1.1 Four Special Matrices

- Matrices
  - Storage of information
  - Operator

$$K_n \xrightarrow{K_n(1,1)=1} T_n \xrightarrow{T_n(n,n)=1} B_n$$

C_n : circulant matrix

	K_n	T_n	B_n	C_n	
Symmetric	O	O	O	O	
Sparse	O	O	O	O	
Tridiagonal	O	O	O		
Constant diagonals	O			O	Fourier?
Invertible	O	O			determinant
Determinant	n+1	1	0	0	
Positive definite	O	O			pivots, eigenvalues

Matrices in MATLAB

- eye, ones, zeros, diag
- toeplitz
- sparse → full, spdiags

- K\f
- lu(K)
- inv(K)
- eig(K)
- chol(K)

Examples

1.1 A $Bu = f$ and $Cu = f$ might be solvable even though B and C are singular!

Show that every vector $f = Bu$ has $f_1 + \cdots f_n = 0$.

$$\rightarrow \begin{cases} \text{physical meaning: the external forces balance} \\ \text{linear algebra meaning: } Bu = f \text{ is solvable when } f \text{ is perpendicular to} \\ \qquad\qquad\qquad\qquad \text{the all-ones column vector } e \end{cases}$$

1.1 B Connect to H("fixed-free") $= \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$ by T("free-fixed")$= \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$

using the reverse identity matrix $J = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$

$$\rightarrow \begin{cases} H = JTJ \\ \text{back=3:-1:1, H=T(back, back)} \end{cases}$$

1.2 Differences, Derivatives, BCs

- Differences replace derivatives: error?

$$-\frac{d^2u}{dx^2} = 1 \rightarrow -\frac{\Delta^2 u}{(\Delta x)^2} = (\text{ones})$$

- Finite differences: derivatives
  - Forward difference
  - Backward difference
  - Centered difference

- Difference of difference: second derivative

Important Multiplications

- Constant, linear, squares

$$\Delta^2(\text{constant}) = 0$$

$$\Delta^2(\text{linear}) = 0$$

$$\Delta^2(\text{squares}) = 2 \cdot (\text{ones})$$

- Delta, step, ramp at k

$$\Delta^2(\text{ramp}) = (\text{delta})$$

- Sines, cosines, exponentials

$$\Delta^2(\text{sines}) = \lambda \cdot (\text{sines})$$

$$\Delta^2(\text{cosines}) = \lambda \cdot (\text{cosines})$$

$$\Delta^2(\text{exponentials}) = \lambda \cdot (\text{exponentials})$$

Finite Difference Equations

$$\begin{cases} -\dfrac{d^2u}{dx^2} = 1 \text{ with } u(0) = 0 \ (\text{fixed end}) \text{ and } u(1) = 0 \rightarrow u(x) = \dfrac{1}{2}x - \dfrac{1}{2}x^2 \\ \dfrac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} = 1 \text{ with } u_0 = 0 \text{ and } u_{n+1} = 0 \quad \rightarrow u_i = \dfrac{1}{2}\left(ih - i^2h^2\right) \end{cases}$$

$$\begin{cases} -\dfrac{d^2u}{dx^2} = 1 \text{ with } u'(0) = 0 \ (\text{free end}) \text{ and } u(1) = 0 \rightarrow u(x) = \dfrac{1}{2}\left(1 - x^2\right) \\ \dfrac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} = 1 \text{ with } \dfrac{u_1 - u_0}{h} = 0 \text{ and } u_{n+1} = 0 \rightarrow u_i = \dfrac{1}{2}h^2(n+i)(n+1-i) \\ e = u(ih) - u_i = \dfrac{1}{2}h(1-x) \sim O(h) \\ \text{more accurate? } \dfrac{u_1 - u_{-1}}{2h} = 0 \sim O\left(h^2\right) \end{cases}$$

