

## Basic identities of matrix/vector ops

$$(A^T)^T = A, (A^T)^T = A^T, (AB)^T = B^T A^T, (A^{-1})^T = (A^T)^{-1}, (AB)^{-1} = B^{-1} A^{-1}$$

For  $A \in \mathbb{R}^{m \times n}$ ,  $A_{ij}$  is the  $i$ th **ROW** then  $j$ th **COLUMN**  
 $(A^T)_{ij} = A_{ji}$ ,  $(AB)_{ij} = \sum_k A_{ik} B_{kj}$   
 $(A+B)^T = A^T + B^T$

$$(AX)^T = X^T A^T, (x \sum_j A_{ij} x_j)^T = x^T y^T = x \cdot y = \sum_j x_j y_j$$
$$x^T A x = \sum_j A_{ij} x_j x_j, x^T x = [0 \dots 1] \cdot [x_1 \dots x_n]^T = \sum_j x_j^2$$

Scalar-multiplication + addition distributes over:  
**column-blocks**  $\rightarrow A \cdot B + C = [A_1 \dots A_n] \cdot [B_1 \dots B_n] + [C_1 \dots C_n] = [A_1 + C_1 \dots A_n + C_n]$   
**row-blocks**  $\rightarrow A \cdot B = [A_1 \dots A_n] \cdot [B_1 \dots B_n] = [A_1 B_1 \dots A_n B_n]$

Matrix-multiplication distributes over:  
**column-blocks**  $\rightarrow AB + AC = A[B_1 \dots B_n] = A[B_1 \dots B_n]$   
**row-blocks**  $\rightarrow AB = [A_1 \dots A_n]B = [A_1 B \dots A_n B]$

**outer-product sum**  
 $AB = [A_1 \dots A_n] \cdot [B_1 \dots B_n] = \sum_j A_j B_j^T$   
e.g. for  $A = [a_1 \dots a_n]$ ,  $B = [b_1 \dots b_n]^T \Rightarrow AB = \sum_j a_j b_j^T$

**Projection: definition & properties**  
A projection  $\Pi: V \rightarrow V$  is an endomorphism such that  $\Pi^2 = \Pi$ . i.e. it leaves its image unchanged (its idempotent).

A square matrix  $P$  such that  $P^2 = P$  is called a **projection matrix**.  
It is called an **orthogonal projection matrix** if  $P^T = P$  (conjugate-transpose).

Eigenvalues of a projection matrix must be 0 or 1  
Because  $\Pi: V \rightarrow V$  is a linear map, its image  $\text{span}(U)$  is  $\Pi(U)$  and null space  $\text{span}(W) = \ker(\Pi)$  are subspaces of  $V$ .  
 $\Pi$  is the identity operator on  $U$ .  
The linear map  $\Pi = I_V - \Pi$  is also a projection with  $W = \Pi(V) = \ker(\Pi)$  and  $\ker(\Pi) = \Pi(V)$ . i.e. they are orthogonal.

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 $\Pi$  is the identity operator on  $W$ .

$V$  can be decomposed as  $V = U \oplus W$  meaning every vector  $x \in V$  can be uniquely written as  $x = u + w$ ,  $u \in U$  and  $w \in W$ .  
 $u = \Pi(x)$ ,  $w = x - \Pi(x)$ .  
 $u \in U$  and  $w \in W$  and  $w = x - \Pi(x) = (I_V - \Pi)x = \Pi^*(x)$ .

An orthogonal projection further satisfies  $U \perp W$ .  
i.e. the image and kernel of  $\Pi$  are orthogonal subspaces.

infact they are each other's orthogonal complements, i.e.  $U^\perp = W$  and  $W^\perp = U$  (because finite-dimensional vector spaces).

so we have  $\Pi(x) \cdot y = \Pi(x) \cdot \Pi(y) = \Pi(x \cdot y)$  or equivalently  $\Pi(x) \cdot \Pi(y) = \Pi(x \cdot y)$ .

By Cauchy-Schwarz inequality we have  $|\Pi(x)| \leq |x|$ .  
The orthogonal projection onto the line containing vector  $u$  is  $\text{proj}_u(u) = \frac{u \cdot u}{u \cdot u} = \frac{u}{|u|}$ .

A special case of  $\Pi(x) = \Pi(y) = 0$  is  $u = (v - \text{proj}_u(v)) = 0$ .  
i.e.  $\text{proj}_u(u) = u$ .

Let  $U = \{u_1, \dots, u_k\} \in \mathbb{R}^{m \times k}$  matrix.  
Orthogonal projection onto  $U$  is  $\Pi_U = U U^T$ .

Can be rewritten as  $\text{proj}_U(u) = \sum_i (u \cdot u_i) u_i$ .  
If  $\{u_1, \dots, u_k\}$  is not orthonormal, then "normalizing factor"  $(U^T U)^{-1}$  is added  $\Rightarrow \Pi_U = U(U^T U)^{-1} U^T$ .

For line subspaces  $U = \text{span}(u)$  we have  $(U^T U)^{-1} = (u^T u)^{-1} = 1/(u \cdot u)$  so  $\Pi_U = \frac{u u^T}{u \cdot u}$ .

**Gram-Schmidt (GS) to gen. ONB from lin. ind. vectors**  
Gram-Schmidt is iterative projection  $\Rightarrow$  we use current  $j$  dim subspace, to get next  $(j+1)$  dim subspace.

Assume orthonormal basis (ONB)  $\{q_1, \dots, q_j\} \in \mathbb{R}^m$ .  
For  $j$  dim subspace  $U_j \subset \mathbb{R}^m$ .  
Let  $Q_j = [q_1 \dots q_j] \in \mathbb{R}^{m \times j}$  be the matrix.  
 $P_j = Q_j Q_j^T$  is orthogonal projection onto  $U_j$ .  
 $P_{j+1} = I_m - Q_j Q_j^T$  is orthogonal projection onto  $(U_j)^\perp$  [orthogonal complement].

