Numerical Analysis - Concise Notes

MATH50003

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

Content from MATH40005 assumed to be known.

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Contents

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
$u = (u_1, \dots, u_n)$ and $v = (v_1, \dots, vn)$

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

Length of $u, ||u|| = \sqrt{u \cdot u}$
Distance between u and $v = ||u - v||$

- P orthogonal if $P^T P = I, (Pu \cdot Pv) = u \cdot v)$
- 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:

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

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

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

Definition - Invariant subspaces
$T : V \to V$ a linear map, W a subspace of V.

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

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.

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

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

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

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 $= \{\lambda_i\}$
- $detA = \prod_{i=1}^{n} \lambda_i$
- AB also upper triangular, with $diag(AB) = \lambda_1\mu_1, \ldots, \lambda_n\mu_n$

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

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 $deg(g) \geq 1$, 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
$f, g \in F[x]\backslash\{0\}$, **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
$d = gcd(f, g) \implies \exists r, s \in F[x]$ s.t $d = rf + sg$

Definiton - Irreducible polynomials
$p(x) \in F[x]$ irreducible over F if $deg(p) \geq 1$ and p not factorisable over F as a product of $\{f_i\} \in F$ s.t $deg(f_i \leq deg(p)$
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 $deg(f) \geq 1$

$$f = p_1 \dots p_r$$

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

- $c_T(x) = c_{T_W}(x)c_{\bar{T}}(x)$
- $m_{T_W}(x)$ 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 $1 \leq i \leq k$, 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 $V_i = ker g_i(T), i = 1, 2$ 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 $J, = (x - \lambda)^n)$
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:

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

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, $dimE_\lambda(A) = \sum_{i=1}^{k} dimE_\lambda(A_i)$
- $\forall q(x) \in F[x]$, $q(A) = q(A_1) \oplus \cdots \oplus q(A_k)$

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;

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

Properties of JCF
J as above, λ an eigenvalue;

1. $n_1 + \cdots + n_a = a(\lambda)$
2. $a =$ number of λ-blocks $= g(\lambda)$
3. $\max(n_1, \dots, n_a) = r$, 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 $\implies \exists$ 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 $u_1, S(u_1), \ldots, S^{m_1-1}(u_1), \ldots u_r, S(u_r), \ldots, S^{m_r-1}(u_r)$

(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

$$\begin{aligned} Z(v,T) &= \{f(T)(v) \ : \ f(x) \in F[x]\} \\ &= \mathrm{Sp}(v, T(v), T^2(v), \ldots) \end{aligned}$$

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

$$\implies T^k(v) = -a_0 v - a_1 T(v) - \cdots - a_{k-1} T(v)$$

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

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

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 $f(x) \in F[x]$
$\implies \exists v_1, \ldots, v_r \in V$ 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 $1 \leq i \leq r, \ k = k_1 \geq k_2 \geq \cdots \geq k_r$

(2) r and $k_1, \ldots, k_r$ uniquely determined by T

Corollary 12.3
T a finite dimensional vector space over F
$\implies \exists$ basis B of V 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

$$[T]_B = C(f_1(x)^{k_{11}}) \oplus \cdots \oplus C(f_1(x)^{k_{1r_1}}) \oplus \ldots$$
$$\oplus C(f_t(x)^{k_{t1}}) \oplus \cdots \oplus C(f_t(x)^{k_{tr_t}})$$

where for each i
$$k_i = k_{i1} \geq \cdots \geq k_{ir_i}$$
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) $(\phi_1 + \phi_2)(v) = \phi_1(v) + \phi_2(v), \qquad \forall v \in V$

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

Definition - The dual space

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

V^* a vector space over F w.r.t above multiplication and addition.
Dimension
$\{v_i\}_i$ a basis of V with eigenvalues $\{\lambda\}_i$
$\exists! \phi \in V^*$ 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

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

$\implies \phi_i(\sum \alpha_j v_j) = \alpha_i \implies \{\phi_1, \ldots, \phi_n\}$ 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 $X^0 of X :$

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

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) $(w, v) = (\bar{w, v})$

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

$\forall v_i, v, w \in V$ 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 $\mathbb{R} \implies A$ symmetric

F $\implies A$ 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) $|(u, v)| \leq ||u|| ||v||$ *(Cauchy-Schwarz Inequality)*

(ii) $||u + v|| \leq ||u|| + ||v||$

(iii) $||u - v|| \leq ||u - w|| + ||w - v||$ *(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
$\{v_1, \dots, v_k\}$ 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 $\{w_1, \dots, w_r\}$ can be extended to orthonormal basis of V

Gram-Schmidt Process

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

***Step 2* -** let $u_1 = \frac{v_1}{||v_1||}$ define $w_2 = v_2 - (v_2, u_1)u_1$
$\implies (w_2, u1) = 0, \quad$ 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 $u_3 = \frac{w_3}{||w_3||} \implies \{u_1, u_2, u_3\}$

***Step 4* -** Continue, for i^{th} step

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

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

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

Projections
V an inner product space. $v, w \in V \backslash 0$
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:

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

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

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) $\text{dist}(v, w)$ denotes shortest distance from v to any vector in W
$\implies \text{dist}(v, w) = ||v - \pi_W(v)$

(iii) $\{v_1, \ldots, v_r\}$ 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. $E = \{e_1, \ldots, e_n\}$, $F = \{f_1, \ldots, f_n\}$ 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
- $P \in M_n() : P^T \bar{P} = I \implies$ unitary matrix

Properties of the above matrices

(i) length-preserving maps of $\mathbb{R}^n, ^n$ (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; $U(n,) = \{P \in M_n() : P^T \bar{P} = I$

15 Linear maps on inner product spaces

Proposition 15.1.
V a finite dimensional inner product space. $T : V \to V$ a linear map
$\implies \exists!$ linear map $T^* : V \to V$ s.t $\forall u, v \in V$

