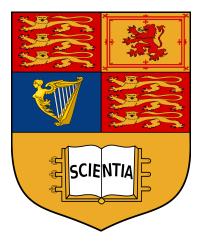
Numerical Analysis - Concise Notes

MATH50003

Arnav Singh



Colour Code - Definitions are green in these notes, Consequences are red and Causes are blue

Content from MATH40005 assumed to be known.

Contents

Ι	Linear Algebra	3		
1	Prelim	3		
3	Algebraic and Geometric multiplicities of eigenvalues	4		
4	Direct Sums	4		
5	Quotient Spaces	5		
6	Triangularisation	5		
7	The Cayley-Hamilton Theorem	5		
8	Polynomials	5		
9	The minimal polynomial of a linear map	6		
10	Primary Decomposition	7		
11	Jordan Canonical Form	7		
12	2 Cyclic Decomposition & Rational Canonical Form 9			
13	3 The Dual Space 10			
14	4 Inner Product Spaces 11			
15	Linear maps on inner product spaces	13		
16	Bilinear & Quadratic Forms	14		

Ι	Computing with Numbers	18
1	Numbers	18
	1.1 Binary Representation	 18
	1.2 Integers	 18
	1.2.1 Signed Integer	 18
	1.2.2 Variable bit representation	 18
	1.2.3 Division	18
	1.3 Floating Point numbers	19
	1.3.1 IEEE Floating-point numbers	19
	1.3.2 Special normal numbers	19
	1.3.3 Special Numbers	20
	1.4 Arithmetic	20
	1.5 Bounding errors in floating-point arithmetic	20
	1.5.1 Arithmetic and Special numbers	21 21
	1.5.2 Special functions	21
	1.0 High-precision noating-point numbers	 21
2	Differentiation	21
	2.1 Finite-differences	 21
	2.1.1 Bounding the error	22
	2.2 Dual numbers	22
	2.2.1 Connection with differentiation	 22
тт	Commention with Matrices	กก
II	Computing with Matrices	23
3	Structured Matrices	23
	3.1 Dense vectors and matrices	 23
	3.2 Triangular Matrices	 24
	3.3 Banded Matrices	 24
	3.4 Permutation Matrices	 25
	3.5 Orthogonal Matrices	25
	3.5.1 Simple Roations	25
	3.5.2 Reflections	 26
1	Decompositions and Langt Squares	26
4	Decompositions and Least Squares 4.1 QR and least squares	20 27
	4.1 QR and least squares	27
	4.2.1 Computing QR decomposition	27
	4.3 Householder reflections and QR	28
	4.4 PLU Decomposition	29
	4.4.1 Special "one-column" Lower triangular matrices	29
	4.4.2 LU Decomposition	29
	4.4.3 PLU Decomposition	30
	4.5 Cholesky Decomposition	 30
	4.6 Timings	 31
_	Cincular Walnes and Conditioning	91
5	Singular Values and Conditioning 5.1 Vector Norms	31 31
	5.1 Vector Norms	31
	5.3 Singular Value Decomposition	32
	5.4 Condition numbers	32
	<u> </u>	 92
6	Differential equations via Finite differences	33
	6.1 Indefinite integration	33
	6.2 Forward Euler	34
	6.3 Backward Euler	35
	6.4 Systems of equations	35
	6.5 Nonlinear problems	35
	6.6 Two-point boundary value problem	35
	6.7 Convergence	35
	6.7.1 Poisson	 36

Part I

Linear Algebra

1 Prelim

Definition - Similair Matrices

 $A, B \in M_n(F)$ similair $(A \sim B)$ if \exists invertible $P \in M_n(F)$ s.t $P^{-1}AP = B$ \sim is an equivalence relation.

Properties of Similair Matrices

- Same Determinant
- Same Char. Poly.
- Same eigenvalues
- Same rank Same Trace

Definition - Companion Matrix

Let p(x) a monic polynomial of degree r; $p(x) = x^r + a_{r-1}x^{r-1} + \cdots + a_0$. Companion matrix of p(x);

$$C(p(x)) = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & -a_0 \\ 1 & 0 & 0 & \dots & 0 & -a_1 \\ 0 & 1 & 0 & \dots & 0 & -a_2 \\ & & & \dots & & \\ 0 & 0 & 0 & \dots & 1 & -a_{r-1} \end{pmatrix}$$

Geometry

Definition - Dot Product

 $u = (u_1, \dots, u_n) \text{ and } v = (v_1, \dots, v_n)$

$$u \cdot v = \sum_{i=1}^{n} u_i v_i$$

Length of $u, ||u|| = \sqrt{u \cdot u}$

Distance between u and v = ||u - v||

- P orthogonal if $P^TP = I, (Pu \cdot Pv) = u \cdot v$
- A symmetric if $A^T = A$, $(Au \cdot v = u \cdot Av)$

Properties of dot product

- linear in u, v
- symmetric; $u \cdot v = v \cdot u$
- $u \cdot v > 0, \forall u, v$

3 Algebraic and Geometric multiplicities of eigenvalues

Definition - Multiplicity of eigenvalues

For $T: V \to V$ a linear map with char. poly. p(x) with roots λ , Then $\exists a(\lambda) \in \mathbb{N}$ the algebraic multiplicity of λ s.t

$$p(x) = (x - \lambda)^{a(\lambda)} q(x)$$

where λ not a root of q(x)

Geometric multiplicity $g(\lambda) = dim E_{\lambda}$, for E_{λ} the eigenspace of T

Theorem 3.2

dimV = n, Let $T: V \to V$ a linear map with finite distinct eigenvalues $\{\lambda_i\}_{i=1}^r$ Characteristic polynomial of T is

$$p(x) = \prod_{i=1}^{r} (x - \lambda_i)^{a(\lambda_i)}$$

so $\sum_{i=1}^{r} a(\lambda_i) = n$. Following are equivalent

- T diagonalisable
- $\sum_{i=1}^{r} g(\lambda_i) = n$
- $g(\lambda_i) = a(\lambda_i) \forall i$ (This can be used to test for diagonalisability.)

4 Direct Sums

Define

For $\{U_i\}_{i=1,\dots,k}$ subspaces of vector space V. Sum of these subspaces is:

$$U_1 + \dots + U_k = \{u_1 + \dots + u_k : u_i \in U_i, \forall i\}$$

Definition - Direct Sums

V a vector space, $\{V_i\}_{i=1,\dots,k}$ subspaces of vector space V. V a direct sum of $\{V_i\}$ if:

$$V = V_1 \oplus \cdots \oplus V_k$$

If $\forall v \in V$ can be expressed as $v = v_1 + \cdots + v_k$ for unique vectors $v_i \in V_i$ Corollary

$$V = V_1 \oplus \cdots \oplus V_k \iff dimV = \sum_{i=1}^k dimV_i \text{ and if } B_i \text{ a basis for } V_i, B = \bigcup_i B_i \text{ is a basis for } V_i$$

Definition - Invariant subspaces

 $T: V \to V$ a linear map, W a subspace of V.

W is T-invariant if
$$T(W) \subseteq W, T(W) = \{T(w) : w \in W\}$$

Write $T_W:W\to W$ for the restriction of T to W

Notation - Direct sums of matrices

$$A_1 \oplus \cdots \oplus A_k = \begin{pmatrix} A_1 & & \\ & \ddots & \\ & & A_k \end{pmatrix}$$

5 Quotient Spaces

Definition - Cosets V a vector space over F, with $W \leq V$ a subspace.

Cosets
$$W + v$$
 for $v \in V$ $W + v := \{w + v : w \in W\}$

Quotient Space

Define V/W as a vector space of vectors W + v over F

- Addition; $(W + v_1) + (W + v_2) = W + v_1 + v_2$
- Scalar Multiplication; $\lambda(W+v)=W+\lambda v$

Can verify this using vector space axioms. Dimension of V/W

$$dimV/W = dimV - dimW$$

Definition - Quotient Map

 $T:V\to V$ a linear map, W a T-invariant subspace of V. Quotient map: $\bar{T}:V/W:\to V/W$ such that

$$\bar{T}(W+v) = W + T(v), \quad \forall v \in V$$

6 Triangularisation

Lemma - Diagonal Matrices

$$A = \begin{pmatrix} \lambda_1 & & & & \\ 0 & \lambda_2 & & * & \\ & & \cdot & & \\ 0 & & & \cdot & \\ 0 & 0 & & & \lambda_n \end{pmatrix}, B = \begin{pmatrix} \mu_1 & & & & \\ 0 & \mu_2 & & * & \\ & & \cdot & & \\ 0 & & & \cdot & \\ 0 & 0 & & & \mu_n \end{pmatrix}$$

- Characteristic polynomial of $A = \prod_{i=1}^{n} (x \lambda_i)$, eigenvalues = $\{\lambda_i\}$
- $det A = \prod_{i=1}^{n} \lambda_i$
- AB also upper triangular, with $diag(AB) = \lambda_1 \mu_1, \dots, \lambda_n \mu_n$

Theorem 6.2 - Triangularisation Theorem

V an n dimensional vector space over $F, T: V \to V$ a linear map, Where $\chi(T) = \prod_{i=1}^{n} (x - \lambda_i)$, where $\lambda_i \in F \ \forall i \implies \exists$ basis B of V s.t $[T]_B$ upper triangular

7 The Cayley-Hamilton Theorem

Theorem. 7.1 - (Cayley-Hamilton Theorem)

V a finite dimensional vector space over F. $T: V \to V$ a linear map with char. poly. p(x)

$$p(T) = 0$$

8 Polynomials

 ${\bf Definition - Polynomials \ over \ a \ field}$

F a field, p(x) over F, for $p(x) = \sum_i a_i x^i$, $F[x] = \{p(x) : a_i \in F\}$

Degree of polynomial

deg(p(x)) =the highest power of x in p(x)

Euclidean Algorithm

 $f, g \in F[x]$ with $deg(g) \ge 1$, Then $\exists q, r \in F[x] s.t$

$$f = gq + r$$

for either r = 0 or deg(r) < deg(g)

Definition - Greatest Common Divisor (GCD) of polynomials

 $f,g \in F[x] \setminus \{0\}$, Say $d \in F[x]$ the gcd of f,g if:

- (i) d|f and d|g
- (ii) if $e(x) \in F[x]$ and e|f and e|g Then e|d

Say f, g are co-prime if gcd(f, g) = 1

Corollary

 $d = gcd(f, g) \implies \exists r, s \in F[x] \text{ s.t } d = rf + sg$

Definiton - Irreducible polynomials

 $p(x) \in F[x]$ irreducible over F if $deg(p) \ge 1$ and p not factorisable over F as a product of $\{f_i\} \in F$ s.t $deg(f_i \le deg(p))$

Corollary

 $p(x) \in F[x]$ irreducible, $\{g_i\} \in F[x]$, if $p|g_1 \dots g_r \implies p|g_i$ for some i

Theorem 8.7 - (Unique Factorization Theorem)

$$f(x) \in F[x]$$
 s.t $deg(f) \ge 1$

$$f = p_1 \dots p_r$$

where each $p_i \in F[x]$ irreducible. Factorisation of f is unique up to scalar multiplication

9 The minimal polynomial of a linear map

Definition - Minimal polynomial

Say $m(x) \in F[x]$ a minimal polynomial for $T: V \to V$ if

- (i) m(T) = 0
- (ii) m(x) monic
- (iii) deg(m) is as small as possible s.t (i) and (ii)