Uniquely decompose next  $u_j \in U_{j+1} = v_j + u_j$ .  
 $u_j = P_j u_j + (I - P_j) u_j = (U_j)^\perp$  we're after this!!

Let  $q_{j+1} = \frac{u_j}{|u_j|} \Rightarrow$  we have next ONB  $\{q_1, \dots, q_{j+1}\}$ .  
For  $u_j$  start next iteration.

$u_j = (I - Q_j Q_j^T) u_j + Q_j Q_j^T u_j$  where  $Q_j = [q_1 \dots q_j]$ .

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For matrix  $A \in \mathbb{R}^{m \times n}$  and for row-space  $R(A)$ , column-space  $C(A)$  and null space  $\ker(A)$ .  
 $R(A)^\perp = \ker(A)$  and  $C(A)^\perp = \ker(A^T)$ .  
Any  $b \in \mathbb{R}^m$  can be uniquely decomposed into  $b = b_C + b_K$  where  $b_C \in C(A)$  and  $b_K \in \ker(A)$ .  
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**Inverse of square-diagonals**  
 $\text{diag}(a_1, \dots, a_n)^{-1} = \text{diag}(a_1^{-1}, \dots, a_n^{-1})$  i.e. diagonals  $b = b_C + b_K$  where  $b_C \in C(A)$  and  $b_K \in \ker(A)$ .

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Notice:  $Q_j = [q_1 \dots q_j]$  is orthogonal projection onto  $U_j$ .  
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rewrite as  
 $u_{j+1} = A_{j+1} - \sum_{i=1}^j Q_i A_{j+1} = A_{j+1} - \sum_{i=1}^j \text{proj}_{Q_i}(A_{j+1})$

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## Vector norms (beyond euclidean)

vector norms are such that:  $|x| = 0 \iff x = 0$   
 $|x| \geq 0$ ,  $|x+y| \leq |x| + |y|$

$p$  norms:  $|x|_p = (\sum_i |x_i|^p)^{1/p}$   
 $p=1$ :  $|x|_1 = \sum_i |x_i|$   
 $p=2$ :  $|x|_2 = \sqrt{\sum_i x_i^2} = \sqrt{x \cdot x}$   
 $p=\infty$ :  $|x|_\infty = \max_i |x_i|$

Any two norms in  $\mathbb{R}^n$  are equivalent, meaning there exist  $c_1, c_2 > 0$  such that:  
 $c_1 |x|_1 \leq |x|_2 \leq c_2 |x|_1$

Equivalence of  $l_1, l_2$  and  $l_\infty$ :  
 $|x|_1 \leq |x|_2 \leq |x|_\infty$   
 $|x|_2 \leq |x|_1 \leq \sqrt{2} |x|_2$

Induce metric  $d(x, y) = |x - y|$  has additional properties:  
Translation invariance:  $d(x + y, y + y) = d(x, y)$   
Scaling:  $d(\lambda x, \lambda y) = |\lambda| d(x, y)$

**Properties: dot-product & norm**  
 $x^T y = y^T x = x \cdot y = \sum_i x_i y_i$   
 $x \cdot y = |x| |y| \cos \theta$

**Matrix norms** are such that:  $|A| = 0 \iff A = 0$   
 $|A| \geq 0$ ,  $|A+B| \leq |A| + |B|$   
 $|A| = \max_i \sum_j |A_{ij}|$  (row-sum)  
 $|A| = \max_j \sum_i |A_{ij}|$  (column-sum)

**Sub-multiplicative matrix norm** (assumed by default) is also such that  $|AB| \leq |A| |B|$   
Common matrix norms, for some  $A \in \mathbb{R}^{m \times n}$ :  
 $|A|_1 = \max_j \sum_i |A_{ij}|$   
 $|A|_2 = \sqrt{\lambda_{\max}(A^T A)}$   
 $|A|_\infty = \max_i \sum_j |A_{ij}|$

**Properties of determinants**  
Consider  $A \in \mathbb{R}^{n \times n}$ , then  $A_{ij}^T \in \mathbb{R}^{(n-1) \times (n-1)}$  the  $(i,j)$ -minor matrix of  $A$  obtained by deleting  $i$ th row and  $j$ th column from  $A$ .  
Then  $\det(A) = \sum_j (-1)^{i+j} A_{ij} \det(A_{ij}^T)$

**Probenius norm**:  $|A|_F = \sqrt{\sum_{i,j} |A_{ij}|^2}$   
A matrix norm  $\| \cdot \|$  on  $\mathbb{R}^{n \times n}$  is consistent with the vector norms  $\| \cdot \|_p$  on  $\mathbb{R}^n$  and  $\| \cdot \|_q$  on  $\mathbb{R}^m$  if for all  $A \in \mathbb{R}^{n \times n}$  and  $x \in \mathbb{R}^n$ :  $\|Ax\|_q \leq \|A\| \|x\|_p$   
If  $A \in \mathbb{R}^{n \times n}$  is compatible with  $\| \cdot \|_p$  then  $\|A\|_p = \max_i \sum_j |A_{ij}|$

For a vector norm  $\| \cdot \|$  on  $\mathbb{R}^n$ , the subordinate matrix norm  $\| \cdot \|$  on  $\mathbb{R}^{n \times n}$  is:  
 $|A| = \max_i \sum_j |A_{ij}|$

And the exact same linearity property for rows immediately leads to:  $|A| = |A^T|$  ( $|A| = |A^T|$ ) and  $|AB| = |A| |B|$  (if  $AB \in \mathbb{R}^{n \times n}$ )

**Alternating**: if any two columns of  $A$  are equal (or any two rows of  $A$  are equal), then  $|A| = 0$  (its singular immediately from this (and multi-linearity)  $\Rightarrow$  if columns (or rows) are linearly dependent  $\Rightarrow$  some linear combinations of others) then  $|A| = 0$ .

Stated in other terms  $\rightarrow |A| \cdot \det(A) = 0 \iff \text{RREF}(A) \neq I_n \iff |A| = 0$  (reduced row-echelon form)  $\iff C(A) \neq \mathbb{R}^n \iff |A| = 0$  (column-space).