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

Say T^* - **adjoint of T**
T **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, $A = [T]_E$
$\implies [T^*]_E = \bar{A}^T$ 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
- $A \in M_n() \implies \exists$ unitary P s.t $P^{-1}AP$ 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 $A \in M_n(F)$
$\implies (u, v) = u^T Av \quad \forall u, v \in V$ 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

$$(v, w) = 0 \iff (w, v) = 0$$
$$\iff$$
$$(,) \text{ skew-symmetric or symmetric}$$

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

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

$V^\perp = \{0\} \iff$ 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 $B = \{e_1, f_1, \ldots, e_m, f_m\}$ 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 $B = \{v_1, \ldots, v_n\}$

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

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

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

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

$(,)$ 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

$$(x, y) = x^T Ay \qquad \text{for } A = A^T, (x, y \in V)$$

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

$$\begin{aligned} Q(x) &= x^T Ax \\ &= \sum_{i,j} a_{ij} x_i x_j \\ &= \sum_{i=1}^{n} a_{ii} x_i^2 + 2 \sum i < j a_{ij} x_i x_j \end{aligned}$$

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

Change of variables

Definition - **Equivalent Quadratic Forms**

$V = F^n,\ Q : V \to F$
$Q(x) = x^T Ax\ \forall x \in V, A$ symmetric
Take $y = (y_1, \ldots, y_n)^T$ s.t $x = Py$ for P invertible
$\implies Q(x) = y^T P^T APy = Q'(y)$
If such a P exists we say Q, Q' **equivalent**
note:
Congruent matrices $A, P^T AP$
$A \sim P^T AP \iff P$ orthogonal

Theorem 16.8.
$V = F^n$, $Q : V \to F$ non-degenerate quadratic form

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

$$Q_0(x) = x_1^2 + \cdots + x_n^2 \quad (x \in^n)$$

Has matrix I_n

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

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

Has matrix $I_{p,q} = \begin{pmatrix} \mathrm{I}_p & 0 \\ 0 & \text{-}\mathrm{I}_q \end{pmatrix}$

(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 $[T]_B = X \implies T \in I(V, f) \iff X^T AX = A$

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

- f skew-symmetric $\implies$ there is only one form (up to equivalence) so we get one isometry group; Classical ***symplectic group*** $\text{Sp}(V, f)$
- 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**

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

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

$$(B_p \ldots B_0.b_1 b_2 b_3 \ldots)_2 = (B_p \ldots B_0)_2 + \frac{b_1}{2} + \frac{b_2}{2^2} + \frac{b_3}{2^3} + \cdots$$

1.2 Integers

Definition 1.2 ***Ring of integers modulo*** m

$$\mathbb{Z}_m := \{0\ (mod\ m), 1\ (mod\ m), \ldots, m-1\ (mod\ m)\}$$

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.

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

$2^p - y$ interpreted as $-y$
e.g

```
11001001 = -55       01001001 = 73
```

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

```
typemax(Int8) + Int8(1)# returns typemin(Int8)
127 + 1 = -128
```

```
 01111111
 00000001+
 --------
=10000000
```

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 ($\div$)
$5 \div 2$ 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

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

With each component as such

$$\begin{aligned} F^{normal}_{\sigma,Q,S} &= \{\pm 2^{q-\sigma} \times (1.b_1 b_2 \dots b_S)_2 : 1 \leq q < 2^Q - 1\} \\ F^{sub-normal}_{\sigma,Q,S} &= \{\pm 2^{1-\sigma} \times (0.b_1 b_2 b_3 \dots b_S)_2\}. \\ F^{special} &= \{-\infty, \infty, \texttt{NaN}\} \end{aligned}$$

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

$$s q_{Q-1} \dots q_0 b_1 \dots b_S$$

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) $1 \leq q < 2^Q - 1$ - Bits represent normal number

$$x = \pm 2^{q-\sigma} \times (1.b_1 b_2 b_3 \dots b_S)_2$$

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

$$x = \pm 2^{1-\sigma} \times (0.b_1 b_2 b_3 \dots b_S)_2.$$

(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

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

`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:

$$\epsilon_{m,S} := 2^{-S}$$
$$\min |F^{normal}_{\sigma,Q,S}| = 2^{1-\sigma}$$

Largest (postive) normal number is

$$\max F^{normal}_{\sigma,Q,S} = 2^{2^Q-2-\sigma}(1.11\dots1)_2 = 2^{2^Q-2-\sigma}(2 - \epsilon_m)$$

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***

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

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.

$$
\begin{aligned}
x \oplus y &:= fl(x+y) \\
x \ominus y &:= fl(x-y) \\
x \otimes y &:= fl(x*y) \\
x \oslash y &:= fl(x/y)
\end{aligned}
$$

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:

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

Proposition. - *Rounding arithmetic*

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

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

With relative error:

$$
\begin{aligned}
|\delta_x^{nearest}| &\leq \frac{\epsilon_m}{2} \\
|\delta_x^{up/down}| &< \epsilon_m.
\end{aligned}
$$

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
                             1/Inf        #  0.0          NaN == NaN   #  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 $x \in F^{normal}$

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
```

```
(0.3333333333333333333333333333333333333333333333333333333333333333333333333333305,
 0.3333333333333333333333333333333333333333333333333333333333333333333333333333348)
```

2 Differentiation

Considering functions:

(i) *Black-box function* $f^{FP} : D \to F,\ D \subset F \equiv F_{\sigma,Q,S}$
Only know function pointwise, F discrete $\implies f^{FP}$ 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 $f^{FP} : D \cap F \to F$, 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

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

where $M = \sup_{x \leq t \leq x+h} |f''(t)|$. 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 $f^{FP} = f(x) + \delta_x^f$ has uniform absolute accuracy in that neighbourhood i.e $|\delta_x^f| \leq c\epsilon_m$ for fixed constant c.

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

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

Where

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

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

$$\implies q(x) := f(g(x)) \text{ a dual extension at a}$$

f, g dual extensions at a

$$\implies r(x) := f(x)g(x) \text{ a dual extension at a}$$

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

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

Transposing `A` done lazily, `A'` stores entries by row

Matrix multiplication done as expected `A*x`

Implemented 2 ways

Using Traditional definition

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

Or going column-by-column

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

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

Solving a linear system done by `\`