Boundary Conditions

$$u(0)=0,\ u(1)=0 \quad \to \boldsymbol{K},\ u_0=u_{n+1}=0$$

$$u'(0)=0,\ u'(1)=0 \quad \to \boldsymbol{B},\ u_0=u_1,\ u_n=u_{n+1}$$

$$u'(0)=0,\ u(1)=0 \quad \to \boldsymbol{T},\ u_0=u_1,\ u_{n+1}=0$$

$$u(0)=u(1),\ u'(0)=u'(1) \to \boldsymbol{C},\ u_0=u_n,\ u_1=u_{n+1}$$

1.3 Elimination Leads to $K=LDL^T$

- Solving a system of n linear equations Ku = f
- Gaussian elimination
  – Forward elimination: K = LU
  – Backward substitution

$$\text{multiplier } l_{ij} = \frac{\text{entry to eliminate}\left(\text{in row } i\right)}{\text{pivot } \left(\text{in row } j\right)}$$

- Three possibilities to get n pivots of A
  – No row change: A = LU (invertible)
  – Row changes by P: PA = LU (invertible)
  – No way: singular A
- Symmetric factorization: $K=LDL^T$
- Cholesky factorization: $K=A^TA$ (upper triangular A)
- Determinant of K_n = n+1

1.4 Inverses and Delta Functions

equation	–u''(x) = f(x)	Ku = f
solution	u(x): function	u: vector
f: uniform load	parabola	parabola
f: point load	Green's function	Discrete Green's function

equation	fixed-fixed	free-fixed
$-u''(x) = \delta(x-a)$	$u(x) = \begin{cases} (1-a)x & \text{for } x \le a \\ (1-x)a & \text{for } x \ge a \end{cases}$	$u(x) = \begin{cases} 1-a & \text{for } x \le a \\ 1-x & \text{for } x \ge a \end{cases}$
$-\Delta^2 u_i = \delta_j \to Ku = \delta_j$	$u_i = \begin{cases} \left(\dfrac{n+1-j}{n+1}\right) i & \text{for } i \le j \\ \left(\dfrac{n+1-i}{n+1}\right) j & \text{for } i \ge j \end{cases}$ column j of K^{-1}	$u_i = \begin{cases} n+1-j & \text{for } i \le j \\ n+1-i & \text{for } i \ge j \end{cases}$ column j of T^{-1}

1.5 Eigenvalues & Eigenvectors

- *Ax*=*b*: steady-state problem, *Ax*=*λx* : dynamic problem
- Eigenvectors: certain exceptional vectors *x* lie along the same line as *Ax*
- Eigenvalues: *Ax* is a number *λ* times the original *x*
  - Whether the special vector *x* is stretched(*λ* = 2) or shrunk(*λ* = 1/2) or reversed(*λ* = −1) or left unchanged(*λ* = 1, steady state), when it is multiplied by *A*
  - *λ* = 0: nullspace contains eigenvectors
  - Separate *λ* from *x*

$$Ax = \lambda x \rightarrow \underbrace{\left(A - \lambda I\right)}_{\text{singular}} x = 0 \rightarrow \underbrace{\det\left(A - \lambda I\right) = 0}_{\text{characteristic equation}}$$

$$\det A = \prod_{i=1}^{n} \lambda_i, \quad \text{trace}\, A = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \lambda_i$$

- If A is triangular then its eigenvalues lie along its main diagonal
- The eigenvalues of A^2 are $\lambda_1^2, \ldots, \lambda_n^2$. The eigenvalues of A^{-1} are $1/\lambda_1, \ldots, 1/\lambda_n$.
- Eigenvalues of A + B and AB are not known from eigenvalues of A and B.

- Markov matrix
  - No negative entries, each column adds to 1
  - eigshow

  - *no* real eigenvectors
  - only *one* line of eigenvectors (unusual)
  - *two* independent eigenvectors

Diagonalization

- Powers of a matrix

$$u_0 = Sa \xrightarrow{a=S^{-1}u_0} \Lambda^k a \to u_k = S\Lambda^k a = S\Lambda^k S^{-1} u_0 \leftrightarrow u_k = A^k u_0$$

- Diagonalization: $A = S\Lambda S^{-1}$
- Differential equation: u' = Au
- Symmetric matrices have real eigenvalues and orthonormal eigenvectors.
- Symmetric diagonalization $A = S\Lambda S^{-1} = Q\Lambda Q^T$ with $Q^T = Q^{-1}$.