For more equivalence to the above, see invertible matrix theorem.

**Swapping rows/columns flips the sign**  
Scaling a row/column by  $\lambda$  will scale the determinant by  $|\lambda|$  (by multi-linearity).

Remember to scale by  $\lambda^{-1}$  to maintain equality, i.e.  $\det(A \cdot \lambda^{-1}) = \det(A) \cdot \lambda^{-n}$

Invariant under addition of rows/columns  
Link to invertible matrices  $\rightarrow |A^{-1}| = |A|^{-1}$  which means  $A$  is invertible  $\iff |A| \neq 0$  i.e. singular matrices are not invertible

For block-matrices:  
 $\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A) \det(D - CA^{-1}B)$  if  $A$  or  $D$  are invertible, respectively.

**Sylvester's determinant theorem**:  
 $\det(M \cdot A \cdot B) = \det(B \cdot A \cdot M)$   
Matrix determinant lemma:  
 $\det(A + uv^T) = (1 + v^T A^{-1} u) \det(A)$   
 $\det(A \cdot UV^T) = \det(U^T \cdot V^T A^{-1} U) \det(A)$

**Tricks for computing determinant**  
If block-triangular matrix then apply  $\det \begin{pmatrix} A & B \\ 0 & D \end{pmatrix} = \det(A) \det(D)$

If close to triangular matrix apply EROs/ECOs to get it there, then use product of diagonals

If Cholesky/LLQR is possible and cheap then do it, then apply  $|A| = |L| |B|$

**Properties of matrices**  
Consider  $A \in \mathbb{R}^{m \times n}$   
If  $Ax = x$  for all  $x$  then  $A = I$   
For square  $A$  the trace of  $A$  is the sum of its diagonals, i.e.  $\text{tr}(A) = \sum_i A_{ii}$

$A$  is symmetric  $\iff A = A^T$ ,  $A$  is Hermitian,  $\iff A = A^H$  i.e. its equal to its conjugate-transpose  
 $AA^T$  and  $A^T A$  are symmetric (and positive semi-definite).

For real matrices, Hermitian/symmetric are equivalent conditions  
Every eigenvalue  $\lambda$  of  $A$  is Hermitian matrices is real (geometric multiplicity of  $\lambda$  is geometric multiplicity of  $\lambda$ )  
eigenvectors  $x_1, x_2$  associated to distinct eigenvalues  $\lambda_1, \lambda_2$  are orthogonal, i.e.  $x_1 \perp x_2$

$A$  is triangular  $\iff$  all entries above (lower-triangular) or below (upper-triangular) the main diagonal are zero  
Determinant  $\rightarrow |A| = \prod_i A_{ii}$  i.e. the product of diagonal elements

$A$  is diagonal  $\iff A_{ij} = 0, i \neq j$  i.e. if all off-diagonal entries are zero  
Written as  $\text{diag}_{m \times n}(a) = \text{diag}_{m \times n}(a_1, \dots, a_p, 0, \dots, 0)$  where  $a = [a_1, \dots, a_p]^T \in \mathbb{R}^p$  diagonal entries of  $A$

For  $x \in \mathbb{R}^n$ ,  $Ax = \text{diag}_{m \times n}(a_1, \dots, a_p, 0, \dots, 0)x = [a_1 x_1, \dots, a_p x_p, 0, \dots, 0]^T \in \mathbb{R}^m$  iff  $p = m$  (those tail-zeros don't exist)

$\text{diag}_{m \times n}(a) \cdot \text{diag}_{n \times m}(b) = \text{diag}_{m \times m}(a \cdot b)$   
Consider  $\text{diag}_{m \times m}(c_1, \dots, c_n, 0, \dots, 0)$  then  $R^n = U \oplus U^\perp$  and  $(U^\perp)^\perp = U$

$U \perp V \iff U \cdot V = 0$  and vice-versa  
 $Y \perp X \iff X^T Y = 0$  and  $X \cdot X = 0$   
Any  $x \in \mathbb{R}^n$  can be uniquely decomposed into  $x = x_C + x_K$  where  $x_C \in C(A)$  and  $x_K \in \ker(A)$

For matrix  $A \in \mathbb{R}^{m \times n}$  and for row-space  $R(A)$ , column-space  $C(A)$  and null space  $\ker(A)$ .  
 $R(A)^\perp = \ker(A)$  and  $C(A)^\perp = \ker(A^T)$ .  
Any  $b \in \mathbb{R}^m$  can be uniquely decomposed into  $b = b_C + b_K$  where  $b_C \in C(A)$  and  $b_K \in \ker(A)$ .  
 $b = b_C + b_K$  where  $b_C \in C(A)$  and  $b_K \in \ker(A)$ .

**Inverse of square-diagonals**  
 $\text{diag}(a_1, \dots, a_n)^{-1} = \text{diag}(a_1^{-1}, \dots, a_n^{-1})$  i.e. diagonals  $b = b_C + b_K$  where  $b_C \in C$

$Q_1, Q_2, \dots, Q_n \in \mathbb{R}^{n \times 1} \mid \dots \mid Q_n \in \mathbb{R}^{n \times n}$  notice its semi-orthogonal since  $Q^T Q = I_n$

Notice  $\Rightarrow a_j = Q_j c_j = Q_1 c_1 + \dots + Q_j c_j + \dots + Q_n c_n = Q_j^T c_j$

Let  $R = [r_1 \mid \dots \mid r_n] \in \mathbb{R}^{n \times n}$

$A \cdot QR = Q \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n & \\ & & & 0 \end{bmatrix}$  notice its

upper-triangular.

### Full QR Decomposition

Consider  $\text{Full QR decomposition}$   $A = [a_1 \mid \dots \mid a_n] \in \mathbb{R}^{m \times n}$   $[m \geq n]$ , i.e.  $a_1, \dots, a_n \in \mathbb{R}^m$  are linearly independent.