```
A = [1 2 3;         returns # 41.000000000000036
     1 2 4;                  -17.000000000000014
     3 7 8]                   1.0
b = [10; 11; 12]
A \ b
```

3.2 Triangular Matrices

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

```
A = [1 2 3;
     4 5 6;
     7 8 9]
```

```
U = UpperTriangular(A)
#  1  2  3
      5  6
         9
```

```
L = LowerTriangular(A)
# 1
  4  5
  7  8  9
```

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 $x_n, x_{n-1}, \ldots, x_1$ 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 `Vector`s in Julia.

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

Definition 3.3 ***Bidiagonal***

Matrix bidiagonal if square and has bandwidths

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

```
Bidiagonal([1,2,3], [4,5], :L)
# 1
  4  2
     5  3
```

```
Bidiagonal([1,2,3], [4,5], :U)
# 1  4
     2  5
        3
```

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

Definition 3.4 ***Tridiagonal***

Matrix tridiagonal if square and has bandwidths $l = u = 1$

```
Tridiagonal([1,2], [3,4,5], [6,7])
#  3  6
   1  4  7
      2  5
```

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 $\{1, 2, \ldots, n\}$ and itself.

Cauchy Notation

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

Where $\{\sigma_1, \ldots, \sigma_n\} = \{1, 2, \ldots, n\}$
Inverse permutation given by σ^{-1}, found by swapping rows of cauchy notation and reordering.

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

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

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

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 $Q^T Q = QQ^T = I$
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 $[a, b]^T$

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

```
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 $\mathbf{v}$ 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 $A \in \mathbb{R}^{m\times n},\ m \geq n$)

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

   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)

$$A = P^T LU$$

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

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

$$A = LL^T$$

Useful as component pieces easily inverted on a computer.

$$
\begin{aligned}
A = P^T LU &\implies A^{-1}\mathbf{b} = U^{-1}L^{-1}P\mathbf{b} \\
A = QR &\implies A^{-1}\mathbf{b} = R^{-1}Q^{\top}\mathbf{b} \\
A = LL &\implies A^{-1}\mathbf{b} = L^{-}L^{-1}\mathbf{b}
\end{aligned}
$$

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

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

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 $A = \left[\mathbf{a}_1|\ldots|\mathbf{a}_n\right]$, $a_k \in \mathbb{R}^m$
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 $\hat{Q}$

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

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

$$
\begin{aligned}
\mathbf{v} &= \left[\mathbf{a}_1|\ldots|\mathbf{a}_j\right]\mathbf{c} \\
&= \left[\mathbf{q}_1|\ldots|\mathbf{q}_j\right]\hat{R}[1:j, 1:j]\mathbf{c} \\
&\in \mathit{span}(\mathbf{q}_1, \ldots, \mathbf{q}_n)
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbf{w} &= \left[\mathbf{q}_1|\ldots|\mathbf{q}_j\right]\mathbf{d} \\
&= \left[\mathbf{a}_1|\ldots|\mathbf{a}_j\right]\hat{R}[1:j, 1:j]^{-1}\mathbf{d} \\
&\in \mathit{span}(\mathbf{a}_1, \ldots, \mathbf{a}_j)
\end{aligned}
$$

We can find an orthogonal basis using Gram-Schmidt.

1. By assumption of full rank of A
$$\mathit{span}(\mathbf{a}_1, \ldots, \mathbf{a}_n) = \mathit{span}(\mathbf{q}_1, \ldots, \mathbf{q}_n)$$

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 $k < j$

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

5. Define further

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

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

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

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

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 $r_{11} = -(a_1 1)\|a_1\|$ with all entries of $\mathbf{a}_1^1$ zero.
Now consider,

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

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 $\mathbf{a}_j^0 := \mathbf{a}_j$ we have

$$Q_j := \begin{bmatrix} I_{j-1j-1} & \\ & Q_{\mathbf{a}_j^j}^{,H} \end{bmatrix}$$

$$\mathbf{a}_j^k := (Q_k \mathbf{a}_j^{k-1})[2 : m - k + 1]$$

$$r_{kj} := (Q_k \mathbf{a}_j^{k-1})[1]$$

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

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

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

With the following properties:

- $L_j^{-1} = I - \begin{bmatrix} \mathbf{0}_j \\ \mathbf{l}_j \end{bmatrix} \mathbf{e}_j^T = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -\ell_{j+1,j} & 1 & \\ & & \vdots & & \cdots \\ & & -\ell_{n,j} & & & 1 \end{bmatrix} \in \mathcal{L}_j$
- $L_j L_k = I + \begin{bmatrix} \mathbf{0}_j \\ \mathbf{l}_j \end{bmatrix} \mathbf{e}_j^T + \begin{bmatrix} \mathbf{0}_k \\ \mathbf{l}_k \end{bmatrix} \mathbf{e}_k^T$
- 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 $k \geq j$ whose entry is maximal in magnitude.

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

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

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

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

$$x^TAx > 0$$

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

$$\implies V^TAV \text{ pos. definite}$$

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

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

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:

