

$Q = Q_0 + Q_1 + \dots + Q_n \in \mathbb{R}^{m \times n}$ notice its semi-orthogonal since $Q^T Q = I_n$

Notice $\Rightarrow a_j = Q_j c_j = Q Q_1^T c_1 + \dots + Q_j c_j$, $a_j \cdot a_j = 0, \dots, 0$ $\Rightarrow Q_j^T = Q_j^T$

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

$A = QR = Q \begin{bmatrix} q_1^T & \dots & q_n^T \\ 0 & \dots & 0 \end{bmatrix}$ notice its

upper-triangular

Full QR decomposition

Consider $\text{Full QR decomposition}$ $A = [a_1 | \dots | a_n] \in \mathbb{R}^{m \times n}$ ($m \geq n$),

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 $\text{Col}(A)$

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

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 $\text{Col}(A)^\perp = \ker(A^T)$

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 $R = [R_1 | 0_{(m-n) \times n}] \in \mathbb{R}^{m \times n}$

Then **Full QR decomposition** is

$A = QR = [Q_1 | Q_2] \begin{bmatrix} R_1 & 0 \\ 0_{(m-n) \times n} \end{bmatrix} = Q_1 R_1$

Q_1 is orthogonal, i.e. $Q_1^T = Q_1^{-1}$ so its a basis transformation

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

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

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

Generalizable to $\mathbb{C} \in \mathbb{C}^{m \times n}$ 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 $L = \text{span}\{c\}$ is characterized by direction $c \in \mathbb{R}^n$ ($n \geq 1$) and offset from origin $c \in L$

It is customary that:

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

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

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

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

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

If $c \perp n$ i.e. $L = \text{span}\{c\} \Rightarrow L$ 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 an orthonormal basis (ONB) $\{\hat{n}\}$

A hyperplane $P = (\mathbb{R}^n)^{\perp} = \{x + c \mid x \in \mathbb{R}^n, x \perp n\}$ is

characterized by normal $n \in \mathbb{R}^n$ ($n \neq 0$) 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. $\|n\| = \|\tilde{n}\| = 1$

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

With those $\Rightarrow P = \{x \in \mathbb{R}^n \mid x \cdot n = c\}$

If $c \cdot n = 0 \Rightarrow P$ 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. $P = (\mathbb{R}^n)^{\perp} \Rightarrow P$ is vector-subspace of \mathbb{R}^n

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

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

$\text{proj}_{L^{\perp}} = uu^T$ and $\text{proj}_P = I_n - uu^T \Rightarrow$

$R = \text{proj}_P u - \text{proj}_L u$

Visualize as preserving component in u then flipping component in L

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 $P_1 \perp q_1 = q_1 - \text{proj}_{\{q_1\}} q_1$ [be projector onto hyperplane

$(Rq_1)^{\perp}$] i.e. orthogonal complement of line Rq_1

Re-state: $u_{j+1} = (I - \text{proj}_{\{u_1, \dots, u_j\}}) u_{j+1}$

$u_{j+1} = (I - \text{proj}_{\{u_1, \dots, u_j\}}) u_{j+1} = (I - \text{proj}_{\{u_1, \dots, u_j\}}) u_{j+1}$

Projectors P_1, \dots, P_n are iteratively applied to

u_{j+1} removing its components along q_1 then along

q_2 and so on...

Let $u_j = (I - \text{proj}_{\{u_1, \dots, u_{j-1}\}}) u_j$ 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: $u_j = u_j^{(j-1)} = u_j^{(j-1)} - (q_j \cdot u_j^{(j-1)}) q_j$

i.e. each $\text{proj}_{\{u_j\}}$ of MGS computes P_{j+1} (and

projections under it) in one go

At start of iteration $j=1, n$ we have ONB

$q_1, \dots, q_{j-2} \in \mathbb{R}^m$ 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 $r_{jk} = q_j \cdot u_k^{(j-1)} \Rightarrow$

$u_k = u_k^{(j-1)} - r_{jk} q_j$

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

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

$\{q_1, \dots, q_n\} \in \mathbb{R}^m$

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

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 $R \in \mathbb{R}^{n \times n}$ upper-triangular

Classical vs. Modified Gram-Schmidt

These algorithms both compute thin QR decomposition

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: $Q^T Q = I_n$ 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. $c \in \mathbb{R}$ are 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:

$\frac{\partial^2 f}{\partial x_1^2} = \frac{\partial}{\partial x_1} \left(\frac{\partial f}{\partial x_1} \right) = \frac{\partial^2 f}{\partial x_1^2}$

Its an N th order partial derivative where $N = \sum_{k=1}^n n_k$

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

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

$\frac{\partial f}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x+h e_i) - f(x)}{h}$ is

directional-derivative of f in direction $u \in \mathbb{R}^n$ is

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

$\frac{\partial_u f(x)}{\partial x_i} = \nabla f(x) \cdot u = \nabla f(x) \cdot \frac{u}{\|u\|} \cos(\theta) \Rightarrow \frac{\partial_u f(x)}{\partial x_i} = \nabla f(x) \cdot u$ is maximized when $\cos(\theta) = 1$

when u and $\nabla f(x)$ are parallel \Rightarrow 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. $\forall x \in B(r, x_{\text{loc}})$ we have $f(x_{\text{loc}}) \leq f(x)$

f has global minimum x_{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 $f'(x) = 0$

$\nabla^2 f(x)$ 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)

$J(f) = [\nabla^T F_1, \dots, \nabla^T F_m]$ is Jacobian $\Rightarrow J(f)_{ij} = \frac{\partial F_i}{\partial x_j}$

Conditioning

A problem is some $f: X \rightarrow Y$ 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 $\Rightarrow \delta f = f(x + \delta x) - f(x)$

A problem (instance) is:

Well-conditioned if all small δx lead to small δf i.e. if δx is small (e.g. 10^{-10} to 10^{-2})

ill-conditioned if some small δx lead to large δf i.e. if δx is large (e.g. 10^{-6} to 10^{16})

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

$R = \lim_{\delta x \rightarrow 0} \sup \frac{\|\delta f\|}{\|\delta x\|} \leq \frac{\|\nabla f(x)\|}{\|\nabla f(x)\|}$

\Rightarrow for most problems simplified to $R = \sup_{\delta x} \frac{\|\nabla f(x)\|}{\|\nabla f(x)\|}$

if Jacobian $J_f(x)$ exists then $R = \|J_f(x)\|$ where matrix norm $\|\cdot\|$ induced by norms on X and Y

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

$\kappa = \lim_{\delta x \rightarrow 0} \sup \frac{\|\delta f\|}{\|f(x)\|} \frac{\|x\|}{\|\delta x\|} = \frac{\|\nabla f(x)\| \cdot \|x\|}{\|f(x)\| \cdot \|x\|}$

\Rightarrow for most problems simplified to

$\kappa = \sup_{\delta x} \frac{\|\nabla f(x)\| \cdot \|x\|}{\|f(x)\| \cdot \|x\|}$

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

More important than κ for numerical analysis

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

\Rightarrow comes up so often that has its own name

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

ill-conditioned if large

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

For $A \in \mathbb{C}^{m \times n}$ the problem $f_A(x) = Ax$ has

$\kappa = \|A\| \frac{\|x\|}{\|Ax\|} \Rightarrow$ if A^{-1} exists then $\kappa \leq \text{Cond}(A)$

if $Ax=b$ problem of finding x given b is just

$f_{A^{-1}}(b) = A^{-1}b \Rightarrow \kappa = \|A^{-1}\| \frac{\|b\|}{\|x\|} \leq \text{Cond}(A)$

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 $f: X \rightarrow Y$ an algorithm for f is $f: X \rightarrow Y$

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

Absolute error $\Rightarrow \frac{\|f(x) - f(\tilde{x}(x))\|}{\|f(x)\|}$

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

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

f is stable if $\forall x \in X$ $\exists \tilde{x} \in X$ s.t.

$\frac{\|f(x) - f(\tilde{x}(x))\|}{\|f(x)\|} = O(\epsilon_{\text{mach}})$

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

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

if backwards stable f and f has condition number

$\kappa(x)$ then relative error $\frac{\|f(x) - f(\tilde{x}(x))\|}{\|f(x)\|} = O(\kappa(x) \epsilon_{\text{mach}})$

Accuracy, stability, backwards stability are non-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. the

$\limsup_{\epsilon \rightarrow 0} \frac{\|f(x) - f(\tilde{x}(x))\|}{\|f(x)\|} / \log(\epsilon) < \infty$

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