Apply QR decomposition to obtain:

ONB  $\{q_1, \dots, q_n\} \in \mathbb{R}^m$  for  $\text{C(A)}$

Semi-orthogonal  $Q_1 = [q_1 \mid \dots \mid q_n] \in \mathbb{R}^{m \times n}$  and upper-triangular  $R_1 \in \mathbb{R}^{n \times n}$  where  $A = Q_1 R_1$

Compute basis extension to obtain remaining  $q_{n+1}, \dots, q_m \in \mathbb{R}^m$  where  $\{q_1, \dots, q_m\}$  is ONB for  $\mathbb{R}^m$

Notice  $\{q_{n+1}, \dots, q_m\}$  is ONB for  $\text{C(A)}^\perp = \ker(A^T)$

Apply  $Q_2$  decomposition to obtain:

Let  $Q_2 = [q_{n+1} \mid \dots \mid q_m] \in \mathbb{R}^{m \times (m-n)}$  let  $Q = [Q_1 \mid Q_2] \in \mathbb{R}^{m \times m}$

Let  $R = [R_1 \mid 0] \in \mathbb{R}^{n \times m}$

Then **Full QR decomposition** is

$A = QR = [Q_1 \mid Q_2] \begin{bmatrix} R_1 & 0 \\ 0 & 0 \end{bmatrix}$

$Q$  is orthogonal, i.e.  $Q^T = Q^{-1}$  so its a basis transformation

$\text{proj}_{\text{C(A)}}(Q_1) = Q_1 Q_1^T$   $\text{proj}_{\text{C(A)}^\perp} = Q_2 Q_2^T$  are orthogonal

projections onto  $\text{C(A)}$   $\text{C(A)}^\perp = \ker(A^T)$  respectively.

Notice:  $Q^T = I_m = Q_1^T Q_1 + Q_2^T Q_2$

**Generalizable** to  $A \in \mathbb{C}^{m \times n}$  by changing transpose to conjugate-transpose

### Lines and hyperplanes in $E^n (= \mathbb{R}^n)$

Consider standard Euclidean space  $E^n (= \mathbb{R}^n)$

with standard basis  $\{e_1, \dots, e_n\} \in \mathbb{R}^n$

with standard origin  $0 \in \mathbb{R}^n$

A line  $L = \mathbb{R}n + c$  is characterized by direction  $n \in \mathbb{R}^n$  ( $n \neq 0$ ) and offset from origin  $c \in \mathbb{R}^n$

It is customary that:

$n$  is a unit vector, i.e.  $\|n\| = \|n\| = 1$

$c \in L$  is closest point to origin, i.e.  $c \perp n$

If  $c \perp n \Rightarrow \perp$  not vector-subspace of  $\mathbb{R}^n$

i.e.  $0 \notin L$  i.e.  $L$  doesn't go through the origin

$L$  is affine-subspace of  $\mathbb{R}^n$

If  $c \perp n$  i.e.  $L$  goes through  $0$  is vector-subspace of  $\mathbb{R}^n$

i.e.  $0 \in L$  i.e.  $L$  goes through the origin

$L$  has  $\dim(L) = 1$  and an orthonormal basis (ONB)  $\{\hat{n}\}$

A hyperplane  $P = \mathbb{R}^{n-1} + c = \{x + c \mid x \in \mathbb{R}^n, x \perp n\}$

$= \{x \in \mathbb{R}^n \mid \langle x, n \rangle = c\}$

characterized by normal  $n \in \mathbb{R}^n$  ( $n \neq 0$ ) and offset from origin  $c \in \mathbb{R}$

It represents an  $(n-1)$ -dimensional slice of the  $n$ -dimensional space

It is customary that:

$n$  is a unit vector, i.e.  $\|n\| = \|n\| = 1$

$c \in P$  is closest point to origin, i.e.  $c \perp n$

With those  $\Rightarrow P \perp$  not vector-subspace of  $\mathbb{R}^n$

i.e.  $0 \notin P$  i.e.  $P$  doesn't go through the origin

$P$  is affine-subspace of  $\mathbb{R}^n$

If  $c = 0$  i.e.  $P = \mathbb{R}^{n-1} \Rightarrow P$  is vector-subspace of  $\mathbb{R}^n$

i.e.  $0 \in P$  i.e.  $P$  goes through the origin

$P$  has  $\dim(P) = n-1$

Notice  $L = \mathbb{R}n$  and  $P = \mathbb{R}^{n-1}$  are orthogonal complements, so:

$\text{proj}_L = \hat{n}\hat{n}^T$  is the orthogonal projection onto  $L$  (along  $P$ )

$\text{proj}_P = \text{id}_n - \text{proj}_L = I_n - \hat{n}\hat{n}^T$  is orthogonal projection onto  $P$  (along  $L$ )

$L = \text{im}(\text{proj}_L) = \ker(\text{proj}_P)$  and  $P = \ker(\text{proj}_L) = \text{im}(\text{proj}_P)$

$\mathbb{R}^n = \mathbb{R}n \oplus \mathbb{R}^{n-1}$  i.e. all vectors  $v \in \mathbb{R}^n$  uniquely decomposed into  $v = v_L + v_P$

### Householder Maps: reflections

Two points  $x, y \in \mathbb{R}^n$  are reflections w.r.t hyperplane  $P = \mathbb{R}^{n-1} + c$  if:

1) The translation  $\overrightarrow{xy} = y - x$  is parallel to normal  $n$ , i.e.  $\overrightarrow{xy} \propto n$

2) Midpoint  $m = 1/2(x+y) \in P$  lies on  $P$ , i.e.  $m \perp n$

Suppose  $P = \mathbb{R}u$  goes through the origin with unit normal  $u \in \mathbb{R}^n$

Householder matrix  $H_u = I_n - 2uu^T$  is reflection w.r.t. hyperplane  $P_u$

Recall: let  $\hat{u} = \frac{u}{\|u\|}$

$\text{proj}_{\hat{u}} = uu^T$  and  $\text{proj}_{P_u} = I_n - uu^T \Rightarrow$