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

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

4.6 Timings

Different decompositions have trade-offs between stability and speed.

```
n = 100                                       # returns
A = Symmetric(rand(n,n)) + 100I
@btime cholesky(A);                           82.313 s
@btime lu(A);                                 127.977 s
@btime qr(A);                                 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: $\|x + y\| \leq |x| + |y|$

(ii) Homogeneity: $\|cx\| = |c|\|x\|$

(iii) Positive-definiteness: $\|x\| = 0 \iff x = 0$

Definition 5.2 *(p-norm)*

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

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

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)*

A a $m \times n$ 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**

$$\|A\|_{X \to Y} := \sup_{\mathbf{v}:\|\mathbf{v}\|_X = 1} \|A\mathbf{v}\|_Y = \sup_{\in \mathbb{R}^n, x \neq 0} \frac{\|Ax\|_Y}{\|x\|_X}$$

$$\|A\|_X := \|A\|_{X \to X}$$

$$\|A\|_1 = \max_j \|\mathbf{a}\|_1 \qquad \|A\|_\infty = \max_k \|A[k, :\|_1$$

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

$$A = \tilde{U}\tilde{\Sigma}\tilde{V}^T x$$

$\tilde{U} \in \mathbb{R}^{m\times m}, V \in \mathbb{R}^{n\times n}$ orthogonal matrices,
$\tilde{\Sigma} \in \mathbb{R}^{m\times n}$ has only diagonal entries.
For $\sigma_k = 0$ if $k > r$

if $m > n$	if $m < n$
$\tilde{\Sigma} = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & & 0 \\ & & \vdots \\ & & 0 \end{bmatrix}$	$\tilde{\Sigma} = \begin{bmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_m & 0 & \dots & 0 \end{bmatrix}$

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)*

$\forall A \in \mathbb{R}6m \times n$ 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)*

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

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

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

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

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 $A\mathbf{x} \approx (A + \delta A)\mathbf{x}$

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

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 $u_k \approx u(x_k), k\bar{1}, \ldots, n-1$

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

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

$$\underbrace{\frac{1}{h}\begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}}_{D_h} \mathbf{u}^m = \underbrace{\begin{bmatrix} f(m_1) \\ \vdots \\ f(m_{n-1}) \end{bmatrix}}_{\mathbf{f}^m}$$

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 $0 \leq t \leq T$

$$\begin{aligned} u(0) &= c \\ u'(t) - a(t)u(t) &= f(t) \end{aligned}$$

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**

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

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:

$$\begin{bmatrix} \mathbf{e}_1^T \\ D_h - I_n^b A_n \end{bmatrix} \mathbf{u}^f = \underbrace{\begin{bmatrix} 1 & & & \\ -1/h & 1/h - a(t_2) & & \\ & \ddots & \ddots & \\ & & -1/h & 1/h - a(t_n) \end{bmatrix}}_{L} \mathbf{u}^b = \begin{bmatrix} c \\ I_n^b \mathbf{f} \end{bmatrix}$$

Still bidiagonal forward-substitution

$$\begin{aligned} u_1 &= c \\ (1 - ha(t_{k+1}))u_{k+1} &= u_k + hf(t_{k+1}) \\ u_{k+1} &= (1 - ha(t_{k+1}))^{-1}(u_k + hf(t_{k+1}) \end{aligned}$$

6.4 Systems of equations

Solving systems of the form

$$\begin{aligned} \mathbf{u}(0) &= c \\ \mathbf{u}'(t) - A(t)\mathbf{u}(t) = f(t) \end{aligned}$$

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

$$\begin{aligned} \mathbf{u}_1 &= c \\ \mathbf{u}_{k+1} &= (I - hA(t_{k+1}))^{-1}(\mathbf{u}_k + h\mathbf{f}(t_{k+1})) \end{aligned}$$

6.5 Nonlinear problems

Forward-euler extends naturally to nonlinear equations.

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

Becomes:

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

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

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

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

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

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 $O(n^2)$

7 Fourier Series

Definition 7.1 *(Complex Fourier Series)*

$$f(\theta) = \sum_{n=-\infty}^{\infty} \hat{f}_k e^{ik\theta}$$

$$\hat{f}_k := \frac{1}{2\pi}\int_0^{2\pi} f(\theta)e^{-ik\theta}d\theta$$

Written as