Properties of the minimal polynomial

- For T a linear map, its minimal polynomial $m_T(x)$ is unique
- $p(x) \in F[x], p(T) = 0 \iff m_T(x)|p(x)$
- $m_T(x)|c_T(x)$ the char. poly. of T
- $\lambda \in F$ a root of $c_T(x) \implies \lambda$ a root of $m_T(x)$
- $A, B \in M_n(F)$ s.t $A \sim B \implies m_A(x) = m_B(x)$

Theorem 9.3

 $p(x) \in F[x]$ an irreducible factor of $c_T(x) \implies p(x)|m_T(x)$

Corollaries

- $\bullet \ c_T(x) = c_{T_W}(x)c_{\bar{T}}(x)$
- $m_{T_W}(x)$ and $m_{\bar{T}}(x)$ both divide $m_T(x)$

10 Primary Decomposition

Theorem 10.1 - (Primary Decomposition Theorem)

V a finite dimensional vector space over $F, T: V \to V$ a linear map with $m_T(x)$ Let factorisation of $m_T(x)$ into irreducible polynomials be:

$$m_T(x) = \prod_{i=1}^k f_i(x)^{n_i}$$

Where $\{f_i(x)\}$ all distinct irreducible polynomials in F[x] For $1 \le i \le k$, define:

$$V_i = ker(f_i(T)^{n_i})$$

Then

- 1. $V = V_1 \oplus \cdots \oplus V_k$ (Call this the **primary decomposition** of V w.r.t T)
- 2. each V_i is T-invariant
- 3. each restriction T_{V_i} has minimal polynomial $f_i(x)^{n_i}$

In the case where each $f_i(x) = (x - \lambda_i)$

$$\implies m_T(x) = \prod_{i=1}^k (x - \lambda_i)^{n_i}$$

With λ_i distinct eigenvalues of T and $V_i = ker(T - \lambda_i I)^{n_i}$ We call V_i the **generalised** λ_i -eigenspace of T

Corollary

A linear map $T: V \to V$ diagonalisable $\iff m_T(x) = \prod_{i=1}^k (x - \lambda_i)$ a product of distinct linear factors

Corollary

For $T: V \to V$ a linear map, with $g_1(x), g_2(x) \in F[x]$ coprime polynomials s.t $g_1(T)g_2(T) = 0$

- 1. Then $V = V_1 \oplus V_2$, where $V_i = kerg_i(T), i = 1, 2$ with each V_i being T-invariant
- 2. Suppose $m_T(x) = g_1(x)g_2(x) \implies m_{T_{V_i}}(x) = g_i(x), i = 1, 2$

11 Jordan Canonical Form

Definition - Jordan Block

F a field and let $\lambda \in F$. Define $n \times n$ matrix:

$$J_n(\lambda) = \begin{pmatrix} \lambda & 1 & 0 & \dots & 0 & 0 \\ 0 & \lambda & 1 & \dots & 0 & 0 \\ 0 & 0 & \lambda & \dots & 0 & 0 \\ & & & \dots & & \\ 0 & 0 & 0 & \dots & \lambda & 1 \\ 0 & 0 & 0 & \dots & 0 & \lambda \end{pmatrix}$$

Properties of the Jordan Blocks

- 1. characteristic and minimal polynomials of $J_{i} = (x \lambda)^{n}$
- 2. λ the only eigenvalue of J, with $a(\lambda) = n, g(\lambda) = 1$
- 3. $J \lambda I = J_n(0)$, multiplication by $J \lambda I$ sends basis vectors as such:

$$e_n \to e_{n-1} \to \cdots \to e_2 \to e_1 \to 0$$

4. $(J - \lambda I)^n = 0$, and for i < n, $rank((J - \lambda I)^i) = n - i$. And under multiplication:

$$e_n \to e_{n-i}, e_{n-1} \to e_{n-i-1} \dots$$

7

Lemma

Let $A = A_1 \oplus \cdots \oplus A_k$ for each i let A_i have char. poly $c_i(x)$ and min. poly. $m_i(x)$.

- $c_A(x) = \prod_{i=1}^k c_i(x)$
- $m_A(x) = lcm(m_1(x), \dots, m_k(x))$
- $\forall \lambda$ eigenvalues of A, $dim E_{\lambda}(A) = \sum_{i=1}^{k} dim E_{\lambda}(A_i)$
- $\forall q(x) \in F[x], q(A) = q(A_1) \oplus \cdots \oplus q(A_k)$

Theorem 11.3 - (Jordan Canonical Form)

 $A \in M_n(F)$, suppose $c_A(x)$ a product of linear factors over F. Then

1. A similair to matrix of form

$$J = J_{n_1}(\lambda_1) \oplus \cdots \oplus J_{n_k}(\lambda_k)$$

This is the Jordan Canonical Form (JCF) of A

2. Matrix J from above, is uniquely determined by A up to order of Jordan blocks

Computing the JCF

JCF theorem says $A \sim J$, a JCF matrix.

 $A \sim J \implies$ same characteristic polynomial, eigenvalues, geometric multiplicities, minimal polynomial and $q(A) \sim q(J)$ for any polynomial q.

For each eigenvalue λ , collect all Jordan blocks as such;

$$J = \underbrace{\left(J_{n_1}(\lambda) \oplus \cdots \oplus J_{n_a}(\lambda)\right)}_{\lambda - \text{blocks of J}} \oplus \underbrace{\left(J_{m_1}(\mu) \oplus \cdots \oplus J_{m_b}(\mu)\right)}_{\mu - \text{blocks of J}} \oplus \dots$$

Properties of JCF

J as above, λ an eigenvalue;

- 1. $n_1 + \cdots + n_a = a(\lambda)$
- 2. $a = \text{number of } \lambda \text{-blocks} = g(\lambda)$
- 3. $\max(n_1,\ldots,n_a)=r$, where $(x-\lambda)^r$ the highest power of $(x-\lambda)$ dividing $m_A(x)$

Theorem 11.6

 $T:V \to V$ a linear map s.t $c_T(x)$ a product of linear factors $\Longrightarrow \exists$ basis B of V s.t $[T]_B$ a JCF matrix **Definition.- Nilpotent Matrix** $A^k=0$ for some $k \in \mathbb{N}$

Theorem 11.7

 $S: V \to V$ a nilpotent linear map $\implies \exists$ basis B of V s.t

$$[S]_B = J_{n_1}(0) \oplus \cdots \oplus J_{n_k}(0)$$

Computing a Jordan Basis

Finding the Jordan Basis B as above.

We have $V = V_1 \oplus \cdots \oplus V_k$ by Primary Decomposition Theorem.

Take each restriction T_{V_i} each with 1 eigenvalue.

Let $S_i = T_{V_i} - \lambda_i I$ so each S_i nilpotent.

Step 1 - Compute subspaces

$$V \supset S(V) \supset S^2(V) \supset \cdots \supset S^r(V) \supset 0$$

$$S^{r+1}(V) = 0$$

Step 2 - Find basis of $S^r(V)$, Using the following rules extend to basis of $S^{r-1}(V)$:

Given basis $u_1, S(u_1), \dots, S^{m_1-1}(u_1), \dots u_r, S(u_r), \dots, S^{m_r-1}(u_r)$

- (1) for each i add vector $v_i \in V$ s.t $u_i = S(v_i)$
- (2) note ker(S) contains linearly independent vectors

$$S^{m_1-1}(u_1), \ldots, S^{m_r-1}(u_r)$$

extend to basis of ker(S) by adding vectors w_1, \ldots, w_s with dim ker(S) = r + s Yielding

$$v_1, S(v_1), \ldots, S^{m_1}(v_1), \ldots, v_r, S(v_r), \ldots, S^{m_r}(v_r), w_1, \ldots, w_s$$

Step 3 - Repeat successively finding Jordan bases of $S^{r-2}, \ldots, S(V), V$

12 Cyclic Decomposition & Rational Canonical Form

Definition - Cyclic Subspaces

V a finite dimensional vector space over F, and $T:V\to V$ a linear map. Let $0\neq v\in V$ and define

$$Z(v,T) = \{ f(T)(v) : f(x) \in F[x] \}$$

= Sp(v, T(v), T²(v), ...)

Say Z(v,T) the T-cyclic subspace of V generated by v.

Z(v,T) is T-invariant. Write T_v

Definition - T-annihilator of v and Z(v,T)

Considering, $v, T(v), T^2(V), \ldots$ with $T^k(v)$ first vector in span of previous ones

$$\implies T^k(v) = -a_0v - a_1T(v) - \dots - a_{k-1}T(v)$$

T-annihilator of v and Z(v,T) is

$$m_v(x) = x^k + a_{k-1}x^k + \dots + a_0 \in F[x]$$

This is monic polynomial of smallest degree s.t $m_v(T)(v) = 0$ also with $m_v(T)(w) = 0 \ \forall w \in Z(v,T)$

Theorem 12.2 (Cyclic Decomposition Theorem)

V a finite dimensional vector space over F

 $T: V \to V$ a linear map. Suppose $m_T(x) = f(x)^k$ for irreducible $f(x) \in F[x]$ $\Longrightarrow \exists v_1, \dots, v_r \in V \text{ s.t}$

$$V + Z(v_1, T) \oplus \cdots \oplus Z(v_r, T)$$

where

- (1) each $Z(v_i,T)$ has T-annihilator $f(x)^{k_i}$ for $1 \le i \le r, \ k=k_1 \ge k_2 \ge \cdots \ge k_r$
- (2) r and k_1, \ldots, k_r uniquely determined by T

Corollary 12.3

T a finite dimensional vector space over F

 $\implies \exists \text{ basis } B \text{ of } V \text{ s.t.}$

$$[T]_B = C(f(x)^{k_1}) \oplus \cdots \oplus C(f(x)^{k_r})$$

Corollary 12.3

 $A \in M_n(F)$, with $m_A(x) = x^k$

$$\implies A \sim C(x^{k_1} \oplus \cdots \oplus C(x^{k_r}))$$

Theorem 12.5 (Rational Canonical Form Theorem)

V be finite dimensional over field F with $T:V\to V$ a linear map with

$$m_T(x) = \prod_{i=1}^t f_i(x)^{k_i}$$

with $\{f_i(x)\}_{i=1}^t \in F[x]$ set of distinct irreducible polynomials $\implies \exists$ basis B of V s.t

$$[T]_B = C(f_1(x)^{k_{11}}) \oplus \cdots \oplus C(f_1(x)^{k_{1r_1}}) \oplus \cdots \oplus C(f_t(x)^{k_{tr_t}}) \oplus \cdots \oplus C(f_t(x)^{k_{tr_t}})$$

where for each i

$$k_i = k_{i1} \ge \cdots \ge k_{ir_i}$$

with r_i and k_{i1}, \ldots, k_{ir_i} uniquely determined by T

Corollary 12.6

 $A \in M_n(F)$ s.t $m_A(x) = \prod_{i=1}^t f_i(x)^{k_i}$ distinct irreducible polynomials. $\implies A \sim C(f_1(x)^{k_{11}}) \oplus \cdots \oplus C(f_1(x)^{k_{1r_1}}) \oplus \cdots \oplus C(f_t(x)^{k_{t1}}) \oplus \cdots \oplus C(f_t(x)^{k_{tr_t}})$

Computing the RCF

 $T:V \to V$ we have

$$c_T(x) = \prod_{i=1}^t f_i(x)^{n_i}, \quad m_T(x) = \prod_{i=1}^t f_i(x)^{k_i}$$

 $\{f_i(x)\}\$ all distinct irreducible polynomials in F[x] enough to find; $rank(f_i(T)^r)\ \forall i\in\{1,\ldots,t\}, 1\leq r\leq k_i$

13 The Dual Space

Definition - Linear functional

V a vector space over F

A linear functional on V a linear map $\phi: V \to F$ s.t

$$\phi(\alpha v_1 + \beta v_2) = \alpha \phi(v_1) + \beta \phi(v_2) \qquad \forall v_i \in V, \forall \alpha, \beta \in F$$

Operations of linear functionals

(i)
$$(\phi_1 + \phi_2)(v) = \phi_1(v) + \phi_2(v), \quad \forall v \in V$$

(ii)
$$(\lambda \phi)(v) = \lambda \phi(v), \quad \forall \lambda \in F, \forall v \in V$$

Definition - The dual space

$$V^* = \{\phi | \phi : V \text{ to } F \text{ a linear functional } \}$$

 V^* a vector space over F w.r.t above multiplication and addition.