$H_u = \text{proj}_{P_u} - \text{proj}_{\hat{u}} = I_n - 2uu^T$

Visualize as preserving component in  $P_u$  then flipping component in  $L_u$

$H_u$  is involutory, orthogonal and symmetric, i.e.  $H_u = H_u^{-1} = H_u^T$

### Modified Gram-Schmidt

Go check Classical GM first, as this is just an alternative computation method

Let  $P_1, q_1 \in \mathbb{R}^m, q_1^T q_1 = 1$  be projector onto hyperplane

$(Rq_j)^T = 1$  i.e. orthogonal complement of line  $Rq_j$

Notice:  $P_{j+1} = I_m - Q_j Q_j^T = \left( I_m - \sum_{i=1}^j Q_i Q_i^T \right) = \left( I_m - \sum_{i=1}^j P_i P_i^T \right)$

Re-state:  $u_{j+1} = \left( I_m - Q_j Q_j^T \right) u_{j+1}$

$u_{j+1} = \left( \left( I_m - P_1 P_1^T \right) \dots \left( I_m - P_j P_j^T \right) \right) u_{j+1}$

Projectors  $P_1, q_1, \dots, P_j, q_j$  are iteratively applied to  $u_{j+1}$  removing its components along  $q_1$  then along  $q_2$  and so on...

Let  $u_k = \left( \left( I_m - P_1 P_1^T \right) \dots \left( I_m - P_{j-1} P_{j-1}^T \right) \right) u_k$  i.e.  $a_k$  without its components along  $q_1, \dots, q_{j-1}$

Notice:  $u_j = u_j^{(j-1)}$  thus  $q_j = u_j = u_j^{(j-1)} / \|u_j\|$  where  $r_{jj} = \|u_j^{(j-1)}\|$

Iterative step:

Notice:  $Q_j = \frac{1}{r_{jj}} \begin{bmatrix} u_j^{(j-1)} \\ u_j^{(j-1)} \\ \vdots \\ u_j^{(j-1)} \end{bmatrix} = \frac{1}{r_{jj}} \begin{bmatrix} u_j^{(j-1)} \\ u_j^{(j-1)} \\ \vdots \\ u_j^{(j-1)} \end{bmatrix} = \frac{1}{r_{jj}} \begin{bmatrix} u_j^{(j-1)} \\ u_j^{(j-1)} \\ \vdots \\ u_j^{(j-1)} \end{bmatrix}$

i.e. each projection  $Q_j$  of MGS computes  $P_{j+1}$  and projections under iteration  $j$  in one go

At start of iteration  $j \in \{1, \dots, n\}$  we have ONB  $q_1, \dots, q_{j-1} \in \mathbb{R}^m$  and residual  $u_j^{(j-1)}, \dots, u_n^{(j-1)} \in \mathbb{R}^m$

Compute  $r_{jj} = \|u_j^{(j-1)}\| \Rightarrow q_j = u_j^{(j-1)} / r_{jj}$

For each  $k \in \{j+1, \dots, n\}$  compute  $r_{jk} = q_j^T u_k^{(j-1)} \Rightarrow u_k = u_k^{(j-1)} - r_{jk} q_j$

Next ONB  $\{q_1, \dots, q_j\}$  and next residual  $u_{j+1}^{(j)}, \dots, u_n^{(j)}$

NOTE: for  $j=1 \Rightarrow q_1, \dots, q_{j-1} = \emptyset$  i.e. none yet

By end of iteration  $j=n$  we have ONB  $\{q_1, \dots, q_n\} \in \mathbb{R}^m$

$A = [a_1 \mid \dots \mid a_n] = [q_1 \mid \dots \mid q_n] \begin{bmatrix} r_{11} & & 0 \\ & \ddots & \\ 0 & & r_{nn} \end{bmatrix} = QR$

corresponds to thin QR decomposition

Where  $A \in \mathbb{R}^{m \times n}$  is full-rank,  $Q \in \mathbb{R}^{m \times n}$  is semi-orthogonal, and  $R \in \mathbb{R}^{n \times n}$  is upper-triangular

### Classical vs. Modified Gram-Schmidt

These algorithms both compute thin QR decomposition

	Classical Gram-Schmidt	Modified Gram-Schmidt
1. for $j = 1$ to $n$ do	1. for $j = 1$ to $n$ do	1. for $j = 1$ to $n$ do
2. $u_j = a_j$	2. $u_j = a_j$	2. $u_j = a_j$
3. end for	3. end for	3. end for
4. for $i = j+1$ to $n$ do	4. for $i = j+1$ to $n$ do	4. for $i = j+1$ to $n$ do
5. $r_{ij} = u_j^T u_i$	5. $r_{ij} = u_j^T u_i$	5. $r_{ij} = u_j^T u_i$
6. $u_i = u_i - r_{ij} u_j$	6. $u_i = u_i - r_{ij} u_j$	6. $u_i = u_i - r_{ij} u_j$
7. for $k = j+1$ to $n$ do	7. for $k = j+1$ to $n$ do	7. for $k = j+1$ to $n$ do
8. $r_{jk} = u_j^T u_k$	8. $r_{jk} = u_j^T u_k$	8. $r_{jk} = u_j^T u_k$
9. $u_k = u_k - r_{jk} u_j$	9. $u_k = u_k - r_{jk} u_j$	9. $u_k = u_k - r_{jk} u_j$
10. end for	10. end for	10. end for
11. end for	11. end for	11. end for

Computes at  $j$ th step:

Classical GS  $\Rightarrow j$ th column of  $Q$  and the  $j$ th column of  $R$

Modified GS  $\Rightarrow j$ th column of  $Q$  and the  $j$ th row of  $R$

Both have flop (floating-point operation) count of  $O(2mn^2)$

NOTE: Householder method has  $2(mn^2 - n^3)/3$  flop count, but better numerical properties

Recall:  $Q^T Q = I_n \Rightarrow$  check for loss of orthogonality with  $\|I_n - Q^T Q\| = \text{loss}$