Derivatives and Differences

$-y''=\lambda y$:	Eigenfunctions y(x) are cosines and sines		
analogy	BCs	eigenvectors	eigenvalues
K_n	y(0)=0, y(1)=0	$y(x)=\sin k\pi x$	$\lambda=k^2\pi^2$
B_n	y'(0)=0, y'(1)=0	$y(x)=\cos k\pi x$	$\lambda=k^2\pi^2$
C_n	y(0)=y(1), y'(0)=y'(1)	$y(x)=\sin 2\pi kx$, $\cos 2\pi kx$	$\lambda=4k^2\pi^2$
T_n	y'(0)=0, y(1)=0	$y(x)=\cos(k+1/2)\pi x$	$\lambda=(k+1/2)^2\pi^2$

$$\boldsymbol{K}_n \to \lambda_k = 2-2\cos k\pi h \to y_k = \left(\sin k\pi h, \ldots, nk\pi h\right)$$

$$\boldsymbol{B}_n \to \lambda_k = 2-2\cos\frac{k\pi}{n} \to y_k = \left(\cos\frac{1}{2}\frac{k\pi}{n}, \cos\frac{3}{2}\frac{k\pi}{n}, \ldots, \cos\left(n-\frac{1}{2}\right)\frac{k\pi}{n}\right)$$

$$\boldsymbol{C}_n \to \lambda_k = 2-w^k-w^{-k} = 2-2\cos\frac{2\pi k}{n} \to y_k = \left(1, w^k, \ldots, w^{(n-1)k}\right)$$

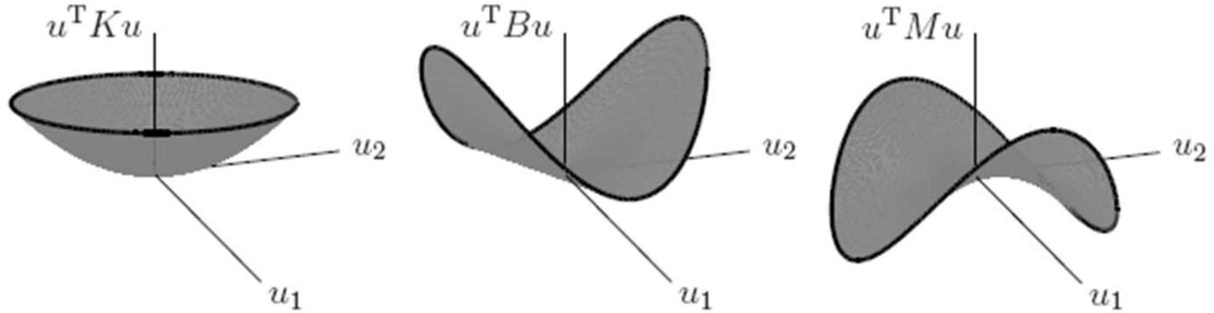
1.6 Positive Definite Matrices

- Every $K = A^T A$ is symmetric and positive definite (or at least semidefinite)
- If K_1 and K_2 are positive definite matrices then so is $K_1 + K_2$
- All pivots and all eigenvalues of a positive definite matrix are positive

- energy-based definition of positive definiteness
  - a point where all partial derivatives are zero, is a minimum (not a maximum or saddle point) if the matrix of second derivatives is positive definite

	Energy-based	Sum of squares
Positive definite	always positive	three($A^T A$), two(LDL^T)
Semidefinite	positive or zero	one
Indefinite	positive or negative	Mixed signs

– The symmetric matrix S is positive definite when $u^T S u > 0$ for every vector u except u = 0



