Welcome to Ma221! Lecture 17, Oct 2

Solving $Ax=b$ for A "structured" or "data sparse": A depends on $O(n)$ parameters

Many Structures...

Examples: Vandermonde: $V(i,j) = x_i^{j-1}$

Cauchy $C(i,j) = \frac{1}{x_i + y_j}$

Toeplitz $T(i,j) = x_{i-j}$ constant along diagonals

Hankel $H(i,j) = x_{i+j}$

Eg: $Vz=b$ mean $\sum_{j=1}^{n} z_j x_i^{j-1} = b_i$

solving for z = polynomial interpolation possible in $O(n^2)$

similar trick for $V^T z = b$

Eg multiplying Tz = convolution use FFT

Eg Solving $Cx=b$, arises in rational interpolation

Common Structure of all these X

$AX + XB =$ low rank, for some simple A, B

Def: This rank called "displacement rank"

Ex: Vandermonde

$D = \mathrm{diag}(x_1, x_2, \dots x_n)$

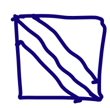
$D \cdot V = V$ "shifted left"

$$V \cdot P = V \cdot \begin{bmatrix} 0 & 0 & & 0 & 1 \\ 1 & 0 & & \vdots & 0 \\ 0 & 1 & \cdots & \vdots & \vdots \\ \vdots & 0 & & 0 & \vdots \\ \vdots & \vdots & & 1 & 0 \end{bmatrix} = V \text{ "shifted left"}$$

$D \cdot V - V \cdot P =$ zero except last column
$=$ rank 1

Ex: Toeplitz

$P \cdot T - T \cdot P = T$ shifted down $- T$ shifted left



$=$ zero except first row, last column

$=$ rank 2

Ex: Cauchy:

$\mathrm{diag}(x_1, \dots, x_n) \cdot C + C \cdot \mathrm{diag}(y_1, \dots y_n) =$ all ones

$=$ rank one

Thm (Kailath et al) There are $O(n^2)$ solvers if displacement rank is $O(1)$

caveat: stability not guaranteed

Chap 3: Least Squares

Ex: polynomial fitting

given sample points (y_i, b_i) $i = 1:m$

find "best" polynomial $p(y)$ of

fixed degree to minimize

$$\sum_{i=1}^{m} (p(y_i) - b_i)^2$$

minimize $\|Ax - b\|_2$

$A(i,j) = y_i^{j-1}$, x coefficients of p

$p(y) = x_1 + x_2 \cdot y + x_3 \cdot y^2 \cdots + x_j y^j$

Try this for $\sin(\frac{\pi y}{5}) + \frac{y}{5}$

at $-5:.5:6$

(polyfit31): loss of stability, big error, for $deg(p) \geq 18$

Standard Notation

$\underset{x}{\mathrm{argmin}} \|Ax - b\|_2$ $A^{m \times n}$ $m > n$

$m > n$ means overdetermined

don't expect $Ax = b$ exactly

Other variants (all in LAPACK)

Constrained LS: $\underset{x:\,Bx=y}{\operatorname{argmin}} \|Ax-b\|_2$

where #rows(B) $\leq$ #cols(A) = dim(x)

$\leq$ #rows(A) + #row(B)

$\Rightarrow$ x unique if A, B full rank

Weighted LS: $\underset{x}{\operatorname{argmin}} \|y\|$ s.t. $b = Ax + By$

if $B = I$: $y = b - Ax$, standard LS

if B square, nonsingular

$\underset{x}{\operatorname{argmin}} \|B^{-1}(Ax-b)\|_2$

Underdetermined LS #rows(A) < #cols(A)

$\underset{x}{\operatorname{argmin}} \|Ax-b\|$ $\Rightarrow$ solution not unique

$\exists$ space of solution: take any null vector z: $A \cdot z = 0$, add it to x

To make solution unique:

$\underset{x}{\operatorname{argmin}} \|x\|_2$ s.t. $Ax = b$

Ridge Regression: (Lecture 1)

$\underset{x}{\operatorname{argmin}} \|Ax-b\|_2^2 + \lambda\|x\|_2^2$

$\lambda > 0$ "tuning parameter"

always unique solution if $\lambda > 0$

Total Least Squares (need SVD)

$$\underset{x:\ (A+E)x=b+r}{\operatorname{argmin}} \quad \|[E,r]\|_2$$

Algorithms for overdetermined LS
(all used in different cases)

Solve: Normal Equations (NE)

$A^T A x = A^T b$

$A^T A$ spd $\rightarrow$ use Cholesky

fastest in dense case
(fewest flops, least comm)

not stable if A ill-conditioned

Use QR decomposition: $A^{m\times n} = QR$

$Q^{m\times n}$ orthonormal columns

$R^{n\times n}$ triangular

$x = R^{-1} Q^T b$

Gram-Schmidt: unstable if
A ill-conditioned (lots of
variants that trade off
speed + stability)

Householder - stable ($x = A \backslash b$
in Matlab)

blocked version to reduce comm.

