Basic identities of matrix/vector ops

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

For $A \in \mathbb{R}^{m\times n}$, A_{ij} is the i-th **ROW** then j-th **COLUMN**
$(A^T)_{ij} = A_{ji}$ $(AB)_{ij} = A_{i*} \cdot B_{*j} = \sum_k A_{ik}B_{kj}$
$(Ax)_i = A_{i*} \cdot x = \sum_j A_{ij}x_j$ $x^T y = y^T x = x \cdot y = \sum_i x_i y_i$
$x^T A x = \sum_i \sum_j A_{ij} x_i x_j$ $\mathbf{x}\mathbf{e}_k^T = [0|\ldots|\mathbf{x}|\ldots|0]$
$\mathbf{e}_k \mathbf{x}^T = [0^T; \ldots; \mathbf{x}^T; \ldots; 0^T]$

Scalar-multiplication + addition distributes over:
column-blocks =>
$\lambda A + B = \lambda[A_1|\ldots|A_c] + [B_1|\ldots|B_c] = [\lambda A_1 + B_1|\ldots|\lambda A_c + B_c]$
row-blocks =>
$\lambda A + B = \lambda[A_1;\ldots;A_r] + [B_1;\ldots;B_r] = [\lambda A_1 + B_1;\ldots;\lambda A_r + B_r]$
Matrix-multiplication distributes over:
column-blocks => $AB = A[B_1|\ldots|B_p] = [AB_1|\ldots|AB_p]$
row-blocks => $AB = [A_1;\ldots;A_p]B = [A_1B;\ldots;A_pB]$
outer-product sum =>
$AB = [A_1|\ldots|A_p][B_1;\ldots;B_p] = \sum_{i=1}^p A_iB_i$
e.g. for $A = [\mathbf{a}_1|\ldots|\mathbf{a}_n]$, $B = [\mathbf{b}_1;\ldots;\mathbf{b}_n]$ => $AB = \sum_i \mathbf{a}_i \mathbf{b}_i$

Projection: definition & properties

A **projection** $\pi: V \to V$ is a **endomorphism** such that $\pi \circ \pi = \pi$, 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 $P^2 = P = P^\dagger$ (conjugate-transpose)
Eigenvalues of a **projection matrix** must be 0 or 1
Because $\pi: V \to V$ is a **linear map**, its **image space** $U = \mathrm{im}(\pi)$ and **null space** $W = \ker(\pi)$ are **subspaces** of V
π is the **identity operator** on U
The **linear map** $\pi^* = I_V - \pi$ is **also** a projection with $W = \mathrm{im}(\pi^*) = \ker(\pi)$ and $U = \ker(\pi^*) = \mathrm{im}(\pi)$, i.e. they swapped
π is a projection **along** W **onto** U
π^* is a projection **along** U **onto** W
π^* 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 $u = \pi(x)$
$w \in W$ 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 π are **orthogonal subspaces**
infact they are eachother's **orthogonal compliments**, i.e. $U^\perp = W, W^\perp = U$ (because finite-dimensional vectorspaces)
so we have $\pi(x) \cdot y = \pi(x) \cdot \pi(y) = x \cdot \pi(y)$
or equivalently, $\pi(x) \cdot (y - \pi(y)) = (x - \pi(x)) \cdot \pi(y) = 0$

By Cauchy–Schwarz inequality we have $\|\pi(x)\| \le \|x\|$
The **orthogonal projection onto the line** containing vector u is $\mathrm{proj}_u = \hat{u}\hat{u}^T$, i.e. $\mathrm{proj}_u(v) = \frac{u \cdot v}{u \cdot u}u$; $\hat{u} = \frac{u}{\|u\|}$
A special case of $\pi(x) \cdot (y - \pi(y)) = 0$ is $u \cdot (v - \mathrm{proj}_u v) = 0$, since $\mathrm{proj}_u(u) = u$
If $U \subseteq \mathbb{R}^n$ is a k-dimensional subspace with **orthonormal basis (ONB)** $\langle \mathbf{u}_1,\ldots,\mathbf{u}_k\rangle \in \mathbb{R}^m$
Let $\mathbf{U} = [\mathbf{u}_1|\ldots|\mathbf{u}_k] \in \mathbb{R}^{m\times k}$ matrix
Orthogonal projection onto U is $\pi_U = \mathbf{U}\mathbf{U}^T$
Can be rewritten as $\pi_U(v) = \sum_i (\mathbf{u}_i \cdot v)\mathbf{u}_i$
If $\langle \mathbf{u}_1,\ldots,\mathbf{u}_k\rangle$ is **not orthonormal**, then "normalizing factor" $(\mathbf{U}^T\mathbf{U})^{-1}$ is added => $\pi_U = \mathbf{U}(\mathbf{U}^T\mathbf{U})^{-1}\mathbf{U}^T$
For **line subspaces** $U = \mathrm{span}\{u\}$, we have $(\mathbf{U}^T\mathbf{U})^{-1} = (u^Tu)^{-1} = 1/(u \cdot u) = 1/\|u\|$

Gram-Schmidt (GS) to gen. ONB from lin. ind. vectors

Gram-Schmidt is **iterative** projection => we use **current** j-**dim subspace**, to get **next** $(j+1)$-**dim subspace**
Assume **orthonormal basis (ONB)** $\langle \mathbf{q}_1,\ldots,\mathbf{q}_j\rangle \in \mathbb{R}^m$ for j-**dim subspace** $U_j \subset \mathbb{R}^m$
Let $Q_j = [\mathbf{q}_1|\ldots|\mathbf{q}_j] \in \mathbb{R}^{m\times j}$ be the matrix
$\mathrm{P}_j = Q_jQ_j^T$ is orthogonal projection **onto** U_j
$\mathrm{P}_{\perp j} = \mathrm{I}_m - Q_jQ_j^T$ is orthogonal projection **onto** $(U_j)^\perp$ (orthogonal compliment)
Uniquely decompose next $U_j \not\ni \mathbf{a}_{j+1} = \mathbf{v}_{j+1} + \mathbf{u}_{j+1}$
$\mathbf{v}_{j+1} = \mathrm{P}_j(\mathbf{a}_{j+1}) \in U_j$ => discard it!!
$\mathbf{u}_{j+1} = \mathrm{P}_{\perp j}(\mathbf{a}_{j+1}) \in (U_j)^\perp$ => we're after this!!
Let $\mathbf{q}_{j+1} = \hat{\mathbf{u}}_{j+1}$ => we have **next ONB** $\langle \mathbf{q}_1,\ldots,\mathbf{q}_{j+1}\rangle$ for U_{j+1} => start next iteration
$\mathbf{u}_{j+1} = (\mathrm{I}_m - Q_jQ_j^T)\mathbf{a}_{j+1} = \mathbf{a}_{j+1} - Q_j\mathbf{c}_j$ where $\mathbf{c}_j = [\mathbf{q}_1 \cdot \mathbf{a}_{j+1},\ldots,\mathbf{q}_j \cdot \mathbf{a}_{j+1}]^T$

Notice: $Q_j\mathbf{c}_j = \sum_{i=1}^j (\mathbf{q}_i \cdot \mathbf{a}_{j+1})\mathbf{q}_i = \sum_{i=1}^j \mathrm{proj}_{\mathbf{q}_i}(\mathbf{a}_{j+1})$, so rewrite as
$\mathbf{u}_{j+1} = \mathbf{a}_{j+1} - \sum_{i=1}^j (\mathbf{q}_i \cdot \mathbf{a}_{j+1})\mathbf{q}_i = \mathbf{a}_{j+1} - \sum_{i=1}^j \mathrm{proj}_{\mathbf{q}_i}(\mathbf{a}_{j+1})$

$\underbrace{\mathbf{a}_1,\ldots,\mathbf{a}_n}_{n} \in \mathbb{R}^m$ $m \ge n$ $U_n = \mathrm{span}\{\mathbf{a}_1,\ldots,\mathbf{a}_n\}$
We apply Gram-Schmidt to build **ONB** $\langle \mathbf{q}_1,\ldots,\mathbf{q}_n\rangle \in \mathbb{R}^m$ for $U_n \subset \mathbb{R}^m$
$j = 1$ => $\mathbf{u}_1 = \mathbf{a}_1$ and $\mathbf{q}_1 = \hat{\mathbf{u}}_1$, i.e. **start of iteration**
$j = 2$ => $\mathbf{u}_2 = \mathbf{a}_2 - (\mathbf{q}_1 \cdot \mathbf{a}_2)\mathbf{q}_1$ and $\mathbf{q}_2 = \hat{\mathbf{u}}_2$, **etc...**
Linear independence **guarantees** that $\mathbf{a}_{j+1} \notin U_j$
For exams: compute $\mathbf{u}_{j+1} = \mathbf{a}_{j+1} - Q_j\mathbf{c}_j$
1) Gather $Q_j = [\mathbf{q}_1|\ldots|\mathbf{q}_j] \in \mathbb{R}^{m\times j}$
2) Compute $\mathbf{c}_j = [\mathbf{q}_1 \cdot \mathbf{a}_{j+1},\ldots,\mathbf{q}_j \cdot \mathbf{a}_{j+1}]^T \in \mathbb{R}^j$
3) Compute $Q_j\mathbf{c}_j \in \mathbb{R}^m$, and subtract from $\mathbf{a}_{j+1}$

Properties: dot-product & norm

$x^Ty = y^Tx = x \cdot y = \sum_i x_iy_i$ $x \cdot y = \|a\|\|b\|\cos\hat{xy}$
$x \cdot y = y \cdot x$ $x \cdot (y+z) = x \cdot y + x \cdot z$ $\alpha x \cdot y = \alpha(x \cdot y)$
$x \cdot x = \|x\|^2 = 0 \iff x = 0$
for $x \neq \mathbf{0}$, we have $x \cdot y = x \cdot z \implies x \cdot (y - z) = 0$
$|x \cdot y| \le \|x\|\|y\|$ (**Cauchy-Schwartz inequality**)
$\|u+v\|^2 + \|u-v\|^2 = 2\|u\|^2 + 2\|v\|^2$ (**parallelogram law**)
$\|u+v\| \le \|u\| + \|v\|$ (**triangle inequality**)
$u \perp v \iff \|u+v\|^2 = \|u\|^2 + \|v\|^2$ (**pythagorean theorem**)
$\|c\|^2 = \|a\|^2 + \|b\|^2 - 2\|a\|\|b\|\cos\hat{ba}$ (**law of cosines**)

Transformation matrix & linear maps

For linear map $f: \mathbb{R}^n \to \mathbb{R}^m$, ordered bases $\langle \mathrm{b}_1,\ldots,\mathrm{b}_n\rangle \in \mathbb{R}^n$ and $\langle \mathrm{c}_1,\ldots,\mathrm{c}_m\rangle \in \mathbb{R}^m$
$A = \mathrm{F}_{CB} \in \mathbb{R}^{m\times n}$ is the **transformation-matrix** of f w.r.t to bases B and C
$f(\mathrm{b}_j) = \sum_{i=1}^m A_{ij}\mathrm{c}_i$ -> each b_j basis gets mapped to a linear combination of $\sum_i a_i\mathrm{c}_i$ bases
If f^{-1} exists (i.e. its bijective and $m = n$) then $(\mathrm{F}_{CB})^{-1} = \mathrm{F}^{-1}{}_{BC}$ (where $\mathrm{F}^{-1}{}_{BC}$ is the **transformation-matrix** of f^{-1})