$$f(\theta) = \underbrace{[\ldots|e^{-2i\theta}|e^{-i\theta}|\underline{1}|e^{i\theta}|e^{2i\theta}|\ldots]}_{F(\theta)} \underbrace{\begin{bmatrix} \vdots \\ \hat{f}_{-2} \\ \hat{f}_{-1} \\ \underline{\hat{f}_0} \\ \hat{f}_1 \\ \hat{f}_2 \\ \vdots \end{bmatrix}}_{\hat{\mathbf{f}}}$$

Build approximation using n approximate coefficients $\hat{f}_k^n \approx \hat{f}_k$
Seperating into 3 cases:

(i) Odd: $n = 2m + 1$ we approximate

$$\begin{aligned} f(\theta) &\approx \sum_{k=-m}^{m} \hat{f}^n e^{ik\theta} \\ &= \underbrace{[e^{-im\theta}|\ldots|e^{-2i\theta}|e^{-i\theta}|1|e^{i\theta}|e^{2i\theta}|\ldots|e^{im\theta}]}_{F_{-m:m}(\theta)} \begin{bmatrix} \hat{f}_{-m}^n \\ \vdots \\ \hat{f}_m^n \end{bmatrix} \end{aligned}$$

(ii) Even: $n = 2m$ we approximate

$$\begin{aligned} f(\theta) &\approx \sum_{k=-m}^{m-1} \hat{f}^n e^{ik\theta} \\ &= \underbrace{[e^{-im\theta}|\ldots|e^{-2i\theta}|e^{-i\theta}|1|e^{i\theta}|e^{2i\theta}|\ldots|e^{i(m-1)\theta}]}_{F_{-m:m-1}(\theta)} \begin{bmatrix} \hat{f}_{-m}^n \\ \vdots \\ \hat{f}_{m-1}^n \end{bmatrix} \end{aligned}$$

(iii) Taylor: if we know negative coefficients vanish ($0 = \hat{f}_{-1} = \hat{f}_{-2} = \ldots$ we approximate:

$$\begin{aligned} f(\theta) &\approx \sum_{k=0}^{n-1} \hat{f}^n e^{ik\theta} \\ &= \underbrace{[1|e^{i\theta}|e^{2i\theta}|\ldots|e^{i(n-1)\theta}]}_{F_{0:n-1}(\theta)} \begin{bmatrix} \hat{f}_0^n \\ \vdots \\ \hat{f}_{n-1}^n \end{bmatrix} \end{aligned}$$

Can be thought of as approximate Taylor expansion using change of var $z = e^{i\theta}$

7.1 Basics of Fourier series

Focus on case where $\hat{f}_k$ absolutely convergent (1-norm of $\mathbf{f}$ bounded)

$$\|\hat{\mathbf{f}}\|_1 = \sum_{k=-\infty}^{\infty} |\hat{f}_k| < \infty$$

Theorem 7.1 *(Convergence)*

if Fourier coefficients absolutely convergent

$$\implies f(\theta) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ik\theta}, \quad \text{Converges Uniformly}$$

Remark
Also have convergence for continuous version of 2-norm

$$\|f\|_2 := \sqrt{\int_0^{2\pi} |f(\theta)|^2 d\theta},$$

for any function s.t $\|f\|_2 < \infty$

Proposition - *(Differentiability and absolutely convergence)*
if $f : \mathbb{R} \to$ and f' periodic, with f' uniformly bounded
$\implies$ fourier coeff satisfy:

$$\|\hat{\mathbf{f}}\|_1 < \infty$$

Remark
More times differentiabel a function $\implies$ faster the coeff. decay $\implies$ faster Fourier series converges.
If function smooth,2π periodic $\implies$ fourier coeffs. decay faster than algebraically; decay like $O(k^{-2})$ $\forall\lambda$

Remark
Let $z = e^{i\theta}$ then if $f(z)$ analytic in a neighbourhood of unit circle
$\implies$ fourier coeff. decay exponentially fast

$f(z)$ entire $\implies$ decay faster than exponentially fast.

7.2 Trapezium rule + discrete Fourier coefficients

$$\theta_j = \frac{2\pi j}{n}, \ j = 0, 1, \ldots, n$$

Gives $n+1$ evenly spaced points over $[0, 2\pi]$

Definition 7.2 *(Trapezium rule)*

Trapezium rule over $[0, 2\pi]$

$$\int_0^{2\pi} f(\theta) d\theta \approx \frac{2\pi}{n} \left[\frac{f(0)}{2} + \sum_{j=1}^{n-1} f(\theta_j) + \frac{f(2\pi)}{2} \right]$$

f periodic; $f(0) = f(2\pi)$

$$\implies \int_0^{2\pi} f(\theta) d\theta \approx 2\pi \underbrace{\frac{1}{n} \sum_{j=0}^{n-1} f(\theta_j)}_{\sum_n [f]}$$

Define Trapezium rule approximation to Fourier coeffs by

$$\hat{f}_k^n := \sum_n [f(\theta) e^{-ik\theta}] = \frac{1}{n} \sum_{j=0}^{n-1} f(\theta_j) e^{-ik\theta_j}$$

Lemma. *(Discrete Orthogonality*
We have:

$$\sum_{j=0}^{n-1} e^{ik\theta_j} = \begin{cases} n & k = \ldots, -2n, -n, 0, n, 2n, \ldots \\ 0 & \text{otherwise} \end{cases}$$

In other words,

$$\sum_n [e^{i(k-j)\theta_j}] = \begin{cases} 1 & k - j = \ldots, -2n, -n, 0, n, 2n, \ldots \\ 0 & \text{otherwise} \end{cases}.$$

Theorem 7.2 *(Discrete Fourier coefficients)*

f absolutely convergent

$$\implies \hat{f}_k^n = \cdots + \hat{f}_{k-2n} + \hat{f}_{k-n} + \hat{f}_k + \hat{f}_{k+n} + \hat{f}_{k+2n} + \ldots$$

Corollary. *(Aliasing)*
$\forall p \in \mathbb{Z}, \hat{f}_k^n = \hat{f}_{k+pn}^n$.
If we know $\hat{f}_0^n, \ldots, \hat{f}_{n-1}^n \implies$ we know $\hat{f}_k^n\ \forall k$ via permutations.
e.g $n = 2m+1$

$$\begin{bmatrix} \hat{f}_{-m}^n \\ \vdots \\ \hat{f}_m^n \end{bmatrix} = \underbrace{\begin{bmatrix} & & & 1 & \\ & & & & \ddots & \\ & & & & & 1 \\ 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \end{bmatrix}}_{P_\sigma} \begin{bmatrix} \hat{f}_0^n \\ \vdots \\ \hat{f}_{n-1}^n \end{bmatrix}$$