Dimension

 $\{v_i\}_i$ a basis of V with eigenvalues $\{\lambda\}_i$

 $\exists ! \phi \in V^* \text{ sending } v_i \to \lambda_i$

$$\phi(\sum \alpha_i v_i) = \sum \alpha_i \lambda_i$$

Proposition 13.1

Let n = dimV with $\{v_1, \ldots, v_n\}$ a basis of V $\forall i$ define $\phi_i \in V^*$ by

$$\phi_i(v_j) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

 $\implies \phi_i(\sum \alpha_j v_j) = \alpha_i \implies \{\phi_1, \dots, \phi_n\}$ a basis of V^* the **dual basis** of B $dimV^* = n = dimV$

Definition - Annihilators

V a finite dimensional vector space over F and V* the dual space. $X \subset V$. Say annihilator $X^0 \circ f X$:

$$X^0 = \{ \phi \in V^* : \phi(x) = 0 \forall x \in X \}$$

 X^0 a subspace of V^*

Proposition 13.2.

W subspace of $V \implies dimW^0 = dimV - dimW$

14 Inner Product Spaces

Definition - Inner Product

 $F = \mathbb{R}$ or . V a vector space over F

Inner product on V a map $(u, v) : V \times V \to F$ satisfying

(i)
$$(\lambda_1 v_1 + \lambda_2 v_2, w) = \lambda_1(v_1, w) + \lambda_2(v_2, w)$$

(ii)
$$(w, v) = (w, v)$$

(iii)
$$(v,v) > 0$$
 if $v \neq 0$

 $\forall v_i, v, w \in V \text{ and } \lambda_i \in F.$ Call such a vector space V with inner product (,) an inner product space.

Properties of Inner Product Space

- right-linear for $F = \mathbb{R}$; $(v, \lambda_1 w_1 + \lambda_2 w_2) = \bar{\lambda_1}(v, w_1) + \bar{\lambda_2}(v, w_2)$
- $(v,v) \in \mathbb{R}$
- $(0, v) = 0 \forall v \in V$
- symmetry; $F = \mathbb{R} \implies (w, v) = (v, w)$
- $(v, w) = (v, x) \forall v \in V \implies w = x$

Matrix of an inner product V a finite dimensional inner product space. $B = \{v_1, \ldots, v_n\}$ a basis. Defining $a_{ij} = (v_i, v_j)$. So we have $a_{ji} = \bar{a_{ij}}$

 $F \mathbb{R} \implies A \text{ symmetric}$

 $F \implies A \text{ hermitian}$

 $v,w \in V \implies (v,w) = [v]_B^T A[\bar{w}]_B$

Definition - Positive definite

Hermitian matrix A positive-definite if $x^T A \bar{x} > 0 \ \forall$ non-zero $x \in F^n$

Proposition 14.1

For $u, v, w \in V$ we have

- (i) $|(u,v)| \le ||u|| ||v||$ (Cauchy-Schwarz Inequality)
- (ii) $||u+v|| \le ||u|| + ||v||$
- (iii) $||u-v|| \le ||u-w|| + ||w-v||$ (Triangle inequalities)

Dual Space

Let V an inner product space over $F = \mathbb{R}$ or $v \in V$ define

$$f_v: V \to F$$

 $f_v(w) = (w, v)$

 $\implies f_v$ linear functional $\in V*$

Definition - \bar{V}

 \bar{V} has same vectors as V

- Addition in \bar{V} same as V
- Scalar multiplication; $\lambda * v = \bar{\lambda}v$

Proposition 14.2.

V finite-dimensional. Define $\pi: \bar{V} \to V*$ as

$$\pi(v) = f_v \quad \forall v \in V$$

 $\implies \pi$ a vector space isomorphism

Definition - Orthogonality

 $\{v_1, \ldots, v_k\}$ orthogonal if $(v_i, v_j) = 0 \ \forall i, j \ i \neq j$ Orthonormal if also $||v_i|| = 1 \ \forall i$

Definition - W^{\perp}

 $W \subseteq V$ define

$$W^{\perp} = \{ u \in V : (u, w) = 0 \ \forall w \in W \}$$

Proposition

V a finite dimensional inner product space. $W \leq V$

$$\implies V = W \oplus W^{\perp}$$

Theorem 14.5

V a finite dimensional inner product space

- (i) V has orthonormal basis
- (ii) Any orthonormal set of vectors $\{w_1, \ldots, w_r\}$ can be extended to orthonormal basis of V

Gram-Schmidt Process

Step 1 - Start with basis $\{v_1, \ldots, v_n\}$ of V

Step 2 - let
$$u_1 = \frac{v_1}{||v_1||}$$
 define $w_2 = v_2 - (v_2, u_1)u_1$
 $\implies (w_2, u_1) = 0$, let $u_2 = \frac{w_2}{||w_2||}$
 $\implies \{u_1, u_2\}$ orthonormal

Step 3 - Let

$$w_3 = v_3 - (v_3, u_1)u_1 - (v_3, u_2)u_2$$

With
$$u_3 = \frac{w_3}{||w_3||} \implies \{u_1, u_2, u_3\}$$

 ${\it Step~4}$ - Continue, for $i^{\rm th}$ step

$$u_i = \frac{w_i}{||w_i||}$$
 $w_i = v_i - (v_i, u_1)u_1 - \dots - (v_i, u_{i-1})u_{i-1}$

Yielding after n steps an orthonormal basis $\{u_1, \ldots, u_n\}$ with

$$\operatorname{Sp}(u_1, \dots, u_i) = \operatorname{Sp}(v_1, \dots, v_i) \quad \forall i \in \{1, \dots, n\}$$

Projections

V an inner product space. $v, w \in V \setminus 0$

Projection of v along w defined to be λw for $\lambda \frac{(v,w)}{(w,w)}$.

For $W \leq V, v \in V$

define projection of V along W as follows:

$$V=W\oplus W^\perp$$

for unique $w \in W, w' \in W^{\perp}$ v = w + w'

Define orthogonal projection map along W.

$$\pi_W:V\to W$$

$$\pi_W(v) = w$$

Proposition 14.7.

V an inner product space. $W \leq V$ with π_W orthogonal projection map along W.

- (i) $v \in V \implies \pi_W$ vector in W closest to V i.e for $w \in W$, ||w - v|| minimum for $w = \pi_W(v)$
- (ii) dist(v, w) denotes shortest distance from v to any vector in W $\implies \operatorname{dist}(v, w) = ||v - \pi_W(v)||$
- (iii) $\{v_1, \dots, v_r\}$ orthonormal basis of W $\implies \pi_W(v) = \sum_{j=1}^r (v, v_j) v_j$

Change of orthonormal basis

Proposition 14.8

V an inner product space. $E = \{e_1, \dots, e_n\}, F = \{f_1, \dots, f_n\}$ orthonormal basis of V $P = (p_{ij})$ change of basis matrix.

$$f_i = \sum_{j=1}^n p_{ji} e_j \implies P^T \bar{P} = I$$

Definition

- $P \in M_n(\mathbb{R}): P^T P = I \implies$ orthogonal matrix
- $P \in M_n(): P^T \bar{P} = I \implies \text{unitary matrix}$

Properties of the above matrices

- (i) length-preserving maps of \mathbb{R}^n , (isometries) i.e $||Pv|| = ||v|| \quad \forall v$
- (ii) Set of all isometries form a group classical group orthogonal group; $O(n, \mathbb{R}) = \{ P \in M_n(\mathbb{R}) : P^T P = I \}$ Unitary Group; $U(n,) = \{P \in M_n() : P^T \bar{P} = I\}$

15Linear maps on inner product spaces

Proposition 15.1.

V a finite dimensional inner product space. $T: V \to V$ a linear map

$$\implies \exists ! \text{ linear map } T^*: V \to V \text{ s.t } \forall u, v \in V$$

$$(T(u), v) = (u, T^*(v))$$

Say T^* - adjoint of TT self-adjoint if $T = T^*$

Proposition 15.2.

V an inner product space with orthonormal basis $E = \{v_1, \ldots, v_n\}$

$$T: V \to V$$
 a linear map, $A = [T]_E$

 $T: V \to V$ a linear map, $A = [T]_E$ $\Longrightarrow [T^*]_E = \bar{A}^T$ if field $\mathbb{R} \implies A$ symmetric, if field $\implies A$ hermitian

Theorem 15.3. Spectral Theorem

V an inner product space. $T: V \to V$ a self-adjoint linear map $\implies V$ has orthonormal basis of T-eigenvectors.

Corollary 15.4.

- $A \in M_n(\mathbb{R}) \implies \exists$ orthogonal P s.t $P^{-1}AP$ diagonal
- $A \in M_n() \implies \exists \text{ unitary } P \text{ s.t } P^{-1}AP \text{ diagonal}$

Lemma 15.5.

 $T: V \to V$ self-adjoint

- (i) eigenvalues of T real
- (ii) eigenvectors for distinct eigenvalues, orthogonal to each other
- (iii) If $W \subseteq V$, T-invariant $\implies W^{\perp}$ is also T-invariant

16 Bilinear & Quadratic Forms

Definition. - Bi-linear form

V a vector space over F

Bi-linear form on V a map; $(,):V\times V\to F$ which is both right and left-linear. i.e $\forall \alpha,\beta\in F$

- $(\alpha v_1 + \beta v_2, w) = \alpha(v_1, w) + \beta(v_2, w)$
- $(v, \alpha w_1 + \beta w_2) = \alpha(v, w_1) + \beta(v, w_2)$

General example

F a field, $V = F^n$ with $A \in M_n(F)$

$$\implies (u, v) = u^T A v \quad \forall u, v \in V \text{ a bilinear form on } V$$

Matrices

(,) a bilinear form on finited dimensional vector space V. With $B = \{v_1, \ldots, v_n\}$ A matrix of (,) w.r.t B, So $(a_{ij}) = (v_i, v_j) \implies \forall u, v \in V \ (u, v) = [u]_B^T A[v]_B$

Definition - Symmetric & Skew-symmetric

Bilinear form (,) on V is

- Symmetric if $(u, v) = (v, u) \ \forall u, v \in V$
- Skew symmetric if $(v, u) = -(u, v) \ \forall u, v \in V$

Definition - Characteristic of Field F

char of field F is the smallest $n \in \mathbb{N}_+$ s.t n = 0. if no such n exists say char(F) = 0

Lemma 16.1.

V a vector space over F with $char(F) \neq 2$

(,) skew-symmetric bilinear form on $V \implies (v,v) = 0 \ \forall v \in V$

$$(v,v) = -(v,v) \implies 2(v,v) = 0 \iff 2 = 0 \text{ or } (v,v) = 0$$

Orthogonality

Theorem 16.2

bilinear form (,) has property that

$$(v, w) = 0 \iff (w, v) = 0$$

(,) skew-symmetric or symmetric

Definition - Non-degenerate

(,) on V non-degenerate if $V^{\perp} = \{0\}$. Where V^{\perp} defined analogously w.r.t bilinear forms.

$$\forall u \in V, \ (u, v) = 0 \forall v \in V \implies u = 0$$

 $V^{\perp} = \{0\} \iff \text{matrix of (,) w.r.t a basis is invertible.}$

Dual Space

Proposition 16.3.