The transformation matrix of the identity map is called change-in-basis matrix
The identity matrix I_m represents $\mathrm{id}_{\mathbb{R}^m}$ w.r.t. the standard basis $E_m = \langle \mathrm{e}_1,\ldots,\mathrm{e}_m\rangle$ => i.e. $\mathrm{I}_m = \mathrm{I}_{EE}$
If $B = \langle \mathrm{b}_1,\ldots,\mathrm{b}_m\rangle$ is a basis of $\mathbb{R}^m$, then $\mathrm{I}_{EB} = [\mathrm{b}_1|\ldots|\mathrm{b}_m]$ is the transformation matrix from B to E
$\mathrm{I}_{BE} = (\mathrm{I}_{EB})^{-1}$, so => $\mathrm{F}_{CB} = \mathrm{I}_{CE}\mathrm{F}_{EE}\mathrm{I}_{EB}$

Dot-product uniquely determines a vector w.r.t. to basis
If $a_i = x \cdot \mathrm{b}_i$; $x = \sum_i a_i\mathrm{b}_i$, we call a the coordinate-vector of x w.r.t. to B
Rank-nullity theorem:
$\dim(\mathrm{im}(f)) + \dim(\ker(f)) = \mathrm{rk}(A) + \dim(\ker(A)) = n$
f is injective/monomorphism **iff** $\ker(f) = \{0\}$ **iff** A is full-rank

Orthogonality concepts

$u \perp v \iff u \cdot v = 0$, i.e. u and v are orthogonal
u and v are orthonormal **iff** $u \perp v$, $\|u\| = 1 = \|v\|$
$A \in \mathbb{R}^{n\times n}$ is orthogonal **iff** $A^{-1} = A^T$
Columns of $A = [a_1|\ldots|a_n]$ are orthonormal basis (ONB) $C = \langle a_1,\ldots,a_n\rangle \in \mathbb{R}^n$, so $A = \mathrm{I}_{EC}$ is change-in-basis matrix
Orthogonal transformations preserve lengths/angles/distances => $\|Ax\|_2 = \|x\|_2$, $\hat{AxAy} = \hat{xy}$
Therefore can be seen as a succession of reflections and planar rotations
$\det(A) = 1$ or $\det(A) = -1$, and all **eigenvalues** of A are s.t. $|\lambda| = 1$
$A \in \mathbb{R}^{m\times n}$ is semi-orthogonal **iff** $A^TA = I$ or $AA^T = I$
If $n > m$ then **all** m **rows** are orthonormal vectors
If $m > n$ then **all** n **columns** are orthonormal vectors
$U \perp V \subset \mathbb{R}^n \iff \mathbf{u} \cdot \mathbf{v} = 0$ for all $\mathbf{u} \in U, \mathbf{v} \in V$, i.e. they are **orthogonal subspaces**
Orthogonal compliment of $U \subset \mathbb{R}^n$ is the subspace
$U^\perp = \{x \in \mathbb{R}^n \mid \forall y \in \mathbb{R}^n : x \perp y\}$
$= \{x \in \mathbb{R}^n \mid \forall y \in \mathbb{R}^n : \|x\| \le \|x + y\|\}$
$\mathbb{R}^n = U \oplus U^\perp$ and $(U^\perp)^\perp = U$
$U \perp V \iff U^\perp = V$ and vice-versa
$Y \subseteq X \implies X^\perp \subseteq Y^\perp$ and $X \cap X^\perp = \{0\}$
Any $\mathbf{x} \in \mathbb{R}^n$ can be uniquely decomposed into $\mathbf{x} = \mathbf{x}_i + \mathbf{x}_k$, where $\mathbf{x}_i \in U$ and $\mathbf{x}_k \in U^\perp$
For matrix $A \in \mathbb{R}^{m\times n}$ and for row-space $\mathrm{R}(A)$, column-space $\mathrm{C}(A)$ and null space $\ker(A)$
$\mathrm{R}(A)^\perp = \ker(A)$ and $\mathrm{C}(A)^\perp = \ker(A^T)$
Any $\mathbf{b} \in \mathbb{R}^m$ can be uniquely decomposed into
$\mathbf{b} = \mathbf{b}_i + \mathbf{b}_k$, where $\mathbf{b}_i \in \mathrm{C}(A)$ and $\mathbf{b}_k \in \ker(A^T)$
$\mathbf{b} = \mathbf{b}_i + \mathbf{b}_k$, where $\mathbf{b}_i \in \mathrm{R}(A)$ and $\mathbf{b}_k \in \ker(A)$

Vector norms (beyond euclidean)

vector norms are such that: $\|x\| = 0 \iff x = \mathbf{0}$, $|\lambda x| = |\lambda|\|x\|$, $\|x + y\| \le \|x\| + \|y\|$
ℓ_p norms: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p\right)^{1/p}$
$p = 1$: $\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|$
$p = 2$: $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{\mathbf{x} \cdot \mathbf{x}}$
$p = \infty$: $\|\mathbf{x}\|_\infty = \lim_{p\to\infty}\|\mathbf{x}\|_p = \max_{1\le i\le n}|x_i|$
Any two norms in $\mathbb{R}^n$ are equivalent, meaning there exist $r > 0; s > 0$ such that: $\forall \mathbf{x} \in \mathbb{R}^n, r\|\mathbf{x}\|_a \le \|\mathbf{x}\|_b \le s\|\mathbf{x}\|_a$
Equivalence of ℓ_1, ℓ_2 and ℓ_∞ => $\|\mathbf{x}\|_\infty \le \|\mathbf{x}\|_2 \le \|\mathbf{x}\|_1$, $\|\mathbf{x}\|_2 \le \sqrt{n}\|\mathbf{x}\|_\infty$, $\|\mathbf{x}\|_1 \le \sqrt{n}\|\mathbf{x}\|_2$
Induce **metric** $d(x,y) = \|y - x\|$, has additional properties:
Translation invariance: $d(x+w, y+w) = d(x,y)$
Scaling: $d(\lambda x, \lambda y) = |\lambda| d(x,y)$

Matrix norms

Matrix norms are such that: $\|A\| = 0 \iff A = \mathbf{0}$, $|\lambda A| = |\lambda|\|A\|$, $\|A + B\| \le \|A\| + \|B\|$
Matrices $\mathbb{F}^{m\times n}$ are a vector space so **matrix norms are vector norms**, all results apply
Sub-multiplicative matrix norm (assumed by default) is also such that $\|AB\| \le \|A\|\|B\|$
Common matrix norms, for some $\mathbf{A} \in \mathbb{R}^{m\times n}$:
$\|\mathbf{A}\|_1 = \max_j \|\mathbf{A}_{*j}\|_1$
$\|\mathbf{A}\|_2 = \sigma_1(\mathbf{A})$ i.e. largest singular value of A (square-root of largest eigenvalue of A^TA or AA^T)
$\|\mathbf{A}\|_\infty = \max_i \|\mathbf{A}_{i*}\|_1$, note that $\|\mathbf{A}\|_1 = \|\mathbf{A}^T\|_\infty$
Frobenius norm: $\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |A_{ij}|^2}$
A matrix norm $\|\cdot\|$ on $\mathbb{R}^{m\times n}$ is **consistent** with the vector norms $\|\cdot\|_a$ on $\mathbb{R}^n$ and $\|\cdot\|_b$ on $\mathbb{R}^m$ if for all $\mathbf{A} \in \mathbb{R}^{m\times n}$ and $\mathbf{x} \in \mathbb{R}^n$ => $\|\mathbf{A}\mathbf{x}\|_b \le \|\mathbf{A}\|\|\mathbf{x}\|_a$
If $a = b$, $\|\cdot\|$ is **compatible** with $\|\cdot\|_a$
Frobenius norm is **consistent** with ℓ_2 norm => $\|Av\|_2 \le \|A\|_F\|v\|_2$
For a vector norm $\|\cdot\|$ on $\mathbb{R}^n$, the **subordinate matrix norm** $\|\cdot\|$ on $\mathbb{R}^{m\times n}$ is
$\|\mathbf{A}\| = \max\{\|\mathbf{A}\mathbf{x}\| : \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\| = 1\}$
$= \max\left\{\frac{\|\mathbf{A}\mathbf{x}\|}{\|\mathbf{x}\|} : \mathbf{x} \in \mathbb{R}^n, \mathbf{x} \neq 0\right\}$
$= \max\{\|\mathbf{A}\mathbf{x}\| : \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\| \le 1\}$
Vector norms are **compatible** with their **subordinate matrix norms**
For $p = 1, 2, \infty$ **matrix norm** $\|\cdot\|_p$ is **subordinate** to the vector norm $\|\cdot\|_p$ (and thus **compatible** with)

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 if its diagonals**, i.e. $\mathrm{tr}(A)$

A is symmetric **iff** $A = A^T$; A is Hermitian, iff $A = A^\dagger$, i.e. its equal to its conjugate-transpose
AA^T and A^TA are **symmetric** (and **positive semi-definite**)
For real matrices, **Hermitian/symmetric** are equivalent conditions
Every eigenvalue λ_i of **Hermitian** matrices is real
geometric multiplicity of λ_i = geometric multiplicity of λ_i
eigenvectors $\mathbf{x}_1, \mathbf{x}_2$ associated to distinct eigenvalues λ_1, λ_2 are **orthogonal**, i.e. $\mathbf{x}_1 \perp \mathbf{x}_2$

A is triangular **iff** all entries above (**lower-triangular**) or below (**upper-triangular**) the main diagonal are **zero**
Determinant => $|A| = \prod_i a_{ii}$, 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
$\mathrm{diag}_{m\times n}(\mathbf{a}) = \mathrm{diag}_{m\times n}(a_1,\ldots,a_p)$, $p = \min(m,n)$, where $\mathbf{a} = [a_1,\ldots,a_p]^T \in \mathbb{R}^p$ diagonal entries of A
For $x \in \mathbb{R}^n$, $Ax = \mathrm{diag}_{m\times n}(a_1,\ldots,a_p)[x_1\ \ldots\ x_n]^T = [a_1x_1\ \ldots\ a_px_p\ \ 0\ldots0]^T \in \mathbb{R}^m$ (if $p = m$ those tail-zeros don't exist)
$\mathrm{diag}_{m\times n}(\mathbf{a}) + \mathrm{diag}_{m\times n}(\mathbf{b}) = \mathrm{diag}_{m\times n}(\mathbf{a} + \mathbf{b})$
Consider $\mathrm{diag}_{n\times k}(c_1,\ldots,c_q)$, $q = \min(n,k)$, then
$\mathrm{diag}_{m\times n}(a_1,\ldots,a_p)\mathrm{diag}_{n\times k}(c_1,\ldots,c_q)$
$= \mathrm{diag}_{m\times k}(a_1c_1,\ldots,a_rc_r,0,\ldots,0) = \mathrm{diag}(\mathbf{s})$
Where $r = \min(p,q) = \min(m,n,k)$, and $\mathbf{s} \in \mathbb{R}^s$, $s = \min(m,k)$
Inverse of square-diagonals =>
$\mathrm{diag}(a_1,\ldots,a_n)^{-1} = \mathrm{diag}(a_1^{-1},\ldots,a_n^{-1})$, i.e. diagonals **cannot be zero** (division by zero undefined)
Determinant of square-diagonals =>
$|\mathrm{diag}(a_1,\ldots,a_n)| = \prod_i a_i$ (since they are technically triangular matrices)