$$\sigma = \begin{pmatrix} 1 & 2 & \ldots & m & m+1 & m+2 & \ldots & n \\ m+2 & m+3 & \ldots & n & 1 & 2 & \ldots & m+1 \end{pmatrix}.$$

Take Case: Taylor (all neg. coeffs = 0)
Let $z = e^{i\theta}$

$$f(z) = \sum_{k=0}^{\infty} \hat{f}_k z^k$$

$\hat{f}_0^n, \ldots, \hat{f}_{n-1}^n$ approx. of Taylor series coeffs. by evalueating on the boundary.

Theorem 7.3 *(Taylor series converge)*

$0 = \hat{f}_{-1} = \hat{f}_{-2} = \ldots$ and $\hat{\mathbf{f}}$ absolutely convergent

$$\implies f_n(\theta) = \sum_{k=0}^{n-1} \hat{f}_k^n e^{ik\theta} \quad \text{converges uniformly to } f(\theta)$$

7.3 Discrete Fourier Transform and Interpolation

Definition 7.3 *(DFT)*

Defined as:

$$Q_n := \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & e^{-i\theta_1} & e^{-i\theta_2} & \ldots & e^{-i\theta_{n-1}} \\ 1 & e^{-i2\theta_1} & e^{-i2\theta_2} & \ldots & e^{-i2\theta_{n-1}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & e^{-i(n-1)\theta_1} & e^{-i(n-1)\theta_2} & \ldots & e^{-i(n-1)\theta_{n-1}} \end{bmatrix} = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega^{-1} & \omega^{-2} & \ldots & \omega^{-(n-1)} \\ 1 & \omega^{-2} & \omega^{-4} & \ldots & \omega^{-2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{-(n-1)} & \omega^{-2(n-1)} & \ldots & \omega^{-(n-1)^2} \end{bmatrix} \quad \left(\omega = e^{i\pi/n}\right)$$

$$Q_n^* = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & e^{i\theta_1} & e^{i2\theta_1} & \ldots & e^{i(n-1)\theta_1} \\ 1 & e^{i\theta_2} & e^{i2\theta_2} & \ldots & e^{i(n-1)\theta_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & e^{i\theta_{n-1}} & e^{i2\theta_{n-1}} & \ldots & e^{i(n-1)\theta_{n-1}} \end{bmatrix} = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega^{1} & \omega^{2} & \ldots & \omega^{(n-1)} \\ 1 & \omega^{2} & \omega^{4} & \ldots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{(n-1)} & \omega^{2(n-1)} & \ldots & \omega^{(n-1)^2} \end{bmatrix}$$

Such that we have

$$\underbrace{\begin{bmatrix} f_0^n \\ \vdots \\ f_{n-1}^n \end{bmatrix}}_{\hat{\mathbf{f}}^n} = \frac{1}{\sqrt{n}} Q_n \underbrace{\begin{bmatrix} f(\theta_0) \\ \vdots \\ f(\theta_n) \end{bmatrix}}_{\mathbf{f}^n}$$

Proposition - *(DFT is Unitary)*
Q_n is unitary: $Q_n^* Q_n = Q_n Q_n^* = I$.
$\implies$ easily inverted with map from DFT $\rightarrow$ values

$$\sqrt{n} Q_n^* \mathbf{f}^n = \mathbf{f}^n$$

Corollary
$f_n(\theta)$ interpolates f at θ_j

$$f_n(\theta_j) = f(\theta_j)$$

7.4 Fast Fourier Transform

Q_n, Q_n^* applied take $O(n^2)$ operations, reduced to $O(n \log n)$ with FFT

$$\omega_n = \exp(\frac{2\pi}{n}); \quad \underbrace{\begin{bmatrix} 1 \\ \omega_{2n} \\ \vdots \\ \omega_{2n}^{2n-1} \end{bmatrix}}_{\vec{\omega}_{2n}} = P_\sigma^T \begin{bmatrix} I_n \\ \omega_{2n} I_n \end{bmatrix} \underbrace{\begin{bmatrix} 1 \\ \omega_n \\ \vdots \\ \omega_n^{n-1} \end{bmatrix}}_{\vec{\omega}_n}$$

$$\text{For } \sigma = \begin{pmatrix} 1 & 2 & 3 & \dots & n & n+1 & \dots & 2n \\ 1 & 3 & 5 & \dots & 2n-1 & 2 & \dots & 2n \end{pmatrix}$$

σ being the permutation that takes:

- Even entries $\rightarrow$ first n entries
- Odd entries $\rightarrow$ last n entries

With P_σ^T reversing that process.

$$\begin{aligned} \implies Q_{2n}^* &= \frac{1}{\sqrt{2n}} \left[\mathbf{1}_{2n} | \vec{\omega}_{2n} | \vec{\omega}_{2n}^2 | \dots | \vec{\omega}_{2n}^{2n-1} \right] = \frac{1}{\sqrt{2n}} P_\sigma^T \begin{bmatrix} \mathbf{1}_n & \vec{\omega}_n & \vec{\omega}_n^2 & \dots & \vec{\omega}_n^{n-1} & \vec{\omega}_n^n & \dots & \vec{\omega}_n^{2n-1} \\ \mathbf{1}_n & \omega_{2n} \vec{\omega}_n & \omega_{2n}^2 \vec{\omega}_n^2 & \dots & \omega_{2n}^{n-1} \vec{\omega}_n^{n-1} & \omega_{2n}^n \vec{\omega}_n^n & \dots & \omega_{2n}^{2n-1} \vec{\omega}_n^{2n-1} \end{bmatrix} \\ &= \frac{1}{\sqrt{2}} P_\sigma^T \begin{bmatrix} Q_n^* & Q_n^* \\ Q_n^* D_n & -Q_n^* D_n \end{bmatrix} = \frac{1}{\sqrt{2}} P_\sigma^T \begin{bmatrix} Q_n^* & \\ & Q_n^* \end{bmatrix} \begin{bmatrix} I_n & I_n \\ D_n & -D_n \end{bmatrix} \end{aligned}$$

Can reduce DFT to 2 DFTs applied to vectors of half dimension.
For $n = 2^q \implies O(n \log n)$ opperations.

8 Orthogonal polynomials

Consider expansions of the form

$$f(x) = \sum_{k=0}^{\infty} c_k p_k(x) \approx \sum_{k=0}^{n-1} c_k^n p_k(x)$$

For:

- $p_k(x)$ - special families of polynomials
- c_k - expansion coefficients
- c_k^n - approximate coefficients

8.1 General properties of orthogonal polynomials

Definition 8.1 *(Graded polynomial basis)*

Set of polynomials; $\{p_0(x), p_1(x), \dots\}$ if p_n is precisely degree n

