rank 1 matrix A matrix with only one linearly independent column or row.

Rayleigh quotient Given an eigenvector v of matrix A , the Rayleigh quotient $(Av)^T v / \|v\|_2^2$ is the eigenvalue corresponding to v .

Reduced QR decomposition If $m \geq n$, a reduced QR decomposition of matrix A can be performed. In this decomposition $A = QR$, where $A^{m \times n} = Q^{m \times n} R^{n \times n}$. If m is quite a bit larger than n , this computation is considerably faster, and uses less memory.

Reduced SVD The singular value decomposition, $A = U \Sigma V^T$, where U is $m \times n$, Σ is $n \times n$, and V is $n \times n$. If m is quite a bit larger than n , this computation is considerably faster, and uses less memory. See “Singular value decomposition” for more information.

Regression line A straight line fit to a set of data points using least squares.

Relative error In floating point conversion, the relative error in converting x is $|\text{fl}(x) - x|/|x|$, $x \neq 0$. In an iteration, the relative error is $|x_{\text{new}} - x_{\text{prev}}|/|x_{\text{prev}}|$. Relative error is used in many other situations.

Residual $r = b - Ax$, where A is $m \times n$, x is $n \times 1$, and b is $m \times 1$. The residual measures error in an iterative method for solving $Ax = b$, and in least squares the residual is minimized.

Resonance The tendency of a system to oscillate at a greater amplitude at some frequencies than at others. These are known as the system’s resonant frequencies. At these frequencies, even small periodic driving forces can produce oscillations of large amplitude.

Rosser matrix Symmetric eigenvalue test matrix. It has eigenvalues with particular properties that challenge a symmetric eigenvalue solver.

Rotation matrix A linear transformation that performs a rotation of an object. $P = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$ is a 2×2 rotation matrix.

Round-off error The error introduced when a real number, x , is approximated using finite-precision computer arithmetic and when floating point operations are performed.

Row-equivalent matrices Matrix B is row-equivalent to matrix A if B can be obtained from A using elementary row operations.

Scalar multiple Multiplying a vector or a row of a matrix by a scalar.

Schur’s Triangularization Every $n \times n$ real matrix A with real eigenvalues can be factored into $A = PTP^T$, where P is an orthogonal matrix, and T is an upper-triangular matrix.

Sensitivity of eigenvalues A measure of how small changes in matrix entries affect the ability to accurately compute an eigenvalue. If λ is an eigenvalue and x, y are right and left eigenvectors corresponding to λ , then the condition number of λ is $1/y^T x$. The condition numbers for the eigenvalues of a symmetric matrix are one.

Similar matrices Matrices A and B are similar if there exists a nonsingular matrix X such $B = X^{-1}AX$.

Singular value decomposition If $A \in \mathbb{R}^{m \times n}$, then there exist orthogonal matrices $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ such that $A = U \tilde{\Sigma} V^T$, where $\tilde{\Sigma}$ is an $m \times n$ diagonal matrix. The diagonal entries of $\tilde{\Sigma}$ are all nonnegative and are arranged as follows: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$, with $\sigma_{r+1} = \dots = \sigma_n = 0$.

Singular values The square root of the eigenvalues of $A^T A$ for any matrix A . The singular values are the entries on the diagonal of the matrix $\tilde{\Sigma}$ in the singular value decomposition.

Sparse matrix A matrix most of whose entries are 0.

Spectral radius If A is an $n \times n$ matrix, the spectral radius of A , written $\rho(A)$, is the maximum eigenvalue in magnitude; in other words, $\rho(A) = \max_{1 \leq i \leq n} |\lambda_i|$.

Spectral theorem If A is a real symmetric matrix, there exists an orthogonal matrix P such that $D = P^T A P$, where D is a diagonal matrix containing the eigenvalues of A , and the columns of P are an orthonormal set of eigenvalues that form a basis for \mathbb{R}^n .

Stable algorithm An algorithm is stable if it performs well in general, and an algorithm is unstable if it performs badly in significant cases. In particular, an algorithm should not be unduly sensitive to errors in its input or errors during its execution.

Sub-multiplicative norm A matrix norm is sub-multiplicative if $\|AB\| \leq \|A\| \|B\|$. The induced matrix norms and the Frobenius norm are sub-multiplicative.

Successive overrelaxation (SOR) An iterative method for solving the linear system $Ax = b$. A relaxation parameter, ω , $0 < \omega < 2$, provides a weighted average of the newest value, $x_i^{(k)}$, and the previous one, $x_{i-1}^{(k)}$, $1 \leq i \leq n$, $k = 1, 2, 3, \dots$, until meeting an error tolerance.

SVD See “Singular value decomposition.”

Symmetric matrix A square matrix such that $a_{ij} = a_{ji}$, $i \neq j$. In other words, $A^T = A$.