The **(column) rank** of A is number of linearly independent columns, i.e. $\mathrm{rk}(A)$
I.e. its the **number of pivots** in **row-echelon-form**
I.e. its the **dimension** of the **column-space**
$\mathrm{rk}(A) = \dim(\mathrm{C}(A))$
I.e. its the **dimension** of the **image-space**
$\mathrm{rk}(A) = \dim(\mathrm{im}(f_A))$ of linear map $f_A(x) = Ax$
The **(row) rank** of A is number of linearly independent rows
The **row/column ranks** are **always the same**, hence $\mathrm{rk}(A) = \dim(\mathrm{C}(A)) = \dim(\mathrm{R}(A)) = \dim(\mathrm{C}(A^T)) = \mathrm{rk}(A^T)$
A is full-rank **iff** $\mathrm{rk}(A) = \min(m,n)$, i.e. its as linearly independent as possible

Two matrices $\mathbf{A}, \tilde{\mathbf{A}} \in \mathbb{R}^{m\times n}$ are **equivalent** if there exist two invertible matrices $\mathbf{P} \in \mathbb{R}^{m\times m}$ and $\mathbf{Q} \in \mathbb{R}^{n\times n}$ such that $\mathbf{A} = \mathbf{P}\tilde{\mathbf{A}}\mathbf{Q}^{-1}$
Two matrices $\mathbf{A}, \tilde{\mathbf{A}} \in \mathbb{R}^{n\times n}$ are **similar** if there exists an invertible matrix $\mathbf{P} \in \mathbb{R}^{n\times n}$ such that $\mathbf{A} = \mathbf{P}\tilde{\mathbf{A}}\mathbf{P}^{-1}$
Similar matrices are equivalent, with $\mathbf{Q} = \mathbf{P}$
A is diagonalisable **iff** A is similar to some diagonal matrix D

Properties of determinants

Consider $A \in \mathbb{R}^{n\times n}$, then $A_{ij}{}' \in \mathbb{R}^{(n-1)\times(n-1)}$ the (i,j)-**minor matrix** of A, obtained by deleting i-**th row** and j-**th column** from A
Then we define **determinant** of A, i.e. $\det(A) = |A|$, as
$\det(A) = \sum_{k=1}^n (-1)^{i+k}A_{ik}\det(A_{ik}{}')$, i.e. expansion along i-**th row** *(for any i)
$\det(A) = \sum_{k=1}^n (-1)^{k+j}A_{kj}\det(A_{kj}{}')$, i.e. expansion along j-**th column** (for any j)
When $\det(A) = 0$ we call A a **singular matrix**
Common determinants
For $n = 1$, $\det(A) = A_{11}$
For $n = 2$, $\det(A) = A_{11}A_{22} - A_{12}A_{21}$
$\det(I_n) = 1$
Multi-linearity in columns/rows: if
$A = [a_1|\ldots|a_j|\ldots|a_n] = [a_1|\ldots|\lambda x_j + \mu y_j|\ldots|a_n]$ then
$\det(A) = \lambda\det([a_1|\ldots|x_j|\ldots|a_n]) + \mu\det([a_1|\ldots|y_j|\ldots|a_n])$
And the exact same linearity property for **rows**
Immediately leads to: $|A| = |A^T|$, $|\lambda A| = \lambda^n|A|$, and $|AB| = |BA| = |A||B|$ (for any $B \in \mathbb{R}^{n\times n}$)
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**) => if **columns** (or **rows**) are linearly-dependent (some are linear combinations of others) then $|A| = 0$
Stated in other terms => $\mathrm{rk}(A) < n \iff |A| = 0$ <=> $\mathrm{RREF}(A) \neq I_n \iff |A| = 0$ (reduced row-echelon-form)
<=> $\mathrm{C}(A) \neq \mathbb{R}^n \iff |A| = 0$ (column-space)
For more equivalence to the above, see invertible matrix theorem
Interaction with **EROs**/**ECOs**:
Swapping rows/columns **flips the sign**
Scaling a row/column by $\lambda \neq 0$ will **scale the determinant** by λ (by multi-linearity)
Remember to **scale by** λ^{-1} to **maintain equality**, i.e. $\det(A) = \lambda^{-1}\det([a_1|\ldots|\lambda a_j|\ldots|a_n])$
Invariant under **addition** of rows/columns
Link to invertable matrices => $|A^{-1}| = |A|^{-1}$ which means A is invertible $\iff |A| \neq 0$, i.e. **singular matrices are not invertible**
For block-matrices:
$\det\begin{pmatrix}A & B\\ \mathbf{0} & D\end{pmatrix} = \det(A)\det(B) = \det\begin{pmatrix}A & \mathbf{0}\\ C & D\end{pmatrix}$
$\det\begin{pmatrix}A & B\\ C & D\end{pmatrix} = \det(A)\det(D - CA^{-1}B) = \det(D)\det(A - BD^{-1}C)$ if A or D are invertible, respectively
Sylvester's determinant theorem:
$\det(I_m + AB) = \det(I_n + BA)$
Matrix determinant lemma:
$\det(\mathbf{A} + \mathbf{u}\mathbf{v}^T) = (1 + \mathbf{v}^T\mathbf{A}^{-1}\mathbf{u})\det(\mathbf{A})$
$\det(\mathbf{A} + \mathbf{U}\mathbf{V}^T) = \det(\mathbf{I}_m + \mathbf{V}^T\mathbf{A}^{-1}\mathbf{U})\det(\mathbf{A})$
$\det(\mathbf{A} + \mathbf{U}\mathbf{W}\mathbf{V}^T) = \det(\mathbf{W}^{-1} + \mathbf{V}^T\mathbf{A}^{-1}\mathbf{U})\det(\mathbf{W})\det(\mathbf{A})$

Tricks for computing determinant

If block-triangular matrix then apply $\det\begin{pmatrix}A & B\\ 0 & D\end{pmatrix} = \det(A)\det(B)$
If close to triangular matrix apply **EROs**/**ECOs** to get it there, then its just product of diagonals
If **Cholesky/LU/QR** is possible and cheap then do it, then apply $|AB| = |A||B|$
If all else fails, try to find row/column with **MOST** zeros
Perform minimal **EROs**/**ECOs** to get that row/column to be **all-but-one** zeros
Don't forget to keep track of sign-flipping & scaling-factors
Do Laplace expansion along that row/column => notice **all-but-one** minor matrix determinants **go to zero**

Representing EROs/ECOs as transformation matrices

For $A \in \mathbb{R}^{m\times n}$, suppose a sequence of:
EROs transform $A \rightsquigarrow_{\mathrm{EROs}} A'$ => there is matrix R s.t. $RA = A'$
ECOs transform $A \rightsquigarrow_{\mathrm{ECOs}} A'$ => there is matrix C s.t. $AC = A'$
Both transform $A \rightsquigarrow_{\mathrm{EROs+ECOs}} A'$ => there are matrices R, C s.t. $RAC = A'$

FORWARD: to compute these **transformation matrices**:
Start with $[I_m \mid A \mid I_n]$, i.e. A and identity matrices
For every **ERO** on A, do the same to **LHS** (i.e. I_m)
For every **ECO** on A, do the same to **RHS** (i.e. I_n)
Once done, you should get $[I_m \mid A \mid I_n] \rightsquigarrow [R \mid A' \mid C]$ with $RAC = A'$

If the sequences of **EROs** and **ECOs** were $R_1,\ldots,R_\lambda$ and $C_1,\ldots,C_\mu$ respectively
$R = R_\lambda \cdots R_1$ and $C = C_1 \cdots C_\mu$, so
$(R_\lambda \cdots R_1)A(C_1 \cdots C_\mu) = A'$
$R^{-1} = R_1^{-1} \cdots R_\lambda^{-1}$ and $C^{-1} = C_\mu^{-1} \cdots C_1^{-1}$, where R_i^{-1}, C_j^{-1} are **inverse EROs/ECOs** respectively

BACKWARD: once $R_1,\ldots,R_\lambda$ and $C_1,\ldots,C_\mu$ for which $RAC = A'$ are **known**, starting with $[I_m \mid A \mid I_n]$
For $i = 1 \to \lambda$ perform R_i on A, perform $R_{\lambda-i+1}^{-1}$ on **LHS** (i.e. I_m)
For $j = 1 \to \mu$ perform C_j on A, perform $C_{\mu-j+1}^{-1}$ on **RHS** (i.e. I_n)
You should get $[I_m \mid A \mid I_n] \rightsquigarrow [R^{-1} \mid A' \mid C^{-1}]$ with $A = R^{-1}A'C^{-1}$

You can mix-and-match the **forward/backward** modes
i.e. inverse operations in inverse order for one, and operations in normal order for the other
e.g. you can do $[I_m \mid A \mid I_n] \rightsquigarrow [R^{-1} \mid A' \mid C]$ to get $AC = R^{-1}A'$ => useful for LU factorization