Suppose (,) non-degenerate bilinear form on a finite dimensional vector space V.

- (i) $v \in V$ define $f_v \in V^*$ $f_v(u) = (v, u) \quad \forall u \in V$ $\implies \phi: V \to V^*$ mapping $v \mapsto f_v \ (v \in V)$ an isomorphism
- (ii) $\forall W \leq V$ we have $dim(W^{\perp}) = dim(V) dim(W)$

Bases

Definition

 $A, B \in M_n(F)$ congruent if \exists invertible $P \in M_n(F)$ s.t

$$B = P^T A P$$

A, B congruent \implies bilinear forms $(u, v)_1 = u^T A v$ and $(u, v)_2 = u^T B v$ are equivalent

Skew-symmetric bilinear forms

Theorem 16.4.

V a finite dimensional vector space over F where $char(F) \neq 2$

- (,) non-degenerate skew-symmetric bilinear form on V. Then
 - (i) dim(V) even
- (ii) \exists basis $B = \{e_1, f_1, \dots, e_m, f_m\}$ of V s.t matrix of (,) w.r.t B is a block-diagonal matrix

$$J_m = \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{m \text{ blocks}}$$

So that
$$(e_i, f_i) = -(f_i, e_i) = 1$$

 $(e_i, e_j) = (f_i, f_j) = (e_i, f_j) = (f_j, e_i) = 0 \quad \forall i \neq j$

Corollary 16.5.

If A invertible skew-symmetric $n \times n$ matrix over F where $char(F) \neq 2 \implies n$ even and A congruent to J_m

Symmetric bilinear forms

Theorem 16.6.

V a finite dimensional vector space over F where $char(F) \neq 2$

- (,) a non-degenerate symmetric bilinear form on V
- $\implies V$ has orthogonal basis $B = \{v_1, \dots, v_n\}$

$$(v_i, v_j) = 0$$
 for $i \neq j$
 $(v_i, v_i) = \alpha_i \neq 0 \quad \forall i$

Matrix of (,) w.r.t $B = diag(\alpha_1, ..., \alpha_n)$

Corollary 16.7.

A invertible symmetric matrix over F, $char(F) \neq 2$

 \implies A congruent to diagonal matrix

Computing orthogonal basis for 16.6

- 1. find v_1 s.t $(v_1, v_1) \neq 0$
- 2. Compute v_1^{\perp} and find $v_2 \in v_1^{\perp}$ s.t $(v_2, v_2) \neq 0$
- 3. Compute $Sp(v_1, v_2)^{\perp}$ and find $v_3 \in Sp(v_1, v_2)^{\perp}$ s.t $(v_3, v_3) \neq 0$
- 4. Continue until you get orthogonal basis

Quadratic Form

Assume from now F s.t $char(F) \neq 2$, V a finite dimensional vector space over F

Definition - Quadratic form

Quadratic form on V a map $Q: V \to F$ of form

$$Q(v) = (v, v) \quad \forall v \in V$$

(,) a symmetric bilinear form on V

Q non-degenerate if (,) non-degenerate.

Remarks

- (i) given Q we find $(u, v) = \frac{1}{2}[Q(u+v) Q(u) Q(v)]$
- (ii) $V = F^n$ every symmetric bilinear forms s.t

$$(x,y) = x^T A y$$
 for $A = A^T, (x, y \in V)$

For
$$\mathbf{x} = (x_1, \dots, x_n)^T$$

$$Q(x) = x^{T} A x$$

$$= \sum_{i,j} a_{ij} x_{i} x_{j}$$

$$= \sum_{i=1}^{n} a_{ii} x_{i}^{2} + 2 \sum_{i=1}^{n} i < j a_{ij} x_{i} x_{j}$$

A general homogeneous quadratic polynomial in x_1, \ldots, x_n (all terms of degree 2)

Change of variables

Definition - Equivalent Quadratic Forms

$$V=F^n,\ Q:V\to F$$

$$Q(x) = x^T A x \ \forall x \in V, A \text{ symmetric}$$

Take
$$y = (y_1, \dots, y_n)^T$$
 s.t $x = Py$ for P invertible $\Rightarrow Q(x) = y^T P^T A P y = Q'(y)$

$$\implies Q(x) = y^T P^T A P y = Q'(y)$$

If such a P exists we say Q, Q' equivalent

note:

Congruent matrices A, P^TAP

 $A \sim P^T A P \iff P \text{ orthogonal}$

Theorem 16.8.

 $V = F^n, Q: V \to F$ non-degenerate quadratic form

(i) if $F = \Longrightarrow Q$ equivalent to form

$$Q_0(x) = x_1^2 + \dots + x_n^2 \quad (x \in {}^n)$$

Has matrix I_n

(ii) if $F = \mathbb{R} \implies Q$ equivalent to unique $Q_{p,q}; p + q = n$

$$Q_{p,q}(x) = x_1^2 + \dots + x_p^2 - (x_{p+1}^2 + \dots + x_{p+q}^2) \quad (x \in \mathbb{R}^n)$$

16

Has matrix $I_{p,q} = \begin{pmatrix} I_p & 0 \\ 0 & -I_q \end{pmatrix}$

(iii) if $F = \mathbb{Q} \implies \exists$ infinitely many inequivalent non-degenerate quadratic forms on \mathbb{Q}^n

Definition - isometry

f = (,) a non-degenerate symmetric/skew-symmetric bilinear form on finite dimensional vector space V **Isometry** of f a linear map $T: V \to V$ s.t

$$(T(u), T(v)) = (u, v) \quad \forall u, v \in V$$

T invertible since f non-degenerate.

Definition - Isometry Group

$$I(V, f) = \{T : T \text{ an isometry } \}$$

forms a subgroup of general linear group GL(V)

Equivalently;

fix basis B of V, A matrix of f w.r.t B if $[T]_B = X \implies T \in I(V, f) \iff X^T A X = A$

$$\implies I(v, f) \cong \{X \in GL(n, F) : X^T A X = A\}$$

- f skew-symmetric \implies there is only one form (up to equivalence) so we get one isometry group; Classical symplectic group Sp(V, f)
- f symmetric \implies there are many forms, forming the isometry groups; the classical orthogonal groups O(V, f)

Part I

Computing with Numbers

1 Numbers

1.1 Binary Representation

Definition 1.1

 $B_0, \ldots, B_p \in 0, 1$ denote $x \in \mathbb{N}_0$ in binary format

$$(B_p \dots B_1 B_0)_2 := 2^p B_p + \dots + 2B_1 + B_0$$

For $b_1, b_2, \ldots \in \{0, 1\}$, Denote $x \in \mathbb{R}^+$ in binary format by:

$$(B_p \dots B_0 \cdot b_1 b_2 b_3 \dots)_2 = (B_p \dots B_0)_2 + \frac{b_1}{2} + \frac{b_2}{2^2} + \frac{b_3}{2^3} + \dots$$

1.2 Integers

Definition 1.2 Ring of integers modulo m

$$\mathbb{Z}_m := \{0 \pmod{m}, 1 \pmod{m}, \dots, m-1 \pmod{m}\}$$

Integers with p-bits represent elements in \mathbb{Z}_{2^p}

Integer arithmetic equivalent to arithmetic module 2^p

1.2.1 Signed Integer

Use Two's complement convention.

Integer is
$$\begin{cases} \text{negative,} & \text{if 1st bit} = 1\\ \text{positive,} & \text{if 1st bit} = 0 \end{cases}$$

 $2^p - y$ interpreted as -y

e.g

$$11001001 = -55$$
 $01001001 = 73$

Overflow

Given arithmetic is modulo 2^p we often get overflow errors

1.2.2 Variable bit representation

Can represent integers using a variable number of bits, hence avoiding overflow. In Julia we have BigInts created by big()

1.2.3 Division

We have 2 types of division

- (i) Integer division (÷)
 5 ÷ 2 equivalent to div(5,2) rounds down returning 2
- (ii) Standard Division (/)

Returns floating-point number

5 / 2

Can also create rationals using (//)

$$(1//2) + (3//4)$$

Rational arithmetic often leads to overflow so combine it with big() often.

1.3 Floating Point numbers

Subset of real numbers representable using a fixed number of bits.

Definition 1.3 Floating-point numbers

Given integers

 σ - (Exponential shift)

Q - (Number of exponent bits)

S - (The precision)

Define set of floating-point numbers as

$$F_{\sigma,Q,S} := F_{\sigma,Q,S}^{normal} \cup F_{\sigma,Q,S}^{sub-normal} \cup F^{special}$$

With each component as such

$$\begin{split} F_{\sigma,Q,S}^{normal} &= \{ \pm 2^{q-\sigma} \times (1.b_1b_2 \dots b_S)_2 : 1 \leq q < 2^Q - 1 \} \\ F_{\sigma,Q,S}^{sub-normal} &= \{ \pm 2^{1-\sigma} \times (0.b_1b_2b_3 \dots b_S)_2 \}. \\ F^{special} &= \{ -\infty, \infty, \text{NaN} \} \end{split}$$

Floating point numbers stored in 1 + Q + S total bits as such

$$sq_{Q-1}\dots q_0b_1\dots b_S$$

With first bit the sign bit: 0 positive, 1 negative Bits $q_{Q-1} \dots q_0$ the exponent bits - binary digits of unsigned integer q Bits $b_1 \dots b_S$ the significand bits.

For $q = (q_{Q-1} \dots q_0)_2$

(i) $1 \le q < 2^Q - 1$ - Bits represent normal number

$$x = \pm 2^{q-\sigma} \times (1.b_1b_2b_3...b_S)_2$$

(ii) q = 0. (All bits are 0) - Bits represent sub-normal number.

$$x = \pm 2^{1-\sigma} \times (0.b_1b_2b_3 \dots b_S)_2.$$

(iii) $q = 2^Q - 1$ (All bits are 1) - Bits represent special number. $\pm \infty$

1.3.1 IEEE Floating-point numbers

Definition 1.4 IEEE Floating-point numbers

IEEE has 3 standard floating-point formats defined as such with corresponding types in Julia

$$\begin{split} F_{16} &:= F_{15,5,10} & \text{Float16} - \text{Double-precision} \\ F_{32} &:= F_{127,8,23} & \text{Float32} - \text{Single-precision} \\ F_{64} &:= F_{1023,11,52} & \text{Float64} - \text{Half-precision} \end{split}$$

Float64 - created by using decimals. e.g 1.0 Float32 - created by using f0 e.g 1f0

1.3.2 Special normal numbers

Definition 1.5 Machine epsilon

Denoted:

$$\epsilon_{m,S} := 2^{-S}$$

$$\min |F_{\sigma,Q,S}^{\text{normal}}| = 2^{1-\sigma}$$

Largest (postive) normal number is

$$\max F_{\sigma,Q,S}^{\text{normal}} = 2^{2^Q - 2 - \sigma} (1.11 \dots 1)_2 = 2^{2^Q - 2 - \sigma} (2 - \epsilon_{\text{m}})$$

1.3.3 Special Numbers

Definition 1.6 Not a Number

We have NaN represent "not a number"

1.4 Arithmetic

Arithmetic on floating-points exact up to rounding.