$$p_n(x) = k_n x^n + k_n^{(n-1)} x^{n-1} + \dots + k_n^{(1)} x + k_n^{(0)}$$

If p_n graded $\implies \{p_0(x), \dots, p_n(x)\}$ a basis of all polynomials of degree n

Definition 8.2 *(Orthogonal polynomial)*

Given integrable weight $w(x)$ for $x \in (a,b)$, define continuous inner product

$$\langle f, g \rangle = \int_a^b f(x)g(x)w(x)dx$$

Graded polynomial basis $\{p_0(x), p_1(x), \dots\}$ are orthogonal polynomials (OPs) if

$$<p_n, p_m> = 0 \quad \text{when } m \neq n$$

Definition 8.3 *(Orthonormal polynomials)*

A set of OPs $\{p_0(x), p_1(x), \dots\}$ **orthonormal** if $\|q_n\| = 1 \ \forall n$

Definition 8.4 *(Monic OP)*

A set of OPs $\{p_0(x), p_1(x), \dots\}$ **monic** if $k_n = 1$

Proposition - *(Expansion)* If $r(x)$ a degree n poly., $\{p_n\}$ orthogonal and $\{q_n\}$ orthonormal $\implies$

$$\begin{aligned} r(x) &= \sum_{k=0}^{n} \frac{<p_k, r>}{\|p_k\|^2} p_k(x) \\ &= \sum_{k=0}^{n} <q_k, r> q_k(x) \end{aligned}$$

Corollary - *Zero inner product*
If degree n polynomial r satisfies

$$0 = <p_0, r> = \cdots = <p_n, r> \implies r = 0$$

Corollary - *(Uniqueness)*
Monic OPs are unique

Proposition - *Orthogonal to lower degree*
Given weigth $w(x)$, polynomial p of precisely degree n satisfies

$$<p, r> = 0$$

$\forall$ degree $m < n$, polynmial $r \iff p(x) = ap_n(x)$ where $p_n(x)$ are monic OPs.
$\implies$ OP uniquely defines by k_n

8.1.1 3-term Recurrence

Theorem 8.1 *(3-term recurrence, 2nd form)*

If $\{p_n\}$ are OPs $\implies \exists a_n, b_n \neq 0, c_{n-1} \neq 0 \in \mathbb{R}$ s.t

$$\begin{aligned} xp_0(x) &= a_0 p_0(x) + b_0 p_1(x) \\ xp_n(x) &= c_{n-1} p_{n-1}(x) + a_n p_n(x) + b_n p_{n+1}(x) \end{aligned}$$

p_n monic $\implies xp_n$ monic

Corollary - *(monic 3-term recurrence)*
If $\{p_n\}$ are monic $\implies b_n = 1$.

8.1.2 Jacobi Matrix

Corollary - *(Jacobi Matrix)*
For

$$P(x) := [p_0(x)|p_1(x)|\ldots]$$

$$\implies xP(x) = P(x)\underbrace{\begin{bmatrix} a_0 & c_0 & & \\ b_0 & a_1 & c_1 & \\ & b_1 & a_2 & \ddots \\ & & \ddots & \ddots \end{bmatrix}}_{X}$$

More generally, for any polynomial $a(x)$ we have

$$a(x)P(x) = P(x)a(X).$$

Corollary - *(Orthonormal 3-term recurrence)*
$\{q_n\}$ are orthonormal $\implies$ recurrence coefficients satisfy $c_n = b_n$.
The Jacobi matrix is symmetric:

$$X = \begin{bmatrix} a_0 & b_0 & & \\ b_0 & a_1 & b_1 & \\ & b_1 & a_2 & \ddots \\ & & \ddots & \ddots \end{bmatrix}$$

Remark
Typically Jacobi matrix is the transpose $J := X^T$.
If the basis orthonormal $\implies$ X is symmetric and they are the same.

8.2 Classical Orthogonal Polynomials

Classic OPs special families of OPs with special properties

- Their derivatives are also OPs
- They are eigenfunctions of simple differential operators

We consider:

1. Chebyshev polynomials (1st kind) $T_n(x)$:
   $w(x) = 1/\sqrt{1-x^2}$ on $[-1, 1]$.
2. Chebyshev polynomials (2nd kind) $U_n(x)$:
   $w(x) = \sqrt{1-x^2}$ on $[-1, 1]$.
3. Legendre polynomials $P_n(x)$:
   $w(x) = 1$ on $[-1, 1]$.
4. Hermite polynomials $H_n(x)$:
   $w(x) = \exp(-x^2)$ on $(-\infty, \infty)$

Other important families discussed are

1. Ultraspherical polynomials
2. Jacobi polynomials
3. Laguerre polynomials

8.2.1 Chebyshev

Definition 8.5 *(Chebyshev polynomials, 1st kind)*

$T_n(x)$ are orthogonal with respect to $1/sqrt1 - x^2$ and satisfy:

$$T_0(x) = 1, T_n(x) = 2^{n-1}x^n + O(x^{n-1})$$

Definition 8.6 *(Chebyshev polynomials, 2nd kind)*

$T_n(x)$ are orthogonal with respect to $1/sqrt1 - x^2$.

$$U_n(x) = 2^n x^n + O(x^{n-1})$$

Theorem 8.2 *(Chebyshev T are* cos*)*

$$T_n(x) = \cos(n \cdot acosx) \quad T_n(cos(\theta)) = \cos n\theta.$$

Corollary

$$\begin{aligned} xT_0(x) &= T_1(x) \\ xT_n(x) &= \frac{T_{n-1}(x) + T_{n+1}(x)}{2} \end{aligned}$$

Chebyshev polynomials particularly powerful

$$f(x) = \sum_{k=0}^{\infty} \check{f}_k T_k(x), \quad f(x) = \sum_{k=0}^{\infty} \check{f}_k \cos(k\theta)$$

$\implies$ coefficients recovered fast using FFT-based techniques.

Theorem 8.3 *(Chebyshev U are* sin*)*

For $x = \cos\theta$,

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}$$

which satisfy:

$$\begin{aligned} xU_0(x) &= U_1(x)/2 \\ xU_n(x) &= \frac{U_{n-1}(x)}{2} + \frac{U_{n+1}(x)}{2}. \end{aligned}$$

8.3 Legendre

Definition 8.7 *(Pochammer symbol)*

The Pochammer symbol is

$$\begin{aligned} (a)_0 &= 1 \\ (a)_n &= a(a+1)(a+2)\dots(a+n-1). \end{aligned}$$

Definition 8.8 *(Legendre)*

Legendre polynomials $P_n(x)$ are OPs w.r.t $w(x) = 1$ on $[-1, 1]$, with