Positive definite K	K = toeplitz([2 − 1 0])
All pivots are positive	$K = LDL^T$ with pivots 2, 3/2 , 4/3
Upper left determinants > 0	K has determinants 2, 3, 4
All eigenvalues are positive	$K = Q\Lambda Q^T$ with $\lambda = 2, 2+\sqrt{2}, 2-\sqrt{2}$
$u^T K u > 0$ if $u = 0$	$u^T K u = 2\left(u_1 - \frac{1}{2}u_2\right)^2 + \frac{3}{2}\left(u_2 - \frac{2}{3}u_3\right)^2 + \frac{4}{3}u_3^2$
$K = A^T A$, indep. columns	A can be the Cholesky factor chol(K)

Minimum Problems

$$P(u) = \frac{1}{2}u^T K u - u^T f = \left(u_1{}^2 - u_1 u_2 + u_2{}^2\right) - u_1 f_1 - u_2 f_2$$

$$P(u) - P_{\min} \geq 0$$

	Quadratic function	Not a quadratic function
1st derivative vector	linear	$\frac{\partial P}{\partial u_i} = 0$
2nd derivative matrix	K	$H_{ij} = \frac{\partial^2 P}{\partial u_i \partial u_j}$: positive definite

- Newton's method

1.7 Numerical Linear Algebra

- "build up, break down" process
  - Ku = f, Kx = λx, Mu''+Ku = 0
- A: may be rectangular, better conditioned and more sparse
  - *A:* independent columns → $K = A^T A$: symmetric positive definite
- K: symmetric and more beautiful
- Three essential factorization
  - Elimination: A = LU (triangular matrices)
  - Orthogonalization: A = QR (orthogonal matrices)
    - Gram-Schmidt algorithm
    - Householder algorithm
  - Singular value decomposition: $A = U\Sigma V^T$ (very sparse matrices)
    - Positive definite K: U=Q, $V=Q^T$, $\Sigma=\Lambda$, $K=Q\Lambda Q^T$

Orthogonalization

- Orthonormal: Orthogonality + Normalization to unit vectors
- Q: square → orthogonal matrix
  - $Q^{-1} = Q^T$
  - $\| Qx \| = \| x \|$ (length preserved)
- Permutation, Rotation, Reflection
- A: (m x n), linearly independent columns a_n → orthonormal vectors q_n
  - Gram-Schmidt: (m x n) (n x n)
  - Householder: qr(A), (m x m) (m x n)
- Why Q? stability

Diagonalization

- $A = S\Lambda S^{-1}$: orthogonal S?
- Two different orthogonal matrices: $A = U\Sigma V^T$
- Find V and Σ from $K = A^TA$
- Diagonal matrix Σ
  - Singular values instead of eigenvalues
- $AV = U\Sigma \rightarrow u_i = Av_i/\sigma_i$ (orthonormal eigenvectors of AA^T)
- $A^+ = \text{pinv}(A) = V\Sigma^+U^T \rightarrow A^+u_i = v_i/\sigma_i$

Condition Numbers and Norms

- Condition number of a positive definite matrix
  - $c(K) = \lambda_{max} / \lambda_{min}$
  - Sensitivity of the linear system Ku = f
  - maximum “blowup factor” in the relative error
- When A is not symmetric
  - Other vectors can blow up more than eigenvectors
  - Norm $\|A\| = \max(\|Ax\| / \|x\|)$: measure of size A
  - $c(A) = \|A\| \|A^{-1}\|$
  - order $1/(\Delta x)^2$ in approximating a 2nd-order differential equation

1.8 Best Basis from the SVD

- A: measurement data
  - Measuring m properties (or features) of n samples
- Correlation
  - Sample correlation: A^TA, Property correlation: AA^T
- Principal component analysis
  - To identify the most important properties revealed by the measurements in *A*
  - Covariance matrix
- Gene expression data
- Model order reduction
  - To identify the components in a *dynamic* problem that are most important to follow
  - Proper orthogonal decomposition