Classical GS  $\Rightarrow \|I_n - Q^T Q\| = \text{Cond}(A)^2 \epsilon_{\text{mach}}$

Modified GS  $\Rightarrow \|I_n - Q^T Q\| = \text{Cond}(A) \epsilon_{\text{mach}}$

NOTE: Householder method has  $\|I_n - Q^T Q\| \leq \epsilon_{\text{mach}}$

### Multivariate Calculus

Consider  $f: \mathbb{R}^n \rightarrow \mathbb{R}$

When clear write  $j$ th component of input as  $x_j$  instead of  $x$

Level curve w.r.t.  $c \in \mathbb{R}$  is all points  $s.t. f(x) = c$

Projecting level curves onto  $\mathbb{R}^n$  gives  $f$ 's contour-map

$n_k$ th order partial derivative w.r.t  $x_k$  of  $\dots$  of  $n_1$ th order partial derivative w.r.t  $x_1$  of  $f$  is:

$f$  is backwards stable if  $\forall x \in X \exists \epsilon \in X.s.t. f(x) = f(x)$  and  $\frac{\|x - \tilde{x}\|}{\|x\|} = O(\epsilon_{\text{mach}})$

i.e. exactly the right answer to nearly the right question, a subset of stability

$\Theta, \otimes, \odot$  inner-product, back-substitution w/ triangular systems, are backwards stable

if backwards stable  $f$  and  $f$  has condition number  $\kappa(x)$  then relative error  $\frac{\|f(x) - f(\tilde{x})\|}{\|f(x)\|} = O(\kappa(x) \epsilon_{\text{mach}})$

Accuracy, stability, backwards stability are norm-independent for fin-dim  $X, Y$

Big-O meaning for numerical analysis

In complexity analysis  $f(n) = O(g(n))$  as  $n \rightarrow \infty$

But in numerical analysis  $f(n) = O(g(n))$  as  $\epsilon \rightarrow 0$  i.e. when  $x, u$  are parallel  $\Rightarrow$  hence  $\nabla f(x)$  is direction of max. rate-of-change

$f$  has local minimum at  $x_{\text{loc}}$  if there's radius  $r > 0$  s.t.  $\forall x \in B(r, x_{\text{loc}})$  we have  $f(x_{\text{loc}}) \leq f(x)$

$f$  has global minimum  $x_{\text{glob}}$  if  $\forall x \in \mathbb{R}^n$  we have  $f(x_{\text{glob}}) \leq f(x)$

A local minimum satisfies optimality conditions:  $\nabla f(x) = 0$  if, for  $n=1$  its  $f'(x) = 0$

$\nabla f(x)$  is positive-definite, e.g. for  $n=1$  its  $f''(x) > 0$

$H(f) = \nabla^2 f = J(f \nabla f)^T$  is Hessian  $\Rightarrow H(f)_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$

Interpret  $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$  as  $m$  functions  $f_i: \mathbb{R}^n \rightarrow \mathbb{R}$  (one per output-component)

$J(f) = [\nabla f^T; \dots; \nabla f_m^T]$  is Jacobian  $\Rightarrow J(f)_{ij} = \frac{\partial f_i}{\partial x_j}$

Using functions  $f_1, \dots, f_n$  let  $\Phi(f_1, \dots, f_n)$  be formula defining some function

Then  $\Phi(O(g_1), \dots, O(g_n))$  is the class of functions  $\{\Phi(f_1, \dots, f_n) : f_1 \in O(g_1), \dots, f_n \in O(g_n)\}$

e.g.  $\epsilon \cdot O(1) = \{e f(x) : f \in O(1)\}$

General case:  $\Phi_1(O(f_1), \dots, O(f_m)) = \Phi_2(O(g_1), \dots, O(g_n))$  means  $\Phi_1(O(f_1), \dots, O(f_m)) \subseteq \Phi_2(O(g_1), \dots, O(g_n))$

e.g.  $\epsilon \cdot O(1) = O(\epsilon^2)$  means  $\{e f(x) : f \in O(1)\} \subseteq O(\epsilon^2)$

Special case:  $f = \Phi(O(g_1), \dots, O(g_n))$  means  $f \in \Phi(O(g_1), \dots, O(g_n))$

e.g.  $\epsilon \cdot O(1)^2 = \epsilon^2 \cdot O(1)$  means  $\{e \cdot e f(x) : f \in O(1)\} \subseteq \{e^2 f(x) : f \in O(1)\}$

$\{e \cdot e f(x) : f \in O(1)\} \subseteq \{e^2 f(x) : f \in O(1)\}$  not necessarily true

Let  $f_1 = O(g_1), f_2 = O(g_2)$  and let  $k \neq 0$  be a constant

$f_1 f_2 = O(g_1 g_2) : f \cdot O(g) = O(fg) : O(k \cdot |g|) = O(g)$

$f_1^2 = O(\max\{|g_1|, |g_2|\})$

$\Rightarrow$  if  $g_1 = g_2 = 0$  then  $f_1^2 = f_2^2 = 0$

$\epsilon$  is sign-bit,  $m/\epsilon^2$  is mantissa,  $\epsilon$  is exponent (8-bit for single, 11-bit for double)

Equivalently, can restrict to  $\text{double}^1 s.m \leq \epsilon^2 - 1$  for unique  $m$  and  $\epsilon$

$P$  and  $g$  are idealized (ignores over/underflow), so is countably infinite and self-similar (i.e.  $P = P \cdot P$ )

For all  $x \in \mathbb{R}$  there exists  $f(x) \in P$  s.t.