Eigen-values/vectors

Consider $A \in \mathbb{R}^{n\times n}$, non-zero $\mathbf{x} \in \mathbb{C}^n$ is an **eigenvector** with **eigenvalue** $\lambda \in \mathbb{C}$ for A if $A\mathbf{x} = \lambda\mathbf{x}$
If $A\mathbf{x} = \lambda\mathbf{x}$ then $A(k\mathbf{x}) = \lambda(k\mathbf{x})$ for $k \neq 0$, i.e. $k\mathbf{x}$ is also an **eigenvector**
A has at most n distinct **eigenvalues**
The set of all eigenvectors associated with eigenvalue λ is called **eigenspace** E_λ of A
$E_\lambda = \ker(A - \lambda I)$
The **geometric multiplicity** of λ is $\dim(E_\lambda) = \dim(\ker(A - \lambda I))$
The **spectrum** $Sp(A) = \{\lambda_1,\ldots,\lambda_n\}$ of A is the set of all eigenvalues of A
The **characteristic polynomial** of A is $P(\lambda) = |A - \lambda I| = \sum_{i=0}^n a_i\lambda^i$
$a_0 = |A|$, $a_{n-1} = (-1)^{n-1}\mathrm{tr}(A)$, $a_n = (-1)^n$
$\lambda \in \mathbb{C}$ is eigenvalue of A **iff** λ is a root of $P(\lambda)$
The **algebraic multiplicity** of λ is the **number of times** it is **repeated as root** of $P(\lambda)$
$1 \le$ geometric multiplicity of λ $\le$ algebraic multiplicity of λ
Let $\lambda_1,\ldots,\lambda_n \in \mathbb{C}$ be (potentially non-distinct) **eigenvalues** of A, with $\mathbf{x}_1,\ldots,\mathbf{x}_n \in \mathbb{C}^n$ their **eigenvectors**
$\mathrm{tr}(A) = \sum_i \lambda_i$ and $\det(A) = \prod_i \lambda_i$
A is diagonalisable **iff** there exist a basis of $\mathbb{R}^n$ consisting of $\mathbf{x}_1,\ldots,\mathbf{x}_n$
A is diagonalisable **iff** $r_i = g_i$, where
r_i = geometric multiplicity of λ_i and
g_i = geometric multiplicity of λ_i
Eigenvalues of A^k are $\lambda_1,\ldots,\lambda_n$
Let $P = [x_1|\ldots|x_n]$, then
$AP = [\lambda_1x_1|\ldots|\lambda_nx_n] = [x_1|\ldots|x_n]\mathrm{diag}(\lambda_1,\ldots,\lambda_n) = PD$
=> if P^{-1} exists then
$A = PDP^{-1}$, i.e. A is diagonalisable
$P = \mathrm{I}_{EB}$ is **change-in-basis** matrix for basis $B = \langle x_1,\ldots,x_n\rangle$ of eigenvectors
If $A = \mathrm{F}_{EE}$ is transformation-matrix of linear map f, then $\mathrm{F}_{EE} = \mathrm{I}_{EB}\mathrm{F}_{BB}\mathrm{I}_{BE}$
Spectral theorem: if A is Hermitian then P^{-1} exists:
If $\mathbf{x}_i, \mathbf{x}_j$ associated to different eigenvalues then $\mathbf{x}_i \perp \mathbf{x}_j$
If associated to same eigenvalue λ then **eigenspace** E_λ has spanning-set $\{\mathbf{x}_{\lambda_i},\ldots\}$
$\mathbf{x}_1,\ldots,\mathbf{x}_n$ are linearly independent => apply Gram-Schmidt $\mathbf{q}_{\lambda_i},\cdots \leftarrow \mathbf{x}_{\lambda_i},\ldots$
Then $\{\mathbf{q}_{\lambda_i},\ldots\}$ is orthonormal basis (ONB) of E_λ
$Q = \langle \mathbf{q}_1,\ldots,\mathbf{q}_n\rangle$ is an ONB of $\mathbb{R}^n$ => $Q = [\mathbf{q}_1|\ldots|\mathbf{q}_n]$ is orthogonal matrix i.e. $Q^{-1} = Q^T$
$\mathbf{q}_1,\ldots,\mathbf{q}_n$ are still eigenvectors of A => $A = QDQ^T$ (**spectral decomposition**)
$A = QDQ^T$ can be interpreted as scaling in direction of its eigenvectors:
1) Perform a succession of reflections/planar rotations to change coordinate-system
2) Apply scaling by λ_i to each dimension $\mathbf{q}_i$
Undo those reflections/planar rotations

Extension to $\mathbb{C}^n$

Standard inner product: $\langle x, y\rangle = x^\dagger y = \sum_i \overline{x_i}y_i$
Conjugate-symmetric: $\langle x, y\rangle = \overline{\langle y, x\rangle}$
Standard (induced) norm: $\|x\| = \sqrt{\langle x, y\rangle} = \sqrt{x^\dagger y}$
We can diagonalise real matrices in $\mathbb{C}$ which lets us diagonalise more matrices than before

Least Square Method

If we are solving $A\mathbf{x} = \mathbf{b}$ and $\mathbf{b} \notin \mathrm{C}(A)$, i.e. no solution, then **Least Square Method** is:
Finding $\mathbf{x}$ which **minimizes** $\|A\mathbf{x} - \mathbf{b}\|_2$
Recall for $A \in \mathbb{R}^{m\times n}$ we have unique decomposition for any $\mathbf{b} \in \mathbb{R}^m$: $\mathbf{b} = \mathbf{b}_i + \mathbf{b}_k$
where $\mathbf{b}_i \in \mathrm{C}(A)$ and $\mathbf{b}_k \in \ker(A^T)$
$\|A\mathbf{x} - \mathbf{b}\|_2$ is minimized $\iff \|A\mathbf{x} - \mathbf{b}_i\|_2 = 0 \iff A\mathbf{x} = \mathbf{b}_i$

$A^TA\mathbf{x} = A^T\mathbf{b}$ is the **normal equation** which gives solution to least square problem:
$\|A\mathbf{x} - \mathbf{b}\|_2$ is minimized $\iff A\mathbf{x} = \mathbf{b}_i \iff A^TA\mathbf{x} = A^T\mathbf{b}$

Linear Regression

Let $y = f(t) = \sum_{j=1}^n s_jf_j(t)$ be a **mathematical model**, where f_j are **basis functions** and s_j are **parameters**
Let (t_i, y_i), $1 \le i \le m$, $m \gg n$ be a set of **observations**, and $\mathbf{t}, \mathbf{y} \in \mathbb{R}^m$ are vectors representing those **observations**
$f_j(\mathbf{t}) = [f_j(t_1),\ldots,f_j(t_m)]^T$ is **transformed vector**
$A = [f_1(\mathbf{t})|\ldots|f_n(\mathbf{t})] \in \mathbb{R}^{m\times n}$ is a matrix of columns
$\mathbf{z} = [s_1,\ldots,s_n]^T$ is vector of parameters
Then we get equation $A\mathbf{z} = \mathbf{y}$ => **minimizing** $\|A\mathbf{z} - \mathbf{y}\|_2$ is the solution to Linear Regression
So applying **LSM** to $A\mathbf{z} = \mathbf{y}$ is precisely what **Linear Regression** is
We can use normal equations for this =>
$\|A\mathbf{z} - \mathbf{y}\|_2$ is minimized $\iff A^TA\mathbf{z} = A^T\mathbf{y}$
Solution to **normal equations** unique **iff** A is full-rank, i.e. it has linearly-independent columns

Positive (semi-)definite matrices

Consider symmetric $A \in \mathbb{R}^{n\times n}$, i.e. $A = A^T$
A is positive-definite **iff** $x^TAx > 0$ for all $x \neq 0$
A is positive-definite **iff** all its eigenvalues are **strictly positive**
A is positive-definite => all its diagonals are **strictly positive**
A is positive-definite => $\max(A_{ii}, A_{jj}) > |A_{ij}|$, i.e. **strictly larger coefficient** on the diagonals
A is positive-definite => all **upper-left submatrices** are also positive-definite
Sylvester's criterion: A is positive-definite **iff** all **upper-left submatrices** have strictly positive determinant

A is positive semi-definite **iff** $x^TAx \ge 0$ for all x
A is positive semi-definite **iff** all its eigenvalues are **non-negative**
A is positive semi-definite => all its diagonals are **non-negative**
A is positive semi-definite => $\max(A_{ii}, A_{jj}) \ge |A_{ij}|$, i.e. **no coefficient larger** than on the diagonals
A is positive semi-definite => all **upper-left submatrices** are also positive semi-definite
A is positive semi-definite => it has a Cholesky Decomposition

For any $M \in \mathbb{R}^{m\times n}$, MM^T and M^TM are symmetric and **positive semi-definite**

Singular Value Decomposition (SVD) & Singular Values

Singular Value Decomposition of $A \in \mathbb{R}^{m\times n}$ is any decomposition of the form $A = USV^T$, where
Orthogonal $U = [\mathbf{u}_1|\ldots|\mathbf{u}_m] \in \mathbb{R}^{m\times m}$ and $V = [\mathbf{v}_1|\ldots|\mathbf{v}_n] \in \mathbb{R}^{n\times n}$
$S = \mathrm{diag}_{m\times n}(\sigma_1,\ldots,\sigma_p)$ where $p = \min(m,n)$ and $\sigma_1 \ge \cdots \ge \sigma_p \ge 0$
$\sigma_1,\ldots,\sigma_p$ are **singular values** of A,
(Positive) **singular values** are (positive) **square-roots of eigenvalues** of AA^T or A^TA
i.e. $\sigma_1^2,\ldots,\sigma_p^2$ are **eigenvalues** of AA^T or A^TA
$\|A\|_2 = \sigma_1$ (link to matrix norms
Let $r = \mathrm{rk}(A)$, then number of strictly positive **singular values** is r
i.e. $\sigma_1 \ge \cdots \ge \sigma_r > 0$ and $\sigma_{r+1} = \cdots = \sigma_p = 0$
$A = \sum_{i=1}^r \sigma_iu_iv_i^T$

SVD is similar to spectral decomposition, except it always exists
If $n \le m$ then work with $A^TA \in \mathbb{R}^{n\times n}$:
Obtain eigenvalues $\sigma_1^2 \ge \cdots \ge \sigma_n^2 \ge 0$ of A^TA
Obtain **orthonormal** eigenvectors $\mathbf{v}_1,\ldots,\mathbf{v}_n \in \mathbb{R}^n$ of A^TA (apply **normalization** e.g. **Gram-Schmidt**!!!! to **eigenspaces** E_{σ_i})
$V = [\mathbf{v}_1|\ldots|\mathbf{v}_n] \in \mathbb{R}^{n\times n}$ is orthogonal so $V^T = V^{-1}$
$r = \mathrm{rk}(A)$ = no. of strictly +ve σ_i
Let $\mathbf{u}_i = \frac{1}{\sigma_i}A\mathbf{v}_i$ then $\mathbf{u}_1,\ldots,\mathbf{u}_r \in \mathbb{R}^m$ are **orthonormal** (therefore linearly independent)
The orthogonal compliment of $\mathrm{span}\{\mathbf{u}_1,\ldots,\mathbf{u}_r\}$ =>
$\mathrm{span}\{\mathbf{u}_1,\ldots,\mathbf{u}_r\}^\perp = \mathrm{span}\{\mathbf{u}_{r+1},\ldots,\mathbf{u}_m\}$
Solve for unit-vector $\mathbf{u}_{r+1}$ s.t. it is orthogonal to $\mathbf{u}_1,\ldots,\mathbf{u}_r$
Then solve for unit-vector $\mathbf{u}_{r+2}$ s.t. it is orthogonal to $\mathbf{u}_1,\ldots,\mathbf{u}_{r+1}$
And so on…
$U = [\mathbf{u}_1|\ldots|\mathbf{u}_m] \in \mathbb{R}^{m\times m}$ is orthogonal so $U^T = U^{-1}$
$S = \mathrm{diag}_{m\times n}(\sigma_1,\ldots,\sigma_n)$, **AND DONE!!!**
If $m < n$ then let $B = A^T$
apply above method to B => $B = A^T = USV^T$
$A = B^T = VS^TU^T$

Tricks: Computing orthonormal vector-set extensions

You have **orthonormal** vectors $\mathbf{u}_1,\ldots,\mathbf{u}_r \in \mathbb{R}^m$ => need to **extend** to **orthonormal** vectors $\mathbf{u}_1,\ldots,\mathbf{u}_m \in \mathbb{R}^m$
Special case => two 3D vectors => use **cross-product** => $a \times b \perp a, b$