Definition 1.7 Rounding

$$\begin{split} & \mathrm{fl}^{\mathrm{UP}}_{\sigma_{\mathrm{Q},\mathrm{S}}}: \mathbb{R} \to F_{\sigma,\mathrm{Q},\mathrm{S}} \text{ rounds up} \\ & \mathrm{fl}^{\mathrm{DOWN}}_{\sigma_{\mathrm{Q},\mathrm{S}}}: \mathbb{R} \to F_{\sigma,\mathrm{Q},\mathrm{S}} \text{ rounds down} \\ & \mathrm{fl}^{\mathrm{Nearest}}_{\sigma_{\mathrm{Q},\mathrm{S}}}: \mathbb{R} \to F_{\sigma,\mathrm{Q},\mathrm{S}} \text{ rounds nearest} \end{split}$$

In case of tie, returns floating-point number whose least significand bit is equal to 0 $fl^{nearest}$ the default rounding mode. Exempt excess notation when implied by context.

Rounding modes in Julia we are going to use: RoundUp, RoundDown, RoundNearest Use setrounding(Float_, roundingmode) to change mode in a chunk of code.

$$x \oplus y := fl(x+y)$$
$$x \ominus y := fl(x-y)$$
$$x \otimes y := fl(x*y)$$
$$x \oslash y := fl(x/y)$$

Each of the above defined in IEEE arithmetic. Warning These operations are not **associative** $(x \oplus y) \oplus z \neq x \oplus (y \oplus z)$

1.5 Bounding errors in floating-point arithmetic

Definition 1.8 Absolute/relative error

if
$$\tilde{x} = x + \delta_{rma} = x(1 + \delta_r)$$

- (i) $|\delta_a|$ absolute error
- (ii) δ_r relative error

Definition 1.9 Normalised Range

Normalised range $\mathcal{N}_{\sigma,Q,S} \subset \mathbb{R}$ - subset of reals, that lies between smallest and largest normal floating-point number:

$$\mathcal{N}_{\sigma,Q,S} := \{x : \min |F_{\sigma,Q,S}| \le |x| \le \max F_{\sigma,Q,S}\}$$

Proposition. - Rounding arithmetic

if
$$x \in \mathcal{N} \implies$$

$$\mathfrak{fl}^{\text{mode}}(x) = x(1 + \delta_x^{\text{mode}})$$

With relative error:

$$|\delta_x^{\mathrm{nearest}}| \le \frac{\epsilon_{\mathrm{m}}}{2}$$
 $|\delta_x^{\mathrm{up/down}}| < \epsilon_{\mathrm{m}}.$

1.5.1 Arithmetic and Special numbers

We have the following identiites

```
1/0.0
             # Inf
                             Inf*0
                                             NaN
                                                          NaN*0
                                                                          NaN
1/(-0.0)
             # -Inf
                             Inf+5
                                             Inf
                                                          NaN+5
                                                                          NaN
0.0/0.0
                NaN
                             (-1)*Inf
                                          # -Inf
                                                          1/NaN
                                                                          NaN
                                                          NaN == NaN
                                                                       #
                             1/Inf
                                          # 0.0
                                                                          false
                             1/(-Inf)
                                          # -0.0
                                                          NaN != NaN
                                                                          true
                             Inf - Inf
                                            NaN
                             Inf == Inf
                                          #
                                             true
                             Inf == -Inf #
                                            false
```

1.5.2 Special functions

Functions such as cos, sin, exp designed to have relative accuracy e.g for s = sin(x) we satisfy

$$s = \sin(x)(1+\delta) \quad |\delta| < c\epsilon_m$$

for reasonable small c > 0 given $x \in F^{\text{normal}}$

1.6 High-precision floating-point numbers

Possible to set precision using BigFloat type created using big()

Use to find rigorous bound on a number.

e.g

```
setprecision(4_000) # 4000 bit precision
setrounding(BigFloat, RoundDown) do
  big(1)/3
end, setrounding(BigFloat, RoundUp) do
  big(1)/3
end
```

2 Differentiation

Considering functions:

- (i) Black-box function $f^{\text{FP}}: D \to F, \ D \subset F \equiv F_{\sigma,Q,S}$ Only know function pointwise, F discrete $\Longrightarrow f^{\text{FP}}$ not differentiable rigorously. Assume f^{RP} approximates a differentiable function f with controlled error.
- (ii) Generic function A formula that can be evaluated on arbitrary types. e.g polynomial $p(x) = p_0 + p_1 x + \cdots + p_n x^n$ Consider both differentiable $f: D \to \mathbb{R}, D \subset \mathbb{R}$ and floating point evaluated $f^{\text{FP}}: D \cap F \to F$, which is actually computed.
- (iii) Graph Function
 Function built by composition of basic "kernels" with known differentiability properties.

2.1 Finite-differences

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \implies f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

for sufficiently small h

Approximation uses only black-box notion of function.

Proposition. - Bounding the derivative

$$\left| f'(x) - \frac{f(x+h) - f(x)}{h} \right| \le \frac{M}{2}h$$

where $M = \sup_{x \le t \le x+h} |f''(t)|$. Given by Taylor's theorem.

Can also use left-side and central differences to compute derivatives.

- $f'(x) \approx \frac{f(x) f(x-h)}{h}$
- $f'(x) \approx \frac{f(x+h) f(x-h)}{2h}$

2.1.1 Bounding the error

Theorem 2.1 (Finite differences error bound)

f twice-differentiable in neighbourhood of x

Assume $f^{\text{FP}} = f(x) + \delta_x^f$ has uniform absolute accuracy in that neighbourhood i.e $|\delta_x^f| \leq c\epsilon_{\text{m}}$ for fixed constant c.

Take $h=2^{-n}$ for $n \leq S$ (no. of Significand bits) and |x| < 1

Finite difference approximation then satisfies

$$(f^{\mathrm{FP}}(x+h) \ominus f^{\mathrm{FP}}(x)) \oslash h = f'(x) + \delta_{x,h}^{\mathrm{FD}}$$

Where

$$|\delta_{x,h}^{\text{FD}}| \leq \frac{|f'(x)|}{2} \epsilon_{\text{m}} + Mh + \frac{4c\epsilon_{\text{m}}}{h}$$

for $M = \sup_{x \le t \le x+h} |f''(t)|$.

3 terms in bound tell us behaviour.

Heuristic - (finite differences with floating po§int step.)

Choose h proportional to $\sqrt{\epsilon_m}$

2.2 Dual numbers

Definition 2.1 Dual numbers

Dual numbers, \mathbb{D} Commutative ring over reals generated by 1 and ϵ with $\epsilon^2 = 0$, written $a + b\epsilon$

2.2.1 Connection with differentiation

Dual numbers not prone to growth due to round-off errors.

Theorem 2.2 (Polynomials on dual numbers)

p a polynomial.

$$p(a + b\epsilon) = p(a) + b'p(a)\epsilon$$

Definition 2.2 Dual extension

f real-valued function differentiable at a, a dual extension at a if

$$f(a + b\epsilon) = f(a) + bf'(a)\epsilon$$

Lemma - (Product and Chain rule)

f a dual extension at g(a), g a dual extension at a

$$\implies q(x) := f(q(x))$$
 a dual extension at a

f, g dual extensions at a

$$\implies r(x) := f(x)q(x)$$
 a dual extension at a

Part II

Computing with Matrices

3 Structured Matrices

Consider the following structures

(i) Dense

Considered unstructured, need to store all entries in vector or Matrix. Reduces directly to standard algebraic operations

(ii) Triangular

A matrix upper of lower triangular, can invert immediately with back-substitution Store as dense and ignore upper/lower entries in practice.

(iii) Banded

A matrix zero, appart from entries a fixed distance from diagonal. Have diagonal, bidiagonal and tridiagonal matrices.

(iv) Permutation

Permutation matrix permutes rows of a vector

(v) Orthogonal

Q orthogonal satisfies $Q^TQ=I$, hence easily inverted

3.1 Dense vectors and matrices

Storage in memory

•	Vector of primitive type		
	stored consecutively in memory.		

A	=	[1	2;	vec(A)	=	1
		3	4;			3
		5	6]			5
						0

• Matrix stored consecutively in memory going down column-by column. (column-major format)

4 6

Transposing A done lazily, A' stores entries by row

Matrix multiplication done as expected A*x

Implemented 2 ways

Using Traditional definition

Or going column-by-column

$$\begin{bmatrix} \sum_{j=1}^{n} a_{1,j} x_j \\ \vdots \\ \sum_{j=1}^{n} a_{m,j} x_j \end{bmatrix}$$

$$x_1\mathbf{a}_1 + \dots + x_n\mathbf{a}_n$$

Both are O(mn) operations, but column-by-column faster due to more efficient memory accessing.

Solving a linear system done by \

3.2 Triangular Matrices

Represented as dense square matrices, where we ignore entries above/below diagonal.

We have U,L both storing all the data of A

Solving upper-triangular system

$$\begin{bmatrix} u_{11} & \cdots & u_{1n} \\ & \ddots & \vdots \\ & & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

by computing x_n, x_{n-1}, \dots, x_1 by the back-substitution formula:

$$x_k = \frac{b_k - \sum_{j=k+1}^n u_{kj} x_j}{u_{kk}}$$

Multiplication and solving linear system $O(n^2)$ for a triangular matrix.

3.3 Banded Matrices

Definition 3.1 Bandwidths

Matrix A has

- lower-bandwidth, l if $A[k,j] = 0 \forall k-j > l$
- upper-bandwidth, u if $A[k,j] = 0 \forall j k > u$
- strictly lower-bandwidth if it has lower-bandwidth l and $\exists j$ such that $A[j+l,j] \neq 0$
- strictly upper-bandwidth if it has upper-bandwidth u and $\exists k$ such that $A[k, k+u] \neq 0$

Definition 3.2 Diagonal

Matrix diagonal if square and l=u=0 the bandwidths. Stored as Vectors in Julia.

Perform multiplication and solving linear systems in O(n) operations.

Definition 3.3 Bidiagonal

Matrix bidiagonal if square and has bandwidths

- $(l, u) = (1, 0) \implies \text{lower-bidiagonal}$
- $(l, u) = (0, 1) \implies \text{upper-bidiagonal}$

Multiplication and solving linear systems still O(n) operations.

3.4 Permutation Matrices

Matrix representation of the symmetric group S_n acting on \mathbb{R}^n $\forall \sigma \in S_n$ a bijection between $\{1, 2, \dots, n\}$ and itself.

Cauchy Notation

$$\begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \sigma_1 & \sigma_2 & \sigma_3 & \cdots & \sigma_n \end{pmatrix}$$

Where $\{\sigma_1, ..., \sigma_n\} = \{1, 2, ..., n\}$

Inverse permutation given by σ^{-1} , found by swapping rows of cauchy notation and reordering.

Permuting a vector $\sigma = [\sigma_1, \dots, \sigma_n]^T$

$$\mathbf{v}[\sigma] = \begin{bmatrix} v_{\sigma} \\ \vdots \\ v_{\sigma_n} \end{bmatrix}$$

Obviously $\mathbf{v}[\sigma][\sigma^{-1}] = \mathbf{v}$

Definition 3.5 Permutation Matrix

Entries of P_{σ} given by

$$P_{\sigma}[k,j] = e_k^T P_{\sigma} e_j = e_k^T e_{\sigma_j^{-1}} = \delta_{k,\sigma_j^{-1}} = \delta_{\sigma_k,j}$$

where $\delta_{k,j}$ is the Kronecker delta

Permutation matrix equal to identity matrix with rows permuted.