$|x - f(x)| \leq \epsilon_{\text{mach}} |x|$

Equivalently  $f(x) = x(1 + \delta), |\delta| \leq \epsilon_{\text{mach}}$

Machine epsilon  $\epsilon_{\text{machine}} = \epsilon_{\text{mach}} = 2^{-1} \cdot 2^{-t}$  is maximum relative gap between FP's

1) the gap between 1 and next largest FP  $2^{-24} \approx 5.96 \cdot 10^{-8}$  and  $2^{-53} \approx 10^{-16}$  for single/double

FP arithmetic: let  $s, \otimes$  be real and floating counterparts of arithmetic operation

For  $x, y \in \mathbb{R}$  we have  $x \otimes y = f(x \otimes y) = (x \otimes y)(1 + \delta), |\delta| \leq \epsilon_{\text{mach}}$

Holds for any arithmetic operation  $\otimes \in \{+, \cdot, \otimes, \ominus, \odot\}$

Complex floats implemented pairs of real floats, so above applies to complex ops as well

Caveat:  $\epsilon_{\text{mach}} = 2^{-1} \cdot 2^{-t}$  must be scaled by factors  $\alpha$

the order of  $2^{3/2}, 2^{5/2}$  for  $\otimes, \odot$  respectively

$(x_1 \oplus \dots \oplus x_n) = \sum_{i=1}^n x_i \left( \sum_{j=1}^i \epsilon_j \right) : \epsilon_j \leq \epsilon_{\text{mach}}$

$(x_1 \otimes \dots \otimes x_n) = (x_1 \otimes \dots \otimes x_n)(1 + \delta), \delta \leq 1.06(n-1) \epsilon_{\text{mach}}$

$f(\sum x_i y_i) = \sum x_i y_i (1 + \epsilon_i)$  where  $1 + \epsilon_i = (1 + \epsilon_j)(1 + \epsilon_k) \dots (1 + \epsilon_n)$  and  $|x_i|, |y_i| \leq \epsilon_{\text{mach}}$

$1 + \epsilon_i \leq 1 + \epsilon_j + (\epsilon_j + \epsilon_k) \dots$

$|f(x^T y) - x^T y| \leq \sum |x_i y_i| |\epsilon_i|$

Assuming  $n \epsilon_{\text{mach}} \leq 0.1 \Rightarrow$

$|f(x^T y) - x^T y| \leq \epsilon_{\text{mach}} \|x\| \|y\|$  where  $|x_i|, |y_i| \leq |x|, |y|$  is vector and  $\Phi(n)$  is small function of  $n$

Summing a series is more stable if terms added in order of increasing magnitude

For FP matrices, let  $M \in \mathbb{R}^{n \times n} \mid \|M\|_1 = \|M\|_1$  i.e. matrix  $\|M\|_1$  of absolute values of  $M$

$f(A) = A + \epsilon; |E|_{ij} \leq |A|_{ij} \epsilon_{\text{mach}}$

$f(A) = AB + \epsilon; |E|_{ij} \leq |A|_{ij} |B|_{ij} \epsilon_{\text{mach}}$

$f(AB) = AB + \epsilon; |E|_{ij} \leq n \epsilon_{\text{mach}} (|A|_{ij} |B|_{ij}) = O(\epsilon_{\text{mach}}^2)$

Taylor series about  $q \in \mathbb{R}$  is

$f(x) = \sum_{k=0}^n \frac{f^{(k)}(q)}{k!} (x - q)^k + O((x - q)^{n+1})$  as  $x \rightarrow q$

Need  $q=0 \Rightarrow f(x) = \sum_{k=0}^n \frac{f^{(k)}(0)}{k!} x^k + O(x^{n+1})$  as  $x \rightarrow 0$

e.g.  $(1 + \epsilon)^x = \sum_{k=0}^n \frac{\epsilon^k}{k!} x^k + O(\epsilon^{n+1})$  as  $\epsilon \rightarrow 0$

### Elementary Matrices

Identity  $I_n = [e_1 \mid \dots \mid e_n] : [e_1; \dots; e_n]$  has elementary vectors  $e_1, \dots, e_n$  for rows/columns

Row/column switching: permutation matrix  $P_{ij}$  obtained by switching  $e_j$  and  $e_j$  in  $I_n$  [same for rows/columns]

Applying  $P_{ij}$  from left will swap rows, from right will swap columns

$P_{ij} = P_{ji}^T$  i.e. applying twice will undo it

Row/column scaling:  $D_i(\lambda)$  obtained by scaling  $e_j$  by  $\lambda$  in  $I_n$  [same for rows/columns]

Applying  $P_{ij}$  from left will scale rows, from right will scale columns

$D_i(\lambda) = \text{diag}(1, \dots, \lambda, \dots, 1)$  so all diagonal properties

Apply, e.g.  $D_i(\lambda)^{-1} = D_i(1/\lambda)$

Row, e.g.  $D_i(\lambda) = D_i(1/\lambda)$  performs

$R_i \leftarrow R_i + R_j$  when applying from left

$\lambda e_i^T$  is zeros except for  $\lambda$  in  $(i, i)$  th entry

$e_i^T e_j = \delta_{ij}$

$LJ$  factorization w/ Gaussian elimination

$L = L_{ij}$  is lower triangular matrices

Recall: you can represent EROs and ECOs as transformation matrices  $R, C$  respectively

$LJ$  factorization  $\Rightarrow$  finds  $A = LU$  where  $L, U$  are lower/upper triangular respectively

Naive Gaussian Elimination performs  $|U| \mid |L| \mid |U| \mid |L|$  to get  $A_{LU} = R^{-1} U$  using only row addition

$R^{-1}$  i.e. inverse EROs in reversed order, is lower-triangular so  $L \leftarrow R^{-1}$

Algorithm 1 Gaussian elimination

1.  $U = A, L = I$
2. for  $k = 1$  to  $m - 1$  do
3. for  $j = k + 1$  to  $m$  do
4.  $\ell_{jk} = u_{jk} / u_{kk}$
5.  $u_{j,k:m} = u_{j,k:m} - \ell_{jk} u_{k,k:m}$
6. end for
7. end for