Also possible to get Q from normal equations $R = \mathrm{chol}(A^T A)$

$Q = A R^{-1}$

but can be unstable

SVD: most "complete" solution: stable, provides condition number + error bound, works in rank deficient, underdetermined cases etc but expensive

Convert to a linear system with matrix $\left[\begin{array}{c|c} I & A \\ \hline A^T & 0 \end{array}\right]$ (Q3.3)

Back to Normal Equations:

Thm: A full column rank then $x = \underset{x}{\mathrm{argmin}} \|Ax - b\|_2$ satisfies

$$A^T A x = A^T b$$

proof: assume $A^T A x = A^T b$, show $\|A(x+e) - b\|_2^2$ minimized at $e = 0$

$$= (A(x+e) - b)^T (A(x+e) - b)$$

$$= (Ax + Ae - b)^T (Ax + Ae - b)$$

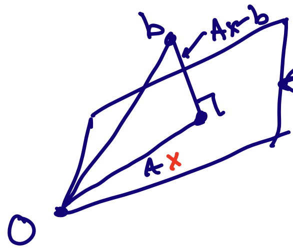
$$= (Ax - b + Ae)^T (Ax - b + Ae)$$

$$= (Ax - b)^T (Ax - b) + (Ae)^T (Ae)$$

$$+ 2e^T \underbrace{A^T(Ax-b)}_{A^TAx - A^Tb = 0 \text{ by NE}}$$

$$= \|Ax-b\|_2^2 + \|Ae\|_2^2$$

minimized at $e=0$



all vectors Ay

$$Ax-b \perp Ay \quad \forall y$$

$$\Rightarrow (Ay)^T(Ax-b) = 0 \quad \forall y$$

$$\Rightarrow y^T(A^TAx - A^Tb) = 0 \quad \forall y$$

$$\Rightarrow A^TAx = A^Tb$$

Cost: to solve $\underbrace{A^TA}_{mn^2}\, x = \underbrace{A^Tb}_{mn}$

cholesky on A^TA: $\frac{n^3}{3}$

cost $= mn^2 + \frac{n^3}{3}$

#words moved: minimized by matmul, Cholesky

QR: $A = QR$ $\quad A^{m\times n}$, $\underset{\text{orth. cols}}{Q^{m\times n}}$, $R^{n\times n}$

$$\underset{x}{\operatorname{argmin}} \|Ax-b\|_2 = R^{-1}Q^Tb$$

proof 1. $A = QR = \begin{array}{c c} & \begin{array}{cc} n & m-n \end{array} \\ m & \left[\begin{array}{c|c} Q & \hat{Q} \end{array}\right] \end{array} \begin{array}{c c} \left[\begin{array}{c} R \\ \hline 0 \end{array}\right] & \begin{array}{c} n \\ m-n \end{array} \end{array}$

$$\|Ax-b\|_2^2 = \Big\|\overbrace{\begin{bmatrix} Q^T \\ \hat{Q}^T \end{bmatrix}}^{\text{orthog}}(Ax-b)\Big\|_2^2$$

$$= \Big\|\begin{bmatrix} Q^T \\ \hat{Q}^T \end{bmatrix}[QRx-b]\Big\|_2^2$$

$$= \Big\|\begin{pmatrix} Q^T(QRx-b) \\ \underbrace{\hat{Q}^T Q}_{0}Rx-b) \end{pmatrix}\Big\|_2^2$$

$$= \Big\|\begin{pmatrix} Rx-Q^Tb \\ \hat{Q}b \end{pmatrix}\Big\|_2^2$$

$$= \|Rx-Q^Tb\|_2^2 + \|\hat{Q}b\|_2^2$$

$$\geq \|\hat{Q}b\|_2^2 \quad \forall x$$

attained by $x = R^{-1}Q^Tb$

Proof 2: NE: $A^TAx = A^Tb$

$$\Rightarrow (QR)^T(QR)x = (QR)^Tb$$

$$R^T\underbrace{\cancel{Q^TQ}}_{I}Rx = R^TQ^Tb$$

$$\cancel{R^T}Rx = \cancel{R^T}Q^Tb$$

$$Rx = Q^Tb$$

$$x = R^{-1}Q^Tb$$