Proposition - Inverse of Permutation Matrix

$$P_{\sigma}^{T} = P_{\sigma^{-1}} = P_{\sigma}^{-1} \implies P_{\sigma} \text{ orthogonal}$$

3.5 Orthogonal Matrices

Definition 3.6 Orthogonal Matrix

Square matrix orthogonal if $Q^TQ = QQ^T = I$ Special cases

3.5.1 Simple Roations

Definition 3.7 Simple Rotation

 2×2 rotation matrix through angle θ

$$Q_{\theta} := \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

Definition 3.8 two-arg arctan

two-argument arctan function gives angle θ through point $[a, b]^T$

$$\operatorname{atan}(b, a) := \begin{cases} \operatorname{atan} \frac{b}{a} & a > 0 \\ \operatorname{atan} \frac{b}{a} + \pi & a < 0 \text{ and } b > 0 \\ \operatorname{atan} \frac{b}{a} + \pi & a < 0 \text{ and } b < 0 \\ \pi/2 & a = 0 \text{ and } b > 0 \\ -\pi/2 & a = 0 \text{ and } b < 0 \end{cases}$$

atan(-1,-2) # angle through [-2,-1]

Proposition - Rotating vector to unit axis

$$Q = \frac{1}{\sqrt{a^2 + b^2}} \begin{bmatrix} a & b \\ -b & a \end{bmatrix}$$

Satisfies
$$Q \begin{bmatrix} a \\ b \end{bmatrix} = \sqrt{a^2 + b^2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

3.5.2 Reflections

Definition 3.9 Reflection Matrix

Given vector **v** satisfying ||v|| = 1, reflection matrix is orthogonal matrix.

$$Q_{\mathbf{v}} := I - 2\mathbf{v}\mathbf{v}^T$$

Reflections in direction of \mathbf{v}

Proposition - Properties of reflection matrix

- (i) 1. Symmetry: $Q_v = Q_v^T$
- (ii) 2. Orthogonality: $Q_v Q_v = I$
- (iii) 2. v is an eigenvector of Q_v with eigenvalue -1
- (iv) 4. Q_v is a rank -1 perturbation of I
- (v) 3. $\det Q_v = -1$

Definition 3.10 Householder reflection

Given vector \mathbf{x} define Householder reflection.

$$Q_{\mathbf{x}}^{\pm,H} := Q_{\mathbf{w}}$$

For $\mathbf{y} = \mp ||\mathbf{x}|| e_1 + x$, $\mathbf{w} = \frac{\mathbf{y}}{||\mathbf{y}||}$ Default choice in sign is

$$Q_x^H := Q_x^{-sign(x_1),H}$$

Lemma

$$Q_x^{\pm,H}\mathbf{x} = \pm ||\mathbf{x}||e_1$$

4 Decompositions and Least Squares

Consider decompositions of matrix into products of structured matrices.

1. QR Decomposition (For square or rectangular matrix $A \in \mathbb{R}^{m \times n}, m \geq n$)

$$A = QR = \underbrace{\begin{bmatrix} \mathbf{q}_1 | \cdots | \mathbf{q}_m \end{bmatrix}}_{m \times m} \begin{bmatrix} \times & \cdots & \times \\ & \ddots & \vdots \\ & & \times \\ & & 0 \\ & & \vdots \\ & & 0 \end{bmatrix}$$

Q orthogonal and R right/upper-triangular

2. Reduced QR Decomposition

$$A = \hat{Q}\hat{R} = \underbrace{\begin{bmatrix} \mathbf{q}_1 | \cdots | \mathbf{q}_m \end{bmatrix}}_{m \times m} \begin{bmatrix} \times & \cdots & \times \\ & \ddots & \vdots \\ & & \times \end{bmatrix}$$

Q has orthogonal columns, and \hat{R} upper-triangular.

3. PLU Decomposition (For square Matrix)

$$A = P^T L U$$

P a permutation matrix, L lower triangular and U upper triangular

4. Cholesky Decomposition (For square, symmetric positive definite matrix $(x^T A x > 0 \forall x \in \mathbb{R}^n, x \neq 0)$)

$$A = LL^T$$

26

Useful as component pieces easily inverted on a computer.

$$A = P^{T}LU \implies A^{-1}\mathbf{b} = U^{-1}L^{-1}P\mathbf{b}$$

$$A = QR \implies A^{-1}\mathbf{b} = R^{-1}Q^{\top}\mathbf{b}$$

$$A = LL \implies A^{-1}\mathbf{b} = L^{-}L^{-1}\mathbf{b}$$

4.1 QR and least squares

Consider matrices with more rows than columns.

QR decomposition contains reduced QR decomposition within it

$$A = QR = \left[\hat{Q}|\mathbf{q}_{n+1}|\cdots|\mathbf{q}_{m}\right] \begin{bmatrix} \hat{R} \\ \mathbf{0}_{m-n\times n} \end{bmatrix} = \hat{Q}\hat{R}.$$

Least squares problem

Find $\vec{x} \in \mathbb{R}^n$ s.t $||A\vec{x} - \vec{b}||$ is minimised

For m = n and A invertible we simply have $\vec{x} = A^{-1}\vec{b}$.

$$||A\mathbf{x} - \mathbf{b}|| = ||QR\mathbf{x} - \mathbf{b}|| = ||R\mathbf{x} - Q^{\top}\mathbf{b}|| = \left\| \begin{bmatrix} \hat{R} \\ \mathbf{0}_{m-n \times n} \end{bmatrix} \mathbf{x} - \begin{bmatrix} \hat{Q}^{\top} \\ \mathbf{q}_{n+1}^{\top} \\ \vdots \\ \mathbf{q}_{m}^{\top} \end{bmatrix} \mathbf{b} \right\|$$

To minimise this norm, suffices to minimise

$$\|\hat{R}\mathbf{x} - \hat{Q}^{\mathsf{T}}\mathbf{b}\| \implies \mathbf{x} = \hat{R}^{-1}\hat{Q}^{\mathsf{T}}\mathbf{b}$$

Provided column rank of A is full, we have \hat{R} invertible

4.2 Reduced QR and Gram-Schmidt

4.2.1 Computing QR decomposition

(i) Write $A = [\mathbf{a}_1 | \dots | \mathbf{a}_n], a_k \in \mathbb{R}^m$ Assume A has full column rank, a_k all linearly independent.

Column span of first j columns in A same as first j columns in \hat{Q}

$$span(\mathbf{a}_1, \dots, \mathbf{a}_n) = span(\mathbf{q}_1, \dots, \mathbf{q}_n)$$

(ii) if $\mathbf{v} \in span(\mathbf{a}_1, \dots, \mathbf{a}_n) \implies \forall \mathbf{c} \in \mathbb{R}^j$

$$\mathbf{v} = \begin{bmatrix} \mathbf{a}_1 | \dots | \mathbf{a}_j \end{bmatrix} \mathbf{c}$$

$$= \begin{bmatrix} \mathbf{q}_1 | \dots | \mathbf{q}_j \end{bmatrix} \hat{R}[1:j,1:j] \mathbf{c}$$

$$\in span(\mathbf{q}_1, \dots, \mathbf{q}_n)$$

(iii) if $\mathbf{w} \in span(\mathbf{q}_1, \dots, \mathbf{q}_n)$, we have for $\mathbf{d} \in \mathbb{R}^j$

$$\mathbf{w} = [\mathbf{q}_1 | \dots | \mathbf{q}_j] \mathbf{d}$$

$$= [\mathbf{a}_1 | \dots | \mathbf{a}_j] \hat{R}[1:j,1:j]^{-1} \mathbf{d}$$

$$\in span(\mathbf{a}_1, \dots, \mathbf{a}_j)$$

We can find an orthogonal basis using Gram-Schmidt.

1. By assumption of full rank of A

$$span(\mathbf{a}_1,\ldots,\mathbf{a}_n) = span(\mathbf{q}_1,\ldots,\mathbf{q}_n)$$

2. $\mathbf{q}_1, \ldots, \mathbf{q}_n$ orthogonal

$$\mathbf{q}_k^T \mathbf{q}_l = \delta_{kl}$$

3. For k, l < j. Define

$$\mathbf{v}_j := \mathbf{a}_j - \sum_{k=1}^{j-1} \underbrace{\mathbf{q}_k^T \mathbf{a}_j}_{\mathbf{r}_{kj}} \mathbf{q}_k$$

4. For k < j

$$\mathbf{q}_k^{\top} \mathbf{v}_j = \mathbf{q}_k^{\top} \mathbf{a}_j - \sum_{k=1}^{j-1} \mathbf{\underline{q}}_k^{\top} \mathbf{a}_j \mathbf{q}_k^{\top} \mathbf{q}_k = 0.$$

5. Define further

$$\mathbf{q}_j = \frac{\mathbf{v}_j}{\|\mathbf{v}_i\|}$$

Define $\mathbf{r}_{jj} := ||\mathbf{v}_j||$, rearrange definition to have

$$\mathbf{a}_j = \begin{bmatrix} \mathbf{q}_1 | \dots | \mathbf{q}_j \end{bmatrix} \begin{bmatrix} r_{1j} \\ \vdots \\ r_{jj} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{a}_1 | \dots | \mathbf{a}_j \end{bmatrix} \begin{bmatrix} r_{11} & \dots & r_{1j} \\ & \ddots & \vdots \\ & & \vdots \end{bmatrix}$$

Compute reduced QR decomposition column-by-column \implies apply for j=n to complete decomposition.

Complexity and Stability

We have a total complexity of $O(mn^2)$ operations, Gram-Schmidt algorithm is unstable, rounding errors in floating point accumulate, \implies lose orthogonality.

4.3 Householder reflections and QR

Consider multiplication by Householder reflection corresponding to first column.

$$Q_1 := Q_{a_1}^H$$

$$Q_1 A = \begin{bmatrix} \times & \times & \cdots & \times \\ & \times & \cdots & \times \\ & \vdots & \ddots & \vdots \\ & \times & \cdots & \times \end{bmatrix} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & \mathbf{a}_2^1 & \cdots & \mathbf{a}_n^1 \end{bmatrix} \qquad r_{1j} := (Q_1 \mathbf{a}_j)[1] \quad \mathbf{a}_1^j := (Q_1 \mathbf{a}_j)[2 : m]$$

Note that $r_{11} = -(a_11)||a_1||$ with all entries of \mathbf{a}_1^1 zero.