The pivot element is simply diagonal entry  $u_{kk}^{(k-1)}$

fails if  $u_{kk}^{(k-1)} = 0$

$\tilde{U} = A + \delta A : \frac{\|\delta A\|}{\|A\|} = O(\epsilon_{\text{mach}})$  only backwards

stable if  $\|L\| \|U\| = \|A\|$

Work required:  $\sim \frac{2}{3} m^3$  flops  $\rightarrow O(m^3)$

Solving  $Ax = LUx$  is  $\sim \frac{2}{3} m^3$  flops (back substitution is  $O(m^2)$ )

NOTE: Householder triangularisation requires  $\sim \frac{4}{3} m^3$

Partial pivoting computes  $PA = LU$  where  $P$  is a permutation matrix  $\Rightarrow PP^T = I$  i.e. orthogonal

For each column  $j$  finds largest entry and row-swaps to make it new pivot  $\Rightarrow$  largest

Then performs normal elimination on that column  $\Rightarrow$  result

Let  $L = L_{m-1} P_{m-1} \dots L_2 P_2 L_1 P_1 A = U$  where  $L_{m-1} P_{m-1} \dots L_2 P_2 L_1 P_1 = L_{m-1} \dots L_1 P_{m-1} \dots P_1$

Setting  $L = \begin{bmatrix} L_{m-1} & & 0 \\ & \ddots & \\ 0 & & I \end{bmatrix} \mid P = P_{m-1} \dots P_1$  gives  $PA = LU$

Algorithm 2 Gaussian elimination with partial pivoting

1.  $U = A, L = I, P = I$
2. for  $k = 1$  to  $m - 1$  do
3.  $i = \text{argmax}_i |u_{ik}|$
4.  $u_{i,k} \leftrightarrow u_{k,k}$
5.  $\ell_{i,k+1} \leftrightarrow \ell_{k,k+1}$
6.  $u_{i,k} \leftrightarrow u_{k,k}$
7. for  $j = k + 1$  to  $m$  do
8.  $\ell_{jk} = u_{jk} / u_{kk}$
9.  $u_{j,k:m} = u_{j,k:m} - \ell_{jk} u_{k,k:m}$
10. end for
11. end for

Work required:  $\sim \frac{2}{3} m^3$  flops  $\rightarrow O(m^3)$  results in  $L_{ij} \leq 1$  so  $\|L\| = O(1)$

Stability depends on growth-factor  $\rho = \frac{\max_{ij} |u_{ij}|}{\max_{ij} |a_{ij}|}$

$\Rightarrow$  for partial pivoting  $\rho \leq 2^{m-1}$

$|U| = O(\rho |A|) \Rightarrow \tilde{U} = PA + \delta A : \frac{\|\delta A\|}{\|A\|} = O(\rho \epsilon_{\text{machine}})$

$\Rightarrow$  only backwards stable if  $\rho = O(1)$

Full pivoting is  $PAQ = LU$  finds largest entry in bottom-right submatrix

Makes it pivot with row/column-swaps before normal elimination

Very expensive  $O(m^3)$  search-ops, partial pivoting only needs  $O(m^2)$

### Metric spaces & limits

Metrics obey these axioms

$d(x, y) \geq 0 \mid x \neq y \Rightarrow d(x, y) = 0 \mid d(x, y) = d(y, x)$

$d(x, z) \leq d(x, y) + d(y, z)$

For metric spaces, mix-and-match these infinite/finite limit definitions

$\lim_{x \rightarrow a} f(x) = L \Leftrightarrow \forall \epsilon \in \mathbb{R}, \exists \delta \in \mathbb{N}, \forall x \in \mathbb{N} : f(x) > r$

$\lim_{x \rightarrow p} f(x) = L \Leftrightarrow \forall \epsilon > 0, \exists \delta > 0, \forall x \in X : 0 < d(x, p) < \delta \Rightarrow d(f(x), L) < \epsilon$

Cauchy sequences, i.e.  $\forall \epsilon > 0, \exists N \in \mathbb{N}, \forall m, n \geq N : d(a_m, a_n) < \epsilon$  converge in complete spaces

You can manipulate matrix limits much like in real analysis, e.g.  $\lim_{n \rightarrow \infty} (A^n + B) = (\lim_{n \rightarrow \infty} A^n + B) \mid B \in \mathbb{C}$

Turn metric limit  $\lim_{n \rightarrow \infty} x_n = L$  into real limit  $\lim_{n \rightarrow \infty} \langle x_n, L \rangle = 0$  to leverage real analysis

Bounded monotone sequences converge in  $\mathbb{R}$

Sandwich theorem for limits in  $\mathbb{R}$   $\Rightarrow$  pick easy upper/lower bounds

$\lim_{n \rightarrow \infty} r^n = 0 \mid r < 1$  and  $\lim_{n \rightarrow \infty} r^n = 0 \mid r = 1$  and  $\lim_{n \rightarrow \infty} r^n = 0 \mid r = 1$

$\lambda^k$  are normalized

$(A - \alpha I)$  has eigenvalues  $\lambda - \alpha$

$\Rightarrow$  power-iteration on  $(A - \alpha I)$  has  $\frac{\lambda_2 - \alpha}{\lambda_1 - \alpha}$

Eigenvector guess  $\Rightarrow$  estimated eigenvalue

Inverse (power)-iteration: perform power iteration on  $(A - \alpha I)^{-1}$  to get  $\lambda_1, \alpha$  closest to  $\lambda_1$

$(A - \alpha I)^{-1}$  has eigenvalues  $(\lambda - \alpha)^{-1}$  so power iteration will yield largest  $(\lambda_1 - \alpha)^{-1}$

i.e. will yield smallest  $\lambda_1 - \alpha$  i.e. will yield  $\lambda_1, \alpha$  closest to  $\lambda_1$

$\|b\|$  has eigenvalues  $\lambda - \alpha$

$\Rightarrow$  power-iteration on  $(A - \alpha I)$  has  $\frac{\lambda_2 - \alpha}{\lambda_1 - \alpha}$

Eigenvector guess  $\Rightarrow$  estimated eigenvalue

Assume  $A$  is diagonal is non-zero w.l.o.g. permute/change basis if isn't then  $A = D \cdot L \cdot U$  where  $D</$