Extension via standard basis $\mathrm{I}_m = [\mathbf{e}_1|\ldots|\mathbf{e}_m]$ using (tweaked) GS:
Choose candidate vector: just work through $\mathbf{e}_1,\ldots,\mathbf{e}_m$ sequentially starting from $\mathbf{e}_1$ => denote the current candidate $\mathbf{e}_k$
Orthogonalize: Starting from $j = r$ going to $j = m$ with each iteration => with current orthonormal vectors $\mathbf{u}_1,\ldots,\mathbf{u}_j$
Compute
$\mathbf{w}_{j+1} = \mathbf{e}_k - \sum_{i=1}^j(\mathbf{e}_k \cdot \mathbf{u}_i)\mathbf{u}_i = \mathbf{e}_k - \sum_{i=1}^j(\mathbf{u}_i)_k\mathbf{u}_i$
$= \mathbf{e}_k - U_j\mathbf{c}_j$
Where $U_j = [\mathbf{u}_1|\ldots|\mathbf{u}_j]$ and $\mathbf{c}_j = [(\mathbf{u}_1)_k,\ldots,(\mathbf{u}_j)_k]^T$
NOTE: $\mathbf{e}_k \cdot \mathbf{u}_i = (\mathbf{u}_i)_k$ i.e. k-th component of $\mathbf{u}_i$
If $\mathbf{w}_{j+1} = \mathbf{0}$ then $\mathbf{e}_k \in \mathrm{span}\{\mathbf{u}_1,\ldots,\mathbf{u}_j\}$ => discard $\mathbf{w}_{j+1}$, choose next candidate $\mathbf{e}_{k+1}$, try this step again
Normalize: $\mathbf{w}_{j+1} \neq \mathbf{0}$ so compute unit vector $\mathbf{u}_{j+1} = \hat{\mathbf{w}}_{j+1}$
Repeat: keep repeating the above steps, now with **new** orthonormal vectors $\mathbf{u}_1,\ldots,\mathbf{u}_{j+1}$

SVD Application: Principal Component Analysis (PCA)

Assume $A_{\text{uncentered}} \in \mathbb{R}^{m\times n}$ represent m **samples** of n-**dimensional data** (with $m \ge n$)
Data centering: subtract mean of each column from that column's elements
Let the **resulting matrix** be $A \in \mathbb{R}^{m\times n}$, who's **columns** have **mean zero**
PCA is done on **centered** data-matrices like A:
SVD exists i.e. $A = USV^T$ and $r = \mathrm{rk}(A)$
Let $A = [\mathbf{r}_1;\ldots;\mathbf{r}_m]$ be rows $\mathbf{r}_1,\ldots,\mathbf{r}_m \in \mathbb{R}^n$ => each row corresponds to a sample
Let $A = [\mathbf{c}_1|\ldots|\mathbf{c}_n]$ be columns $\mathbf{c}_1,\ldots,\mathbf{c}_n \in \mathbb{R}^m$ => each column corresponds to one dimension of the data
Let $X_1,\ldots,X_n$ be **random variables** where each X_i corresponds to column $\mathbf{c}_i$
i.e. each X_i corresponds to i-th component of data
i.e. random vector $X = [X_1,\ldots,X_n]^T$ models the data $\mathbf{r}_1,\ldots,\mathbf{r}_m$
Co-variance matrix of X is $\mathrm{Cov}(A) = \frac{1}{m-1}A^TA$ =>
$(A^TA)_{ij} = (A^TA)_{ji} = \mathrm{Cov}(X_i, X_j)$

$\mathbf{v}_1,\ldots,\mathbf{v}_r$ (columns of V) are **principal axes** of A
Let $\boldsymbol{w} \in \mathbb{R}^n$ be some unit-vector => let $\alpha_j = \mathbf{r}_j \cdot \boldsymbol{w}$ be the **projection/coordinate** of sample $\mathbf{r}_j$ onto $\boldsymbol{w}$
Variance (Bessel's correction) of $\alpha_1,\ldots,\alpha_m$ is
$\mathrm{Var}_{\boldsymbol{w}} = \frac{1}{m-1}\sum_j \alpha_j^2 = \frac{1}{m-1}\boldsymbol{w}^T\left(\sum_j \mathbf{r}_j^T\mathbf{r}_j\right)\boldsymbol{w}$
$= \frac{1}{m-1}\boldsymbol{w}^TA^TA\boldsymbol{w}$
First (principal) axis defined =>
$\boldsymbol{w}_{(1)} = \arg\max_{\|\boldsymbol{w}\|=1}\boldsymbol{w}^TA^TA\boldsymbol{w}$
$= \arg\max_{\|\boldsymbol{w}\|=1}(m-1)\mathrm{Var}_{\boldsymbol{w}} = \mathbf{v}_1$
i.e. $\boldsymbol{w}_{(1)}$ the direction that maximizes variance $\mathrm{Var}_{\boldsymbol{w}}$
i.e. maximizes variance of **projections on line** $\mathbb{R}\boldsymbol{w}_{(1)}$

$\sigma_1\mathbf{u}_1,\ldots,\sigma_r\mathbf{u}_r$ (columns of US) are **principal components/scores** of A
Recall: $A = \sum_{i=1}^r \sigma_i\mathbf{u}_i\mathbf{v}_i^T$ with $\sigma_1 \ge \cdots \ge \sigma_r > 0$, so that relates principal axes and principal components
Data compression: If $\sigma_1 \gg \sigma_2$ then **compress** A by projecting in direction of principal component => $A \approx \sigma_1\mathbf{u}_1\mathbf{v}_1^T$

Cholesky Decomposition

Consider **positive (semi-)definite** $A \in \mathbb{R}^{n\times n}$
Cholesky Decomposition is $A = LL^T$ where L is lower-triangular
For positive semi-definite => **always exists**, but **non-unique**
For positive-definite => **always uniquely exists** s.t. diagonals of L are positive

Finding a Cholesky Decomposition:
Compute LL^T and solve $A = LL^T$ by matching terms
For square roots always pick positive
If there is **exact solution** then **positive-definite**
If there are **free variables** at the end, then **positive semi-definite**
i.e. the decomposition is a **solution-set** parameterized on **free variables**
e.g. $\begin{bmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 2\end{bmatrix} = LL^T$ where $L = \begin{bmatrix}1 & 0 & 0\\ 1 & 0 & 0\\ 1 & c & \sqrt{1-c^2}\end{bmatrix}$, $c \in [0,1]$

If $A = LL^T$ you can use forward/backward substitution to **solve equations**
For $Ax = b$ => let $y = L^Tx$
Solve $Ly = b$ by forward substitution to **find** y
Solve $L^Tx = y$ by backward substitution to **find** x
For $n = 3$ => $L = \begin{bmatrix}l_{11} & 0 & 0\\ l_{21} & l_{22} & 0\\ l_{31} & l_{32} & l_{33}\end{bmatrix}$,
$LL^T = \begin{bmatrix}l_{11}^2 & l_{11}l_{21} & l_{11}l_{31}\\ l_{11}l_{21} & l_{21}^2 + l_{22}^2 & l_{21}l_{31} + l_{22}l_{32}\\ l_{11}l_{31} & l_{21}l_{31} + l_{22}l_{32} & l_{31}^2 + l_{32}^2 + l_{33}^2\end{bmatrix}$

Forward/backward substitution

Forward substitution: for lower-triangular
$L = \begin{bmatrix}\ell_{1,1} & & 0\\ \vdots & \ddots & \\ \ell_{n,1} & \cdots & \ell_{n,n}\end{bmatrix}$
For $Lx = b$, just **solve** the first row
$\ell_{1,1}x_1 = b_1 \implies x_1 = \frac{b_1}{\ell_{1,1}}$ and **substitute down**
Then **solve** the second row
$\ell_{2,1}x_1 + \ell_{2,2}x_2 = b_2 \implies x_2 = \frac{b_2 - \ell_{2,1}x_1}{\ell_{2,2}}$ and **substitute down**
…and so on until all x_i are solved
Backward substitution: for upper-triangular
$U = \begin{bmatrix}u_{1,1} & \cdots & u_{1,n}\\ & \ddots & \vdots\\ 0 & & u_{n,n}\end{bmatrix}$
For $Ux = b$, just **solve** the last row
$u_{n,n}x_n = b_n \implies x_n = \frac{b_n}{u_{n,n}}$ and **substitute up**
Then **solve** the second-to-last row
$u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n = b_{n-1} \implies x_{n-1} = \frac{b_{n-1} - u_{n-1,n-1}x_{n-1}}{u_{n-1,n}}$ and **substitute up**
…and so on until all x_i are solved

Thin QR Decomposition w/ Gram-Schmidt (GS)

Consider **full-rank** $A = [\mathbf{a}_1|\ldots|\mathbf{a}_n] \in \mathbb{R}^{m\times n}$ $(m \ge n)$, i.e. $\mathbf{a}_1,\ldots,\mathbf{a}_n \in \mathbb{R}^m$ are linearly independent
Apply GS $\mathbf{q}_1,\ldots,\mathbf{q}_n \leftarrow \mathrm{GS}(\mathbf{a}_1,\ldots,\mathbf{a}_n)$ to build **ONB** $\langle \mathbf{q}_1,\ldots,\mathbf{q}_n\rangle \in \mathbb{R}^m$ for $\mathrm{C}(A)$
For exams: more efficient to compute as $\mathbf{u}_{j+1} = \mathbf{a}_{j+1} - Q_j\mathbf{c}_j$
1) Gather $Q_j = [\mathbf{q}_1|\ldots|\mathbf{q}_j] \in \mathbb{R}^{m\times j}$ **all-at-once**
2) Compute $\mathbf{c}_j = [\mathbf{q}_1 \cdot \mathbf{a}_{j+1},\ldots,\mathbf{q}_j \cdot \mathbf{a}_{j+1}]^T \in \mathbb{R}^j$ **all-at-once**
3) Compute $Q_j\mathbf{c}_j \in \mathbb{R}^m$, and subtract from $\mathbf{a}_{j+1}$ **all-at-once**
Can now rewrite $\mathbf{a}_j = \sum_{i=1}^j(\mathbf{q}_i \cdot \mathbf{a}_j)\mathbf{q}_i = Q_j\mathbf{c}_j$

Choose $Q = Q_n = [q_1|\dots|q_n] \in \mathbb{R}^{m\times n}$, notice its semi-orthogonal since $Q^TQ = I_n$

Notice => $a_j = Q_jc_j = Q[q_1\cdot a_j,\dots,q_j\cdot a_j,0,\dots,0]^T = Qr_j$

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

$A = QR = Q\begin{bmatrix} q_1^Ta_1 & \cdots & q_1^Ta_n \\ & \ddots & \vdots \\ 0 & & q_n^Ta_n\end{bmatrix}$, notice its upper-triangular

Full QR Decomposition

Consider **full-rank** $A = [a_1|\dots|a_n] \in \mathbb{R}^{m\times n}$, $(m \ge n)$, 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 $C(A)$
- Semi-orthogonal $Q_1 = [q_1|\dots|q_n] \in \mathbb{R}^{m\times n}$ and upper-triangular $R_1 \in \mathbb{R}^{n\times n}$, where $A = Q_1R_1$

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 $C(A)^\perp = \ker(A^T)$
- Let $Q_2 = [q_{n+1}|\dots|q_m] \in \mathbb{R}^{m\times(m-n)}$, let $Q = [Q_1|Q_2] \in \mathbb{R}^{m\times m}$, let $R = [R_1; 0_{m-n}] \in \mathbb{R}^{m\times n}$

Then **full QR decomposition** is

$A = QR = [Q_1|Q_2]\begin{bmatrix}R_1\\0_{m-n}\end{bmatrix} = Q_1R_1$
- Q **is orthogonal**, i.e. $Q^{-1} = Q^T$, so its a basis transformation
- $\text{proj}_{C(A)} = Q_1Q_1^T$, $\text{proj}_{C(A)^\perp} = Q_2Q_2^T$ are orthogonal projections **onto** $C(A)$, $C(A)^\perp = \ker(A^T)$ respectively
- Notice: $QQ^T = I_m = Q_1Q_1^T + Q_2Q_2^T$