Now consider,

$$Q_2 := \begin{bmatrix} 1 & & \\ & Q_{\mathbf{a}_2^1}^H \end{bmatrix} = Q_{\begin{bmatrix} 0 \\ \mathbf{a}_2^1 \end{bmatrix}}^H$$

to achieve the following

$$Q_{2}Q_{1}A = \begin{bmatrix} \times & \times & \times & \cdots & \times \\ & \times & \times & \cdots & \times \\ & & \vdots & \ddots & \vdots \\ & & \times & \cdots & \times \end{bmatrix} = \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1n} \\ & r_{22} & r_{23} & \cdots & r_{2n} \\ & & \mathbf{a}_{3}^{2} & \cdots & \mathbf{a}_{n}^{2} \end{bmatrix} \qquad r_{2j} := (Q_{2}\mathbf{a}_{j}^{1})[1] \quad \mathbf{a}_{j}^{2} := (Q_{2}\mathbf{a}_{j}^{1})[2:m-1]$$

Inductively, we get

Defining $\mathbf{a}_{i}^{0} := \mathbf{a}_{j}$ we have

$$Q_j := \begin{bmatrix} I_{j-1j-1} & Q_{\mathbf{a}_j^j}^{\mathsf{H}} \\ Q_{\mathbf{a}_j^j} \end{bmatrix}$$
$$\mathbf{a}_j^k := (Q_k \mathbf{a}_j^{k-1})[2:m-k+1]$$
$$r_{kj} := (Q_k \mathbf{a}_j^{k-1})[1]$$

Then

$$Q_n \cdots Q_1 A = \underbrace{\begin{bmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \\ & & 0 \\ & & \vdots \\ & & 0 \end{bmatrix}}_{R}$$

$$\implies A = \underbrace{Q_1 \cdots Q_n}_{Q} R.$$

4.4 PLU Decomposition

4.4.1 Special "one-column" Lower triangular matrices

Consider the following set of lower triangular matrices

$$\mathcal{L}_{j} := \left\{ I + \begin{bmatrix} \mathbf{0}_{j} \\ \mathbf{1}_{j} \end{bmatrix} \mathbf{1}_{j}^{\mathbf{1}_{j}^{n-j}} \right\}$$

$$L_{j} = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & \ell_{j+1,j} & 1 & \\ & & \vdots & & \ddots & \\ & & \ell_{n,j} & & & 1 \end{bmatrix}$$

With the following properties:

$$\bullet \ L_j^{-1} = I - \begin{bmatrix} \mathbf{0}_j \\ \mathbf{l}_j \end{bmatrix} \mathbf{e}_j^T = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -\ell_{j+1,j} & 1 & \\ & & \vdots & & \ddots \\ & & -\ell_{n,j} & & 1 \end{bmatrix} \in \mathcal{L}_j$$

$$\bullet \ L_j L_k = I + \begin{bmatrix} \mathbf{0}_j \\ \mathbf{1}_j \end{bmatrix} \mathbf{e}_j^T + \begin{bmatrix} \mathbf{0}_k \\ \mathbf{1}_k \end{bmatrix} \mathbf{e}_k^T$$

• σ a permutation leaving first j rows fixed $(\sigma_{\ell} = \ell \ \forall \ \ell \leq j)$ and $L_j \in \mathcal{L}_{||}$

$$P_{\sigma}L_j = \tilde{L}_j P_{\sigma} \quad \tilde{L}_j \in \mathcal{L}_{|}$$

4.4.2 LU Decomposition

Similarly to QR decomposition we perform a triangularisation using $L_j \in \mathcal{L}_{||}$. Taking the following definitions

$$L_{j} := I - \begin{bmatrix} \mathbf{0}_{j} \\ \frac{\mathbf{a}_{j+1}^{j}[2:n-j]}{\mathbf{a}_{j+1}^{j}[1]} \end{bmatrix} \mathbf{e}_{j}^{T} \qquad \mathbf{a}_{j}^{k} := (L_{k}\mathbf{a}_{j}^{k-1})[2:n-k+1] \qquad u_{kj} := (L_{k}\mathbf{a}_{j}^{k-1})[1]$$

$$\implies L_{n-1} \dots L_{1}A = \underbrace{\begin{bmatrix} u_{11} & \cdots & u_{1n} \\ & \ddots & \vdots \\ & u_{nn} \end{bmatrix}}_{U}$$

$$A = \underbrace{L_{1}^{-1} \dots L_{n-1}^{-1}}_{L}U \qquad L_{j} = I + \begin{bmatrix} \mathbf{0}_{j} \\ \ell_{j+1,j} \\ \vdots \\ \ell_{n,j} \end{bmatrix} \mathbf{e}_{j}^{\top} \implies L = \begin{bmatrix} 1 \\ -\ell_{21} & 1 \\ -\ell_{31} & -\ell_{32} & 1 \\ \vdots & \vdots & \ddots & \ddots \\ -\ell_{n1} & -\ell_{n2} & \cdots & -\ell_{n,n-1} & 1 \end{bmatrix}$$

4.4.3 PLU Decomposition

Achieved by always pivoting when performing Gaussian elimination, swap largest in magnitude entry on the diagonal. This gives us

$$L_{n-1}P_{n-1}\dots P_2L_1P_1A=U$$

for P_j the permutation that leaves rows $1 \to j-1$ fixed, swapping row j with row $k \ge j$ whose entry is maximal in magnitude.

$$L_{n-1}P_{n-1}\dots P_2L_1P_1 = \underbrace{L_{n-1}\tilde{L}_{n-2}\dots \tilde{L}_1}_{L_{n-1}}\underbrace{P_{n-1}\dots P_2P_1}_{P}$$

Tilde denotes combined actions of swapping permutations and lower-triangular matrices.

$$P_{n-1} \cdots P_{j+1} L_j = \tilde{L}_j P_{n-1} \cdots P_{j+1} \implies \tilde{L}_j = I + \begin{bmatrix} \mathbf{0}_j \\ \tilde{\ell}_{j+1,j} \\ \vdots \\ \tilde{\ell}_{n,j} \end{bmatrix} \mathbf{e}_j^\top \implies L = \begin{bmatrix} 1 \\ -\tilde{\ell}_{21} & 1 \\ -\tilde{\ell}_{31} & -\tilde{\ell}_{32} & 1 \\ \vdots & \vdots & \ddots & \ddots \\ -\tilde{\ell}_{n-1,1} & -\tilde{\ell}_{n-1,2} & \cdots & -\tilde{\ell}_{n-1,n-2} & 1 \\ -\tilde{\ell}_{n1} & -\tilde{\ell}_{n2} & \cdots & -\tilde{\ell}_{n,n-2} & -\ell_{n,n-1} & 1 \end{bmatrix}$$

4.5 Cholesky Decomposition

Form of Gaussian elimination (without pivoting) for **symmetric positive definite matrices** Substantially faster.

Definition 4.1 (Positive definite)

A square matrix $A \in \mathbb{R}^{n \times n}$ positived definite if $\forall x \in \mathbb{R}^n, x \neq 0$ we have

$$x^T A x > 0$$

Proposition

 $A \in \mathbb{R}^{n \times n}$ positive deifinite and $V \in \mathbb{R}^{n \times n}$ non-singular

$$\implies V^T A V$$
 pos. definite

Proposition

 $A \in \mathbb{R}^{n \times n}$ positive definite \implies diagonal entries $a_{ii} > 0$

Theorem 4.1 (Subslice positive definite)

 $A \in \mathbb{R}^{n \times n}$ positive definite and $k \in 1, \dots, n^m$ a vector of m integers, each integer appearing only once

$$\implies A[k,k] \in \mathbb{R}^{m \times m}$$
 pos. definite

Theorem 4.2 (Cholesky and symmetric positive definite)

Matrix A symmetric positive definite \iff has Cholesky Decomposition

$$A = LL^T$$

Where diagonals of L positive.

Computing the Cholesky Decomposition

Using the following definitions:

$$\begin{array}{ll} A_1 := A & \alpha_k := A_k[1,1] \\ \mathbf{v}_k := A_k[2:n-k+1,1] & A_{k+1} := A_k[2:n-k+1,2:n-k+1] - \frac{\mathbf{v}_k \mathbf{v}_k^\top}{\alpha_k} \end{array}$$

$$\implies L = \begin{bmatrix} \sqrt{\alpha_1} & & & & \\ \frac{\mathbf{v}_1[1]}{\sqrt{\alpha_1}} & \sqrt{\alpha_2} & & & \\ \frac{\mathbf{v}_1[2]}{\sqrt{\alpha_1}} & \frac{\mathbf{v}_2[1]}{\sqrt{\alpha_2}} & \sqrt{\alpha_2} & & \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{\mathbf{v}_1[n-1]}{\sqrt{\alpha_1}} & \frac{\mathbf{v}_2[n-2]}{\sqrt{\alpha_2}} & \dots & \frac{\mathbf{v}_{n-1}[1]}{\sqrt{\alpha_{n-1}}} & \sqrt{\alpha_n} \end{bmatrix}$$

4.6 Timings

Different decompositions have trade-offs between stability and speed.

n = 100	# returns
A = Symmetric(rand(n,n)) + 100I	
<pre>@btime cholesky(A);</pre>	82.313 s
<pre>@btime lu(A);</pre>	127.977 s
<pre>@btime qr(A);</pre>	255.111 s

Stability

Stable	Unstable
QR with Householder reflections	LU usually, unless diagonally dominant matrix
Cholesky for pos. def.	PLU rarely unstable.

Set of Matrices for which PLU unstable extremely small, often one doesn't run into them.

5 Singular Values and Conditioning

5.1 Vector Norms

Definition 5.1 (Vector-norm)

Norm on $\|\cdot\|$ on \mathbb{R}^n a function satisfying the following, $\forall x, y \in \mathbb{R}^n$, $c \in \mathbb{R}$:

- (i) Triangle inequality: $||x + y|| \le |x| + |y|$
- (ii) Homogeneity: ||cx|| = |c|||x||
- (iii) Positive-definiteness: $||x|| = 0 \iff x = 0$

Definition 5.2 (p-norm)

For $1 \le p < \infty$, $x \in \mathbb{R}^n$

$$||x||_p := (\sum_{k=1}^n |x_k|^p)^{1/p}$$

 x_k k-th entry of x. $p = \infty$ we define

$$||x||_{\infty} := \max_{k} |x_k|$$

5.2 Matrix Norms

Definition 5.3 (Fröbenius norm)

Aa $m\times n$ matrix

$$||A||_F := \sqrt{\sum_{k=1}^m \sum_{j=1]^n} A_{kj}^2}$$

Given by norm(A) in Julia. norm(A) == norm(vec(A))

Definition 5.4 (Matrix-norm)

 $A \in \mathbb{R}^{n \times m}$ for 2 norms $\|\cdot\|_X$ on \mathbb{R}^n and $\|\cdot\|_Y$ on \mathbb{R}^n

We have the induced matrix norm

$$\begin{split} \|A\|_{X \to Y} &:= \sup_{\mathbf{v}: \|\mathbf{v}\|_X = 1} \|A\mathbf{v}\|_Y = \sup_{\in \mathbb{R}^n, x \neq 0} \frac{\|Ax\|_Y}{\|x\|_X} \\ \|A\|_X &:= \|A\|_{X \to X} \\ \|A\|_1 &= \max_j \|\mathbf{a}\|_1 \qquad \|A\|_\infty = \max_k \|A[k,:\|_1] \end{split}$$

Given by opnorm(A,1),opnorm(A,Inf) in Julia

5.3 Singular Value Decomposition

Definition 5.5 (Singular Value Decomposition)

For $A \in \mathbb{R}^{n \times n}$ with rank, r > 0

Reduced singular value decomposition (SVD) is

$$A = U\Sigma V^T$$

 $U \in \mathbb{R}^{m \times r}, V \in \mathbb{R}^{r \times n}$ that have orthonormal columns

 $\Sigma \in \mathbb{R}^{r \times r}$ diagonal of singular values, all positive and decreasing $\sigma_1 \leq \cdots \leq \sigma_r > 0$

Full singular value decomposition (SVD) is

$$A = \tilde{U}\tilde{\Sigma}\tilde{V}^Tx$$

 $\tilde{U} \in \mathbb{R}^{m \times m}, V \in \mathbb{R}^{n \times n}$ orthogonal matrices,

 $\tilde{\Sigma} \in \mathbb{R}^{m \times n}$ has only diagonal entries.