$$k_n = \frac{2^n (1/2)_n}{n!}$$

Theorem 8.4 *(Legendre Rodriguez formula)*

$$P_n(x) = \frac{1}{(-2)^n n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n} (1-x^2)^n$$

Lemma - *(Legendre monomial coefficients)*

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_n(x) &= \underbrace{\frac{(2n)!}{2^n (n!)^2}}_{k_n} x^n - \underbrace{\frac{(2n-2)!}{2^n (n-2)!(n-1)!}}_{k_n^{(2)}} x^{n-2} + O(x^{n-4}) \end{aligned}$$

Theorem 8.5 *(Legendre 3-term recurrence)*

$$\begin{aligned} xP_0(x) &= P_1(x) \\ (2n+1)xP_n(x) &= nP_{n-1}(x) + (n+1)P_{n+1}(x) \end{aligned}$$

9 Interpolation and Gaussian Quadrature

Polynomial Interpolation - process of finding poly. equal to data at precise set of points
Quadrature - act of approximating an integral by a weighted sum

$$\int_a^b f(x)w(x)dx \approx \sum_{j=1}^n w_j f(x_j)$$

9.1 Polynomial Interpolation

Given n distinct points $x_1, \dots, x_n \in \mathbb{R}$, n samples $f_1, \dots, f_n \in \mathbb{R}$
Degree $n-1$ interpolatory poly. $p(x)$ satisfies

$$p(x_j) = f_j$$

Definition 9.1 *(Vandermonde)*

The Vandermonde matrix associated with n distinct points $x_1, \dots, x_n \in \mathbb{R}$ is the matrix

$$V := \begin{bmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \dots & x_n^{n-1} \end{bmatrix}$$

Proposition - *(Interpolatory polynomial uniqueness)*
Interpolatory polynomial is unique and Vandermonde matrix is invertible

Definition 9.2 *(Lagrange basis polynomial)*

$$\ell_k(x) := \prod_{j \neq k} \frac{x - x_j}{x_k - x_j} = \frac{(x - x_1)\dots(x - x_{k-1})(x - x_{k+1})\dots(x - x_n)}{(x_k - x_1)\dots(x_k - x_{k-1})(x_k - x_{k+1})\dots(x_k - x_n)}$$

Proposition - *(Delta interpolation)*

$$\ell_k(x_j) = \delta_{kj}$$

Theorem 9.1 *(Lagrange Interpolation)*

The unique polynomial of degree at most $n-1$ that interpolates f at x_j is

$$p(x) = f(x_1)\ell_1(x) + \dots + f(x_n)\ell_n(x)$$

9.2 Roots of orthogonal polynomials and truncated Jacobi matrices

Lemma
$q_n(x)$ has exactly n distinct roots

Definition 9.3 *(Truncated Jacobi Matrix)*

Given a symmetric Jacobi matrix X, (or weight $w(x)$ with orthonormal polynomials associated with X) the truncated Jacobi matrix is

$$X_n := \begin{bmatrix} a_0 & b_0 & & & \\ b_0 & \ddots & \ddots & & \\ & \ddots & a_{n-2} & b_{n-2} \\ & & b_{n-2} & a_{n-1} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Lemma - *(Zeros)*
The zeros $x_1, \dots, x_n$ of $q_n(x)$ are the eigenvalues of the truncated Jacobi matrix X_n.

$$X_n Q_n = Q_n \begin{bmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{bmatrix}$$

for the orthogonal matrix

$$Q_n = \begin{bmatrix} q_0(x_1) & \dots & q_0(x_n) \\ \vdots & \ddots & \vdots \\ q_{n-1}(x_1) & \dots & q_{n-1}(x_n) \end{bmatrix} \begin{bmatrix} \alpha_1^{-1} & & \\ & \ddots & \\ & & \alpha_n^{-1} \end{bmatrix}$$

where $\alpha_j = \sqrt{q_0(x_j)^2 + \dots + q_{n-1}(x_j)^2}$.

9.3 Interpolatory Quadrature Rules

Definition 9.4 *(interpolatory quadrature rule)*

Set of points $\mathbf{x} = [x_1, \ldots, x_n]$ the interpolatory quadrature rule is:

$$\Sigma_n^{w,\mathbf{x}}[f] := \sum_{j=1}^{n} w_j f(x_j) \quad \text{where} \quad w_j := \int_a^b \ell_j(x) w(x) dx$$

Proposition - *(Interpolatory quadrature is exact for polynomials)*
Interpolatory quadrature is exact for all degree $n-1$ polynomials p:

$$\int_a^b p(x) w(x) dx = \Sigma_n^{w,\mathbf{x}}[f]$$

9.4 Gaussian Quadrature

Definition 9.5 *(Gaussian Quadrature)*

Given weight $w(x)$, the Gauss quadrature rule is:

$$\int_a^b f(x) w(x) dx \approx \underbrace{\sum_{j=1}^{n} w_j f(x_j)}_{\Sigma_n^w[f]}$$

where $x_1, \ldots, x_n$ are the roots of $q_n(x)$ and

$$w_j := \frac{1}{\alpha_j^2} = \frac{1}{q_0(x_j)^2 + \cdots + q_{n-1}(x_j)^2}.$$

Equivalently, $x_1, \ldots, x_n$ are the eigenvalues of X_n and

$$w_j = \int_a^b w(x) dx Q_n[1, j]^2.$$

(Note we have $\int_a^b w(x) dx q_0(x)^2 = 1$.)

Lemma - *(Discrete orthogonality)*
For $0 \leq \ell, m \leq n-1$,

$$\Sigma_n^w[q_\ell \, q_m] = \delta_{\ell m}$$

Theorem 9.2 *(Interpolation via quadrature)*

$$f_n(x) = \sum_{k=0}^{n-1} c_k^n q_k(x) \quad \text{for} \quad c_k^n := \Sigma_n^w[f q_k]$$

interpolates $f(x)$ at the Gaussian quadrature points $x_1, \ldots, x_n$.
Corollary
Gaussian quadrature is an interpolatory quadrature rule with the interpolation points equal to the roots of q_n:

$$\Sigma_n^w[f] = \Sigma_n^{w,\mathbf{x}}[f]$$

Theorem 9.3 *(Exactness of Gauss quadrature)*

If $p(x)$ is a degree $2n-1$ polynomial then Gauss quadrature is exact:

$$\int_a^b p(x) w(x) dx = \Sigma_n^w[p].$$