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

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

Consider **standard Euclidean space** $\mathbb{E}^n (= \mathbb{R}^n)$
- 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 $n \in \mathbb{R}^n$ $(n \ne 0)$ and offset from origin $c \in L$

It is customary that:
- n is a **unit vector**, i.e. $\|n\| = \|\hat n\| = 1$
- $c \in L$ is **closest point to origin**, i.e. $c \perp n$

If $c \ne \lambda n$ => L **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 $c = \lambda n$, i.e. $L = \mathbb{R}n$ => L 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 orthonormal basis (ONB) $(\hat n)$

A **hyperplane** $P = (\mathbb{R}n)^\perp + c = \{x + c \mid x \in \mathbb{R}^n, x \perp n\} = \{x \in \mathbb{R}^n \mid x\cdot n = c\cdot n\}$ is characterized by normal $n \in \mathbb{R}^n$ $(n \ne 0)$ and offset from origin $c \in P$

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

It is customary that:
- n is a **unit vector**, i.e. $\|n\| = \|\hat n\| = 1$
- $c \in P$ is **closest point to origin**, i.e. $c = \lambda n$
- With those => $P = \{x \in \mathbb{R}^n \mid x\cdot n = \lambda\}$

If $c\cdot n \ne 0$ => P **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 $c\cdot n = 0$, i.e. $P = (\mathbb{R}n)^\perp$ => 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 $P = (\mathbb{R}n)^\perp$ are orthogonal compliments, so:
- $\text{proj}_L = \hat n\hat n^T$ is orthogonal projection **onto** L (**along** P)
- $\text{proj}_P = \text{id}_{\mathbb{R}^n} - \text{proj}_L = I_n - \hat n\hat n^T$ is orthogonal projection **onto** P (**along** L)
- $L = \text{im}(\text{proj}_L) = \ker(\text{proj}_P)$ and $P = \ker(\text{proj}_L) = \text{im}(\text{proj}_P)$

$\mathbb{R}^n = \mathbb{R}n \oplus (\mathbb{R}n)^\perp$, i.e. all vectors $v \in \mathbb{R}^n$ uniquely decomposed into $v = v_L + v_P$

Householder Maps: reflections

Two points $x, y \in \mathbb{E}^n$ are **reflections** w.r.t hyperplane $P = (\mathbb{R}n)^\perp + c$ if:
1) The translation $\vec{xy} = y - x$ is **parallel** to normal n, i.e. $\vec{xy} = \lambda n$
2) Midpoint $m = 1/2(x+y) \in P$ **lies** on P, i.e. $m\cdot n = c\cdot n$

Suppose $P_u = (\mathbb{R}u)^\perp$ 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 $L_u = \mathbb{R}u$
- $\text{proj}_{L_u} = uu^T$ and $\text{proj}_{P_u} = I_n - uu^T$ =>
- $H_u = \text{proj}_{P_u} - \text{proj}_{L_u}$
- **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 $P_{\perp q_j} = I_m - q_jq_j^T$ be **projector** onto hyperplane $(\mathbb{R}q_j)^\perp$, i.e. orthogonal compliment of line $\mathbb{R}q_j$
- Notice: $P_{\perp j} = I_m - Q_jQ_j^T = \prod_{i=1}^j(I_m - q_iq_i^T) = \prod_{i=1}^j P_{\perp q_i}$
- Re-state: $u_{j+1} = (I_m - Q_jQ_j^T)a_{j+1}$ =>
- $u_{j+1} = \left(\prod_{i=1}^j P_{\perp q_i}\right)a_{j+1} = (P_{\perp q_j}\cdots P_{\perp q_1})a_{j+1}$

Projectors $P_{\perp q_1},\dots,P_{\perp q_j}$ are iteratively applied to a_{j+1}, removing its components along q_1, then along q_2 and so on...
- Let $u_k^{(j)} = \left(\prod_{i=1}^j P_{\perp q_i}\right)a_k$, i.e. a_k **without** its components along $q_1,\dots,q_j$
- Notice: $u_j = u_j^{(j-1)}$, thus $q_j = \hat u_j = u_j^{(j-1)}/r_{jj}$ where $r_{jj} = \|u_j^{(j-1)}\|$
- Iterative step: $u_k^{(j)} = (P_{\perp q_j})u_k^{(j-1)} = u_k^{(j-1)} - (q_j\cdot u_k^{(j-1)})q_j$
- i.e. each **iteration** j of MGS computes $P_{\perp q_j}$ (and projections under it) **in one go**

At **start** of iteration $j \in 1..n$ 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 $r_{jj} = \|u_j^{(j-1)}\|$ => $q_j = u_j^{(j-1)}/r_{jj}$
- For each $k \in (j+1)..n$, compute $r_{jk} = q_j\cdot u_k^{(j-1)}$ => $u_k^{(j)} = u_k^{(j-1)} - r_{jk}q_j$
- **Next ONB** $(q_1,\dots,q_j)$ and **next residual** $u_{j+1}^{(j)},\dots,u_n^{(j)}$
- NOTE: for $j = 1$ => $q_1,\dots,q_{j-1} = \emptyset$, i.e. none yet

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

$A = [a_1|\dots|a_n] = [q_1|\dots|q_n]\begin{bmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ 0 & & r_{nn}\end{bmatrix} = QR$

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
```
for j = 1 to n do
  u_j = a_j
  for i = 1 to j - 1 do
    r_ij = q_i^T a_j
    u_j = u_j - r_ij q_i
  end for
  r_jj = ||u_j||_2
  q_j = u_j / r_jj
end for
```

Modified Gram-Schmidt
```
for j = 1 to n do
  u_j = a_j
end for
for j = 1 to n do
  r_jj = ||u_j||_2
  q_j = u_j / r_jj
  for k = j + 1 to n do
    r_jk = q_j^T u_k
    u_k = u_k - r_jk q_j
  end for
end for
```

Computes at j-th step:
- **Classical GS** => j-th column of Q and the j-th column of R
- **Modified GS** => 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: $Q^\dagger Q = I_n$ => check for loss of orthogonality with $\|I_n - Q^\dagger Q\| = \text{loss}$
- **Classical GS** => $\|I_n - Q^\dagger Q\| \approx \text{Cond}(A)^2\epsilon_{mach}$
- **Modified GS** => $\|I_n - Q^\dagger Q\| \approx \text{Cond}(A)\epsilon_{mach}$
- NOTE: **Householder method** has $\|I_n - Q^\dagger Q\| \approx \epsilon_{mach}$

Multivariate Calculus

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

When clear write i-**th component** of input as i instead of x_i

Level curve w.r.t. to $c \in \mathbb{R}$ 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 i_k of ..., of n_1-**th order partial derivative** w.r.t i_1 of f is:

$\frac{\partial^{n_k+\dots+n_1} f}{\partial x_{i_k}^{n_k}\cdots\partial x_{i_1}^{n_1}} = \partial_{i_k}^{n_k}\cdots\partial_{i_1}^{n_1} f = f_{i_1\cdots i_k}^{(n_1,\dots,n_k)}$

Its an N-**th order partial derivative** where $N = \sum_k n_k$

$\nabla f = [\partial_1 f,\dots,\partial_n f]^T$ is gradient of f => $(\nabla f)_i = \frac{\partial f}{\partial x_i}$

$\nabla^T f = (\nabla f)^T$ is transpose of ∇f, i.e. $\nabla^T f$ is row vector

$D_uf(x) = \lim_{\delta\to0}\frac{f(x+\delta u) - f(x)}{\delta}$ is **directional-derivative** of f

It is rate-of-change in direction u, where $u \in \mathbb{R}^n$ is unit-vector

$D_uf(x) = \nabla f(x)\cdot u = \|\nabla f(x)\|\cos(\theta)$ => $D_uf(x)$ **maximized** when $\cos\theta = 1$

i.e. when x, u are parallel => hence $\nabla f(x)$ is direction of **max.** rate-of-change

f has **local minimum** at x_{loc} if there's radius $r > 0$ s.t. $\forall x \in B[r; x_{loc}]$ we have $f(x_{loc}) \le f(x)$

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

A **local minimum** satisfies optimality conditions:
- $\nabla f(x) = 0$, e.g. for $n = 1$ its $f'(x) = 0$
- $\nabla^2 f(x)$ is positive-definite, e.g. for $n = 1$ its $f''(x) > 0$

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

Interpret $F: \mathbb{R}^n \to \mathbb{R}^m$ as m functions $F_i: \mathbb{R}^n \to \mathbb{R}$ (one per output-component)

$J(F) = [\nabla^T F_1; \dots; \nabla^T F_m]$ is **Jacobian** => $J(F)_{ij} = \frac{\partial F_i}{\partial x_j}$

Conditioning

A **problem** is some $f: X \to Y$ where X, Y are normed vector-spaces

A problem **instance** is f with fixed input $x \in X$, shortened to **just** "problem" (with $x \in X$ implied)

δx **is small perturbation** of x => $\delta f = f(x+\delta x) - f(x)$

A problem (instance) is:
- **Well-conditioned** if all **small** δx lead to **small** δf, i.e. if κ is **small** (e.g. 1, 10, 10^2)
- **Ill-conditioned** if some **small** δx lead to **large** δf, i.e. if κ is **large** (e.g. 10^6, 10^{16})

Absolute condition number $\text{cond}(x) = \hat\kappa(x) = \hat\kappa$ of f **at** x:

$\hat\kappa = \lim_{\delta\to0}\sup_{\|\delta x\|\le\delta}\frac{\|\delta f\|}{\|\delta x\|}$

=> for most problems simplified to $\hat\kappa = \sup_{\delta x}\frac{\|\delta f\|}{\|\delta x\|}$

If Jacobian $J_f(x)$ exists then $\hat\kappa = \|J_f(x)\|$, where matrix norm $\|\cdot\|$ induced by norms on X and Y

Relative condition number $\kappa(x) = \kappa$ of f **at** x is

$\kappa = \lim_{\delta\to0}\sup_{\|\delta x\|\le\delta}\left(\frac{\|\delta f\|}{\|f(x)\|}\Big/\frac{\|\delta x\|}{\|x\|}\right)$

=> for most problems simplified to $\kappa = \sup_{\delta x}\left(\frac{\|\delta f\|}{\|f(x)\|}\Big/\frac{\|\delta x\|}{\|x\|}\right)$

If Jacobian $J_f(x)$ exists then $\kappa = \frac{\|J_f(x)\|}{\|f(x)\|/\|x\|}$

More important than $\hat\kappa$ for numerical analysis

Matrix condition number $\text{Cond}(A) = \kappa(A) = \|A\|\|A^{-1}\|$

=> comes up so often that has its own name

$A \in \mathbb{C}^{m\times m}$ is well-conditioned if $\kappa(A)$ is small, ill-conditioned if large

$\kappa(A) = \kappa(A^{-1})$, $\kappa(A) = \kappa(\gamma A)$, $\|\cdot\| = \|\cdot\|_2$ => $\kappa(A) = \frac{\sigma_1}{\sigma_m}$

For $A \in \mathbb{C}^{m\times n}$, the problem $f_A(x) = Ax$ has $\kappa = \|A\|\frac{\|x\|}{\|Ax\|}$ => if A^{-1} exists then $\kappa \le \text{Cond}(A)$