For $\sigma_k = 0$ if k > r

$$\tilde{\Sigma} = \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & \\ & & \sigma_n & \\ & & 0 & \\ & & \vdots & \\ & & 0 \end{bmatrix} \qquad \tilde{\Sigma} = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_m & 0 & \dots & 0 \end{bmatrix}$$

Proposition - Gram matrix kernel

Gram-matrix: $A^T A$ Kernel of A also kernel of A^A

Proposition - Gram matrix diagonalisation

Gram-matrix satisfies

$$A^T A = Q \Lambda Q^T$$

Q orthogonal and eigenvalues λ_k non-negative

Theorem 5.1 (SVD existence)

 $\forall A \in \mathbb{R}6m \times n \text{ has a SVD.}$

Corollary

 $A \in \mathbb{R}^{n \times n}$ invertible

$$\implies ||A||_2 = \sigma_1, \quad ||A^{-1}||_2 = \sigma_n^{-1}$$

Theorem 5.2 (Best low rank approximation)

$$A_k := egin{bmatrix} \mathbf{u}_1 | \dots | \mathbf{u}_k \end{bmatrix} egin{bmatrix} \sigma_1 & & & \ & \ddots & & \ & & \sigma_k \end{bmatrix} egin{bmatrix} \mathbf{v}_1 || \mathbf{v}_k \end{bmatrix}^T$$

The best 2-norm approximation of A by a rank k matrix. We have \forall matrices B of rank k, $||A - A_k||_2 \le ||A - B||_2$

5.4 Condition numbers

Proposition

 $|\epsilon_i| \leq \epsilon$ and $n\epsilon < 1$, then

$$\prod_{k=1}^{n} (1 + \epsilon_i) = 1 + \theta_n$$

for constant θ_n s.t $|\theta_n| \leq \frac{n\epsilon}{1-n\epsilon}$

Lemma. - Dot product backward error $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$

$$dot(\mathbf{x}, \mathbf{y}) = (\mathbf{x} + \delta \mathbf{x})^T \mathbf{y}$$

Where we have $|\delta \mathbf{x}| \leq \frac{n\epsilon_m}{2-n\epsilon_m} |\mathbf{x}|$, $|\mathbf{x}|$ absolute value of each entry.

Theorem 5.3 (Matrix-vector backward error)

$$A \in \mathbb{R}^{m \times n}, \mathbf{x} \in \mathbb{R}^n$$

$$mul(A, \mathbf{x}) = (A + \delta A)\mathbf{x}$$

Where $|\delta A| \leq \frac{n\epsilon_m}{2-n\epsilon_m} ||A|| \implies$

$$\begin{split} &\|\delta A\|_1 \leq \frac{n\epsilon_m}{2 - n\epsilon_m)} \|A\|_1 \\ &\|\delta A\|_2 \leq \frac{\sqrt{\min(m,n)}n\epsilon_m}{2 - n\epsilon_m} \|A\|_2 \\ &\|\delta A\|_\infty \leq \frac{n\epsilon_m}{2 - n\epsilon_m)} \|A\|_\infty \end{split}$$

Definition 5.6 (Condition number)

A a square matrix.

Condition number (in p-norm)

$$\kappa_p(A) := ||A||_p ||A^{-1}||_p$$

Under the 2-norm:

$$\kappa_2(A) = \frac{\sigma_1}{\sigma_n}$$

Theorem 5.4 (relative-error for matrix-vector)

Worst-case relative error in $A\mathbf{x} \approx (A + \delta A)\mathbf{x}$

$$\frac{\|\delta A\mathbf{x}\|}{\|A\mathbf{x}\|} \le \kappa(A)\epsilon$$

if we have relative perturbation error $\|\delta A\| = \|A\|\epsilon$

We know for floating point arithmetic the error is bounded by

$$\kappa(A) \frac{n\epsilon_m}{2 - n\epsilon_m}$$

6 Differential equations via Finite differences

6.1 Indefinite integration

For simple differential equation on interval [a, b]

$$u(a) = c$$

$$u'(x) = f(x)$$

We have, for $u_k \approx u(x_k), k\bar{1}, \dots, n-1$

$$f(x_k) = u'(x_k) \approx \frac{u_{k+1} - u_k}{h} = f(x_k)$$

As a linear system

$$\underbrace{\frac{1}{h} \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & -1 & 1 \end{bmatrix}}_{D_h \in \mathbb{R}^{n-1 \times n}} \mathbf{u}^f = \underbrace{\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_{n-1}) \end{bmatrix}}_{\mathbf{f}^f}$$

Super-script f denotes forward differences.

 D_h not square \implies need to add extra row from the initial condition $\mathbf{e}^T \mathbf{u}^f = c$

$$\begin{bmatrix} \mathbf{e}_1^T \\ D_h \end{bmatrix} \mathbf{u}^f = \underbrace{\begin{bmatrix} 1 \\ -1/h & 1/h \\ & \ddots & \ddots \\ & & -1/h & 1/h \end{bmatrix}}_{L_h} \mathbf{u}^f = \begin{bmatrix} c \\ \mathbf{f}^f \end{bmatrix}$$

Lower-triangular bidiagonal system \implies solved using forward substitution in O(n) Can choose either central or backwards-difference formulae too.

 $Central\ differences$

Take $m_k = \frac{x_{k+1} - x_k}{2} \implies u'(m_k) \approx \frac{u_{k+1} - u_k}{h} = f(m_k)$

$$\underbrace{\frac{1}{h} \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}}_{D_{k}} \mathbf{u}^{m} = \underbrace{\begin{bmatrix} f(m_{1}) \\ \vdots \\ f(m_{n-1}) \end{bmatrix}}_{\mathbf{f}^{m}}$$

Convergence

We see experimentally that the error for solutions from forward differences is $O(n^{-1})$ while for central differences it is a faster $O(n^{-2})$ convergence.

Both appearing to be stable.

6.2 Forward Euler

Consider scalar linear time-evolution for $0 \le t \le T$

$$u(0) = c$$

$$u'(t) - a(t)u(t) = f(t)$$

Label *n*-point gird as $t_k = (k-1)h$, $h = \frac{T}{n-1}$

Definition 6.1 (Restriction Matrices)

Define $n-1 \times n$ restriction matrices as

$$I_n^{\mathbf{f}} := \begin{bmatrix} 1 & & & \\ & \ddots & & \\ & & 1 & 0 \end{bmatrix}$$

$$I_n^{\mathbf{b}} := \begin{bmatrix} 0 & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}$$

Can replace discretisation using finite differences. $\frac{u_{k+1}-u_k}{h}-a(t_k)u_k=f(u_k)$ Giving us the linear system

$$\begin{bmatrix} \mathbf{e}_1^T \\ D_h - I_n^f A_n \end{bmatrix} \mathbf{u}^f = \underbrace{\begin{bmatrix} 1 \\ -a(t_1) - 1/h & 1/h \\ & \ddots & \ddots \\ & & -a(t_{n-1}) - 1/h & 1/h \end{bmatrix}}_{L} \mathbf{u}^f = \begin{bmatrix} c \\ I_n^f \mathbf{f} \end{bmatrix}$$

Where we have

$$A_n = \begin{bmatrix} a(t_1) & & \\ & \ddots & \\ & & a(t_n) \end{bmatrix} \quad \mathbf{f} = \begin{bmatrix} f(t_1) \\ \vdots \\ f(t_n) \end{bmatrix}$$

6.3 Backward Euler

Simply replace forward-difference with backward-difference $\frac{u_k - u_{k-1}}{h} - a(t_k)u_k = f(u_k)$ Giving us our system:

$$\begin{bmatrix} \mathbf{e}_{1}^{T} \\ D_{h} - I_{n}^{b} A_{n} \end{bmatrix} \mathbf{u}^{f} = \underbrace{\begin{bmatrix} 1 \\ -1/h & 1/h - a(t_{2}) \\ & \ddots & \ddots \\ & & -1/h & 1/h - a(t_{n}) \end{bmatrix}}_{I} \mathbf{u}^{b} = \begin{bmatrix} c \\ I_{n}^{b} \mathbf{f} \end{bmatrix}$$

Still bidiagonal forward-substitution

$$u_1 = c$$

$$(1 - ha(t_{k+1}))u_{k+1} = u_k + hf(t_{k+1})$$

$$u_{k+1} = (1 - ha(t_{k+1}))^{-1}(u_k + hf(t_{k+1}))^{-1}(u_k + hf(t_k))^{-1}(u_k + hf(t_k))^{-1}(u_$$

6.4 Systems of equations

Solving systems of the form

$$\mathbf{u}(0) = c$$

$$\mathbf{u}'(t) - A(t)\mathbf{u}(t) = f(t)$$

For $\mathbf{u}, \mathbf{f} : [0, T] \to \mathbb{R}^d$ and $A : [0, T] \to \mathbb{R}^{d \times d}$ Once again discretise at the grid t_k approximating $\mathbf{u}(t_k) \approx \mathbf{u}_k \in \mathbb{R}^d$

Forward-Euler

$$\mathbf{u}_1 = c$$

 $\mathbf{u}_{k+1} = (I - hA(t_{k+1}))^{-1}(\mathbf{u}_k + h\mathbf{f}(t_{k+1}))$

6.5 Nonlinear problems

Forward-euler extends naturally to nonlinear equations.

$$\mathbf{u}' = f(t, \mathbf{u}(t))$$

Becomes:

$$\mathbf{u}_{k+1} = \mathbf{u}_k + h f(t_k, \mathbf{u}_k)$$

6.6 Two-point boundary value problem

Consider one discretisation, since symmetric

$$u''(x) \approx \frac{u_{k-1} = 2u_k + u_{k+1}}{h^2}$$

So we use the $n-1 \times n+1$ matrix

$$D^2h := \frac{1}{h^2} \begin{bmatrix} 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \end{bmatrix}$$

6.7 Convergence

Definition 6.2 (Toeplitz)

Toeplitz matrix has constant diagonals

$$T[k,j] = a_{k-j}$$

Proposition. - (Bidiagonal Toeplitz inverse)

Inverse of $n \times n$ bidiagonal Toeplitz matrix is

$$\begin{bmatrix} 1 & & & & & \\ -\ell & 1 & & & & \\ & -\ell & 1 & & & \\ & & \ddots & \ddots & & \\ & & & & -\ell & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & & & & \\ \ell & 1 & & & \\ \ell^2 & \ell & 1 & & \\ \vdots & \ddots & \ddots & \ddots & \\ \ell^{n-1} & \cdots & 2 & \ell & 1 \end{bmatrix}$$

Theorem 6.1 (Forward/Backward Euler Convergence)

Consider equation

$$u(0) = c, \quad u'(t) + au(t) = f(t)$$

Denote

$$\mathbf{u} := \begin{bmatrix} u(t_1) \\ \vdots \\ u(t_n) \end{bmatrix}$$

Assume u twice differentiable with uniformly bounded 2nd derivative.

 \implies error for forwardEuler is

$$\|\mathbf{u}^f - \mathbf{u}\|_{\infty}, \|\mathbf{u}^b - \mathbf{u}\|_{\infty} = O(n^{-1})$$

6.7.1 Poisson

For 2D problems consider Poisson. First stage is to row-reduce to get a summetric tridiagonal pos. def. matrix

$$\begin{bmatrix} 1 & & & & & & \\ -1/h^2 & 1 & & & & & \\ & & 1 & & & & \\ & & & 1 & & & \\ & & & \ddots & & & \\ & & & & 1 & -1/h^2 \\ & & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & & & & \\ 1/h^2 & -2/h^2 & 1/h^2 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1/h^2 & -2/h^2 & 1/h^2 \\ & & & & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ 0 & -2/h^2 & 1/h^2 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1/h^2 & -2/h^2 & 0 \\ & & & & & 1 \end{bmatrix}$$

Consider right-hand side, aside from first and last row, we have

$$\frac{1}{h^{2}} \underbrace{\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix}}_{\Delta} \begin{bmatrix} u_{2} \\ \vdots \\ u_{n-1} \end{bmatrix} = \underbrace{\begin{bmatrix} f(x_{2}) - c_{0}/h^{2} \\ f(x_{3}) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) - c_{1}/h^{2} \end{bmatrix}}_{\mathbf{f}p}$$

Theorem 6.2 (Poisson Convergence)

Suppose u four-times differentiable with uniformly bounded fourth-derivative \implies finite difference approximation to Poisson convergence like $O(n^2)$