Symmetric matrix eigenvalue problem The eigenvectors and eigenvalues of a real symmetric matrix are real and can be computed more efficiently than those of a general matrix. The Jacobi iteration, the symmetric QR iteration, the Francis algorithm, bisection, and divide-and-conquer algorithms are discussed in the book.

Symmetric QR iteration Using orthogonal similarity transformation, create a tridiagonal matrix with the same eigenvalues as A . Using the QR iteration with the Wilkinson shift, transform a symmetric matrix to a diagonal matrix of eigenvalues.

Thomas algorithm An algorithm for solving an $n \times n$ tridiagonal system of equations $Ax = b$ with flop count $O(n)$.

Transpose of a matrix If A is an $m \times n$ matrix, then A^T is the $n \times m$ matrix obtained by exchanging the rows and columns of A ; in other words, $a_{ij}^T = a_{ji}$, $1 \leq i \leq m$, $1 \leq j \leq n$.

Triangle inequality If $\|\cdot\|$ is a vector or matrix norm, then $\|x + y\| \leq \|x\| + \|y\|$.

Tridiagonal matrix A banded matrix whose only nonzero entries are on the main diagonal, the lower diagonal, and the super diagonal. A tridiagonal matrix is both a lower and an upper Hessenberg matrix, and a tridiagonal matrix can be factored into a product of two bidiagonal matrices.

Truncation Convert to finite precision by dropping all digits past the last valid digit without rounding.

Truncation error The error introduced when an operation, like summing a series, is cut off.

Truss A structure normally containing triangular units constructed of straight members with ends connected at joints referred to as pins. Trusses are the primary structural component of many bridges.

Underdetermined system An $m \times n$ linear system for which $n > m$; in other words, there are more unknowns than equations. These are a type of least-squares problems.

Underflow Occurs when a floating point operation produces a result too small for the precision of the computer.

Upper bidiagonal form A matrix having the main diagonal and the super diagonal, with all other entries equal to zero. An orthogonal transformation to upper bidiagonal form is the first step of the Demmel and Kahan zero-shift QR downward sweep algorithm for computing the SVD.

Upper-triangular matrix A linear system whose coefficient matrix has zeros below the main diagonal; in other words, $a_{ij} = 0$, $j < i$, $1 \leq i, j \leq n$.

Vandermonde matrix An $m \times n$ matrix of the form:

$$V = \begin{bmatrix} 1 & t_1 & t_1^2 & \dots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \dots & t_2^{n-1} \\ 1 & t_3 & t_3^2 & \dots & t_3^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_m & t_m^2 & \dots & t_m^{n-1} \end{bmatrix}. \text{ The elements of } V \text{ are represented by the formula } v_{ij} = t_i^{j-1}. \text{ The Vandermonde matrix plays a role in least-squares problems. Note also that if}$$

$$p(x) = a_{n-1}x^{n-1} + a_{n-2}x^{n-2} + \dots + a_2x^2 + a_1x + a_0, \text{ then } V \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{bmatrix} \text{ evaluates } p(x) \text{ at the points } t_1, t_2, \dots, t_m.$$

Vector norm $\|\cdot\| : \mathbb{R}^n \rightarrow \mathbb{R}$ is a vector norm provided:

- $\|x\| \geq 0$ for all $x \in \mathbb{R}^n$. $\|x\| = 0$ if and only if $x = 0$;
- $\|\alpha x\| = |\alpha| \|x\|$ for all $\alpha \in \mathbb{R}$;
- $\|x + y\| \leq \|x\| + \|y\|$ for all $x, y \in \mathbb{R}^n$.

Well-conditioned problem If small perturbations in problem data lead to small relative errors in the solution, a problem is said to be well-conditioned.

Wilkinson bidiagonal matrix The Wilkinson-bidiagonal matrix is $A = \begin{bmatrix} 20 & 20 & 0 & \dots & 0 \\ 0 & 19 & 20 & \dots & 0 \\ \vdots & \vdots & 18 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & 20 \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$. This matrix illustrates that even though the eigenvalues of a matrix are not equal or even close to each other, an eigenvalue problem can very ill-conditioned.

Wilkinson shift A shift used in the computation of the eigenvalues of a symmetric matrix. The shift is the eigenvalue closest to h_{kk} of the 2×2 matrix

$$\begin{bmatrix} h_{k-1,k-1} & h_{k,k-1} \\ h_{k,k-1} & h_{kk} \end{bmatrix},$$

where the entries are from the lower right-hand corner of the tridiagonal matrix being reduced to a diagonal matrix.

Wilkinson test matrices These are symmetric and tridiagonal, with pairs of nearly, but not exactly, equal eigenvalues. The most frequently used case is wilkinson(21). Its two largest eigenvalues are both about 10.746; they agree to 14, but not to 15, decimal places.

Zero matrix An $m \times n$ matrix all of whose entries are 0.