If $Ax = b$, problem of finding x given b is just $f_{A^{-1}}(b) = A^{-1}b$ => $\kappa = \|A^{-1}\|\frac{\|b\|}{\|x\|} \le \text{Cond}(A)$

For $b \in \mathbb{C}^m$, the problem $f_b(A) = A^{-1}b$ (i.e. finding x in $Ax = b$) has $\kappa = \|A\|\|A^{-1}\| = \text{Cond}(A)$

Stability

Given a problem $f: X \to Y$, an **algorithm** for f is $\tilde f: X \to Y$

Input $x \in X$ is first rounded to $\text{fl}(x)$, i.e. $\tilde f(x) = \tilde f(\text{fl}(x))$

Absolute error => $\|\tilde f(x) - f(x)\|$

relative error => $\frac{\|\tilde f(x) - f(x)\|}{\|f(x)\|}$

$\tilde f$ is **accurate** if $\forall x \in X$, $\frac{\|\tilde f(x) - f(x)\|}{\|f(x)\|} = O(\epsilon_{mach})$

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

i.e. nearly the right answer to nearly the right question

outer-product is stable

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

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

$\oplus,\ominus,\otimes,\oslash$, **inner-product**, back-substitution w/ triangular systems, are backwards stable

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

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 $n\to\infty$

But in numerical analysis $f(\epsilon) = O(g(\epsilon))$ as $\epsilon\to0$, i.e. $\limsup_{\epsilon\to0}\|f(\epsilon)\|/\|g(\epsilon)\| < \infty$

i.e. $\exists C,\delta > 0$ s.t. $\forall\epsilon$ we have $0 < \|\epsilon\| < \delta \implies \|f(\epsilon)\| \le C\|g(\epsilon)\|$

$O(g)$ is set of functions $\{f : \limsup_{\epsilon\to0}\|f(\epsilon)\|/\|g(\epsilon)\| < \infty\}$

Smallness partial order $O(g_1) \le O(g_2)$ defined by set-inclusion $O(g_1) \subseteq O(g_2)$

i.e. as $\epsilon\to0$, $g_1(\epsilon)$ goes to zero **faster** than $g_2(\epsilon)$

Roughly same hierarchy as complexity analysis but **flipped** (some don't fit the pattern)

e.g. $\dots O(\epsilon^3) < O(\epsilon^2) < O(\epsilon) < O(1)$

Maximum: $O(\max(|g_1|,|g_2|)) = O(g_2) \iff O(g_1) \le O(g_2)$

e.g. $O(\max(\epsilon^k,\epsilon)) = O(\epsilon)$

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. $e^{O(1)} = \{e^{f(\epsilon)} : f \in O(1)\}$

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. $e^{O(1)} = O(\epsilon^k)$ means $\{e^{f(\epsilon)} : f \in O(1)\} \subseteq O(\epsilon^k)$ not necessarily true

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

e.g. $(\epsilon+1)^2 = \epsilon^2 + O(\epsilon)$ means $\epsilon\mapsto(\epsilon+1)^2 \in \{\epsilon^2 + f(\epsilon) : f \in O(\epsilon)\}$ not necessarily true

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

$f_1f_2 = O(g_1g_2)$, $f\cdot O(g) = O(fg)$, $O(k\cdot g) = O(g)$

$f_1 + f_2 = O(\max(|g_1|,|g_2|))$

=> if $g_1 = g_2 = g$ then $f_1 + f_2 = O(g)$

Floating-point numbers

Consider base/radix $\beta \ge 2$ (typically 2) and precision $t \ge 1$ (24 or 53 for IEEE single/double precisions)

Floating-point numbers are discrete subset

$F = \{(-1)^S(m/\beta^t)\beta^E \mid 1 \le m \le \beta^t, S \in \mathbb{B}, m, E \in \mathbb{Z}\}$

S is **sign-bit**, m/β^t is **mantissa**, E is **exponent** (8-bit for single, 11-bit for double)

Equivalently, can restrict to $\beta^{t-1} \le m \le \beta^t - 1$ for unique m and E

$F \subset \mathbb{R}$ is idealized (ignores over/underflow), so is countably infinite and self-similar (i.e. $F = \beta F$)

For all $x \in \mathbb{R}$ there exists $\text{fl}(x) \in F$ s.t. $|x - \text{fl}(x)| \le \epsilon_{mach}|x|$

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

Machine epsilon $\epsilon_{machine} = \epsilon_{mach} = \frac12\beta^{1-t}$ is maximum relative gap between FPs

Half the gap between 1 and next largest FP

$2^{-24} \approx 5.96\times10^{-8}$ and $2^{-53} \approx 1.11\times10^{-16}$ for single/double

FP arithmetic: let $*, \circledast$ be real and floating counterparts of arithmetic operation

For $x, y \in F$ we have $x\circledast y = \text{fl}(x*y) = (x*y)(1+\epsilon)$, $|\epsilon| \le \epsilon_{mach}$

Holds for **any arithmetic operation** $\circledast = \oplus,\ominus,\otimes,\oslash$

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

Caveat: $\epsilon_{mach} = \frac12\beta^{1-t}$ must be scaled by factors on the order of $2^{3/2}, 2^{5/2}$ for $\otimes,\oslash$ respectively

$(x_1\oplus\dots\oplus x_n) = (x_1+\dots+x_n) + \sum_{i=1}^n x_i\left(\sum_{j=i}^n\delta_j\right)$; $|\delta_j| \le \epsilon_{mach}$

$(x_1\otimes\dots\otimes x_n) = (x_1\times\dots\times x_n)(1+\epsilon)$, $\epsilon \le 1.06(n-1)\epsilon_{mach}$

$\text{fl}(\sum_i x_iy_i) = \sum_i x_iy_i(1+\epsilon_i)$ where $1+\epsilon_i = (1+\delta_i)(1+\eta_i)\cdots(1+\eta_n)$ and $|\delta_i|, |\eta_i| \le \epsilon_{mach}$

$1+\epsilon_i \approx 1+\delta_i+(\eta_i+\dots+\eta_n)$

$|\text{fl}(x^Ty) - x^Ty| \le \sum|x_iy_i||\epsilon_i|$

Assuming $n\epsilon_{mach} \le 0.1$ =>

$|\text{fl}(x^Ty) - x^Ty| \le \phi(n)\epsilon_{mach}|x|^T|y|$, where $|x|_i = |x_i|$ 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 $|M|_{ij} = |M_{ij}|$, i.e. matrix $|M|$ of absolute values of M

$\text{fl}(\lambda A) = \lambda A + E$; $|E|_{ij} \le |\lambda A|_{ij}\epsilon_{mach}$

$\text{fl}(A+B) = (A+B) + E$; $|E|_{ij} \le |A+B|_{ij}\epsilon_{mach}$

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

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

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

Need $a = 0$ => $f(x) = \sum_{k=0}^n\frac{f^{(k)}(0)}{k!}x^k + O(x^{n+1})$ as $x\to0$

e.g. $(1+\epsilon)^p = \sum_{k=0}^n\binom{p}{k}\epsilon^k + O(\epsilon^{n+1}) = \sum_{k=0}^n\frac{p!}{k!(p-k)!}\epsilon^k + O(\epsilon^{n+1})$ as $\epsilon\to0$

Elementary Matrices

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

Row/column switching: permutation matrix P_{ij} obtained by switching e_i and e_j in I_n (same for rows/columns)
- Applying P_{ij} **from left** will swap rows, **from right** will swap columns
- $P_{ij} = P_{ij}^T = P_{ij}^{-1}$, i.e. applying twice will undo it

Row/column scaling: $D_i(\lambda)$ obtained by scaling e_i by λ 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. $D_i(\lambda)^{-1} = D_i(\lambda^{-1})$

Row addition: $L_{ij}(\lambda) = I_n + \lambda e_ie_j^T$ performs $R_i \leftarrow R_i + \lambda R_j$ when applying **from left**
- $\lambda e_ie_j^T$ is zeros except for λ in (i,j)-**th entry**
- $L_{ij}(\lambda)^{-1} = L_{ij}(-\lambda)$ both triangular matrices

LU factorization w/ Gaussian elimination

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

LU **factorization** => finds $A = LU$ where L, U are lower/upper triangular respectively

Naive Gaussian Elimination performs $[I_m|A|I_n] \mapsto [R^{-1}|U|I_n]$ to get $AI_n = R^{-1}U$ using only row addition

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

Algorithm 1 Gaussian elimination
```
U = A, L = I
for k = 1 to m - 1 do
  for j = k + 1 to m do
    ℓ_jk = u_jk / u_kk
    u_j,k:m = u_j,k:m - ℓ_jk u_k,k:m
  end for
end for
```

The **pivot element** is simply diagonal entry $u_{kk}^{(k-1)}$; fails if $u_{kk}^{(k-1)} \approx 0$

$\tilde L\tilde U = A + \delta A$, $\frac{\|\delta A\|}{\|L\|\cdot\|U\|} = O(\epsilon_{mach})$; only **backwards stable** if $\|L\|\cdot\|U\| \approx \|A\|$

Work required: $\sim\frac23m^3$ flops $\sim O(m^3)$

Solving $Ax = LUx$ is $\sim\frac23m^3$ flops (back substitution is $O(m^2)$)

NOTE: Householder triangularisation requires $\sim\frac43m^3$

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

For each column j, finds largest entry and row-swaps to make it new pivot => P_j

Then performs normal elimination on that column => L_j

Result is $L_{m-1}P_{m-1}\dots L_2P_2L_1P_1A = U$, where $L_{m-1}P_{m-1}\dots L_2P_2L_1P_1 = L'_{m-1}\dots L'_1P_{m-1}\dots P_1$

Setting $L = (L'_{m-1}\dots L'_1)^{-1}$, $P = P_{m-1}\dots P_1$ gives $PA = LU$

Algorithm 2 Gaussian elimination with partial pivoting
```
U = A, L = I, P = I
for k = 1 to m - 1 do
  i = argmax_{i≥k} |u_ik|
  u_k,k:m ↔ u_i,k:m
  ℓ_k,1:k-1 ↔ ℓ_i,1:k-1
  p_k,: ↔ p_i,:
  for j = k + 1 to m do
    ℓ_jk = u_jk / u_kk
    u_j,k:m = u_j,k:m - ℓ_jk u_k,k:m
  end for
end for
```

Work required: $\sim\frac23m^3$ flops $\sim O(m^3)$; results in $L_{ij} \le 1$ so $\|L\| = O(1)$

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

=> for partial pivoting $\rho \le 2^{m-1}$

$\|U\| = O(\rho\|A\|)$ => $\tilde L\tilde U = \tilde PA + \delta A$, $\frac{\|\delta A\|}{\|A\|} = O(\rho\epsilon_{machine})$

=> 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

$d(x,x) = 0 \mid x \ne y \implies d(x,y) > 0 \mid d(x,y) = d(y,x)$

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

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

$\lim_{x\to+\infty}f(x) = +\infty \iff \forall R \in \mathbb{R}, \exists N \in \mathbb{N}, \forall x > N: f(x) > r$

$\lim_{x\to p}f(x) = L \iff \forall\epsilon > 0, \exists\delta > 0, \forall x \in X: 0 < d_X(x,p) < \delta \implies d_Y(f(x),L) < \epsilon$

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

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

Turn **metric limit** $\lim_{n\to\infty}x_n = L$ into **real limit** $\lim_{n\to\infty}d(x_n,L) = 0$ to leverage real analysis

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

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

$\lim_{n\to\infty}r^n = 0 \iff |r| < 1$ and $\lim_{n\to\infty}\sum_{i=0}^n ar^i = \frac{a}{1-r} \iff |r| < 1$

Iterative Techniques

Systems of Equations

Let $A, R, G \in \mathbb{R}^{n\times n}$ where G^{-1} exists => **splitting** $A = G + R$ helps iteration

$Ax = b$ rewritten as $x = Mx + c$ where $M = -G^{-1}R$; $c = G^{-1}b$

Define $f(x) = Mx + c$ and sequence $x^{(k+1)} = f(x^{(k)}) = Mx^{(k)} + c$ with starting point $x^{(0)}$

Limit of (x_k) is fixed point of f => unique fixed point of f is **solution** to $Ax = b$

If $\|\cdot\|$ is consistent norm and $\|M\| < 1$ then (x_k) converges for any $x^{(0)}$ (because Cauchy-completeness)

We want to find $\|M\| < 1$ and easy to compute M; c

Stopping criterion usually the relative residual $\frac{\|b - Ax^{(k)}\|}{\|b\|} \le \epsilon$

Assume A's **diagonal is non-zero** (w.l.o.g. permute/change basis if isn't) then $A = D + L + U$ where D is **diagonal** of A, L, U are strict **lower/upper triangular** parts of A

Jacobi Method:

$G = D$; $R = L + U$ => $M = -D^{-1}(L+U)$; $c = D^{-1}b$

$x_i^{(k+1)} = \frac{1}{A_{ii}}\left(b_i - \sum_{j\ne i}A_{ij}x_j^{(k)}\right)$ => $x_i^{(k+1)}$ only needs b_i; $x^{(k)}$; A_{i*} => row-wise parallelization

Gauss-Seidel (G-S) Method:

$G = D + L$; $R = U$ => $M = -(D+L)^{-1}U$; $c = (D+L)^{-1}b$

$x_i^{(k+1)} = \frac{1}{A_{ii}}\left(b_i - \sum_{j=1}^{i-1}A_{ij}x_j^{(k+1)} - \sum_{j=i+1}^nA_{ij}x_j^{(k)}\right)$

Computing $x_i^{(k+1)}$ needs b_i; $x^{(k)}$; A_{i*} and $x_j^{(k+1)}$ for $j < i$ => lower storage requirements

Successive over-relaxation (SOR):

$G = \omega^{-1}D + L$; $R = (1-\omega^{-1})D + U$ =>

$M = -(\omega^{-1}D + L)^{-1}((1-\omega^{-1})D + U)$; $c = (\omega^{-1}D + L)^{-1}b$

$x_i^{(k+1)} = \frac{\omega}{A_{ii}}\left(b_i - \sum_{j=1}^{i-1}A_{ij}x_j^{(k+1)} - \sum_{j=i+1}^nA_{ij}x_j^{(k)}\right) + (1-\omega)x_i^{(k)}$ for **relaxation factor** $\omega > 1$

If A is **strictly row diagonally dominant** then Jacobi/Gauss-Seidel methods converge; A is **strictly row diagonally dominant** if $|A_{ii}| > \sum_{j\ne i}|A_{ij}|$

If A is positive-definite then **G-S** and **SOR** ($\omega \in (0,2)$) converge

Eigenvalue Problems

If A is diagonalizable then eigen-decomposition is $A = X\Lambda X^{-1}$

Dominant λ_1; x_1 are such that $|\lambda_1|$ is strictly largest for which $Ax = \lambda x$

Rayleigh quotient for Hermitian $A = A^\dagger$ is $R_A(x) = \frac{x^\dagger Ax}{x^\dagger x}$
- Eigenvectors are stationary points of R_A
- $R_A(x)$ is closest to being like eigenvalue of x, i.e. $R_A(x) = \text{argmin}_\alpha\|Ax - \alpha x\|_2$
- $R_A(x) - R_A(v) = O(\|x - v\|^2)$ as $x \to v$ where v is eigenvector

Power iteration: define sequence $b^{(k+1)} = \frac{Ab^{(k)}}{\|Ab^{(k)}\|}$ with initial $b^{(0)}$ s.t. $\|b^{(0)}\| = 1$

Assume **dominant** λ_1; x_1 exist for A, and that $\text{proj}_{x_1}(b^{(0)}) \ne 0$

Under above assumptions, $\mu_k = R_A(b^{(k)}) = \frac{b^{(k)\dagger}Ab^{(k)}}{b^{(k)\dagger}b^{(k)}}$ converges to **dominant** λ_1

(b_k) converges to some **dominant** x_1 associated with λ_1 => $\|Ab^{(k)}\|$ converges to $|\lambda_1|$

If $\text{proj}_{x_1}(b^{(0)}) = 0$ then (b_k); (μ_k) converge to second **dominant** λ_2; x_2 instead

If **no dominant** λ (i.e. multiple eigenvalues of maximum $|\lambda|$) then (b_k) will converge to linear combination of their corresponding eigenvectors

Slow convergence if **dominant** λ_1 not "very dominant"

$\|b^{(k)} - \alpha_kx_1\| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$ for **phase factor** $\alpha_k \in \{-1,1\}$, it may alternate if $\lambda_1 < 0$

$\alpha_k = \frac{(\lambda_1)^kc_1}{|\lambda_1|^k|c_1|}$ where $c_1 = x_1^\dagger b^{(0)}$ and assuming $b^{(k)}$; x_1 are normalized

$(A - \sigma I)$ has **eigenvalues** $\lambda - \sigma$

=> power-iteration on $(A - \sigma I)$ has $\frac{\lambda_2 - \sigma}{\lambda_1 - \sigma}$

Eigenvector guess => estimated eigenvalue

Inverse (power-)iteration: perform power iteration on $(A - \sigma I)^{-1}$ to get $\lambda_{1,\sigma}$ **closest** to σ

$(A - \sigma I)^{-1}$ has eigenvalues $(\lambda - \sigma)^{-1}$ so power iteration will yield **largest** $(\lambda_{1,\sigma} - \sigma)^{-1}$

i.e. will yield **smallest** $\lambda_{1,\sigma} - \sigma$, i.e. will yield $\lambda_{1,\sigma}$ **closest** to σ

$\|b^{(k)} - \alpha_kx_{1,\sigma}\| = O\left(\left|\frac{\lambda_{1,\sigma} - \sigma}{\lambda_{2,\sigma} - \sigma}\right|^k\right)$ where $x_{1,\sigma}$ corresponds to $\lambda_{1,\sigma}$ and $\lambda_{2,\sigma}$ is 2nd-closest to σ

Efficiently compute eigenvectors for **known eigenvalues** σ

Eigenvalue guess => estimated eigenvector

Algorithm 3 Inverse iteration
```
for k = 1, 2, 3, ... do
  x̂ = (A - σI)^{-1} x^{(k-1)}
  x^{(k)} = x̂ / max(x̂^{(k)})
  λ^{(k)} = (x^{(k)})^T A x^{(k)}
end for
```

Can reduce matrix inversion $O(m^3)$ to $O(m^2)$ by pre-factorization

Nonlinear Systems of Equations

Recall that $\nabla f(x)$ is direction of **max.** rate-of-change $|\nabla f(x)|$

Idea: Search for stationary point by **gradient descent**: $x^{(k+1)} = x^{(k)} - \alpha\nabla f(x^{(k)})$ for step length α

If A is positive-definite, solving $Ax = b$ and $\min_x f(x) = \frac12x^TAx - x^Tb$ are equivalent

Get iterative methods $x^{(k+1)} = x^{(k)} - \alpha^{(k)}p^{(k)}$ for step length $\alpha^{(k)}$ and directions $p^{(k)}$

Conjugate gradient (CG) method: if $A \in \mathbb{R}^{n\times n}$ symmetric then $\langle u,v\rangle_A = u^TAv$ is an inner-product

GC chooses $p^{(k)}$ that are conjugate w.r.t. A, i.e. $\langle p^{(i)},p^{(j)}\rangle_A = 0$ for $i \ne j$

And chooses $\alpha^{(k)}$ s.t. **residuals** $r^{(k)} = -\nabla f(x^{(k)}) = b - Ax^{(k)}$ are orthogonal
- $k = 0$ => $p^{(0)} = -\nabla f(x^{(0)}) = r^{(0)}$
- $k \ge 1$ => $p^{(k)} = r^{(k)} - \sum_{i<k}\frac{\langle p^{(i)},r^{(k)}\rangle_A}{\langle p^{(i)},p^{(i)}\rangle_A}p^{(i)}$

$\alpha^{(k)} = \text{argmin}_\alpha f(x^{(k)} + \alpha p^{(k)}) = \frac{p^{(k)}\cdot r^{(k)}}{\langle p^{(k)},p^{(k)}\rangle_A}$

Without rounding errors, **CG** converges in $\le n$ iterations

Similar to to Gram-Schmidt (but different inner-product)

$\langle p^{(0)},\dots,p^{(n-1)}\rangle$ and $\langle r^{(0)},\dots,r^{(n-1)}\rangle$ are bases for $\mathbb{R}^n$

QR Algorithm to find Schur decomposition $A = QUQ^\dagger$

Any $A \in \mathbb{C}^{m\times m}$ has **Schur decomposition** $A = QUQ^\dagger$
- Q is unitary, i.e. $Q^\dagger = Q^{-1}$ and upper-triangular U
- Diagonal of U contains **eigenvalues** of A

Algorithm 1 Basic QR iteration
```
for k = 1, 2, 3, ... do
  A^{(k-1)} = Q^{(k-1)} R^{(k-1)}
  A^{(k)} = R^{(k-1)} Q^{(k-1)}
end for
```

For $A \in \mathbb{R}^{m\times m}$ each iteration $A^{(k)} = Q^{(k)}R^{(k)}$ produces orthogonal $Q^{(k)T} = Q^{(k)-1}$

So $A^{(k+1)} = R^{(k)}Q^{(k)} = (Q^{(k)T}Q^{(k)})R^{(k)}Q^{(k)} = Q^{(k)T}A^{(k)}Q^{(k)}$ means $A^{(k+1)}$ **is similar to** $A^{(k)}$

Setting $A^{(0)} = A$ we get $A^{(k)} = (\bar Q^{(k)})^TA\bar Q^{(k)}$ where $\bar Q^{(k)} = Q^{(0)}\dots Q^{(k-1)}$

Under certain conditions **QR algorithm** converges to **Schur decomposition**

We can **apply shift** $\mu^{(k)}$ at iteration k => $A^{(k)} - \mu^{(k)}I = Q^{(k)}R^{(k)}$, $A^{(k+1)} = R^{(k)}Q^{(k)} + \mu^{(k)}I$

If **shifts** are good eigenvalue estimates then last column of $\bar Q^{(k)}$ converges quickly to an **eigenvector**

Estimate $\mu^{(k)}$ with Rayleigh quotient => $\mu^{(k)} = (A_k)_{mm} = (\bar q_m^{(k)})^TA\bar q_m^{(k)}$ where $\bar q_m^{(k)}$ is m-th column of $\bar Q^{(k)}$