

Rank-Deficient Matrices and QR

What happens with QR for rank-deficient matrices?



$$A = Q \left(\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right)$$

n } small diagonal entries

"rank-revealing" } QR \rightarrow HW14
"column-pivoted" }

Rank-Deficient Matrices and Least-Squares

What happens with Least Squares for rank-deficient matrices?

$$Ax \cong b$$



$$\|Ax - b\|_2 \rightarrow \min$$

$$u \in N(A)$$

$$\|A(x+u) - b\|_2 = \|Ax - b\|_2$$

$$\rightarrow \min \|x\|_2$$

"Total least squares"

SVD $A = U\sigma V^T$

SVD: What's this thing good for? (I)

$$A = \begin{pmatrix} | & & | \\ \hline & \sigma_1 & \\ & \vdots & \\ & \sigma_n & \\ & \vdots & \\ & & \end{pmatrix} \begin{pmatrix} \leftarrow v_1 \\ \leftarrow \vdots \\ \leftarrow v_n \end{pmatrix}$$

≥ 0 sorted $|\sigma_1| \geq |\sigma_2| \dots$

$$\|A\|_2 = \sigma_1$$

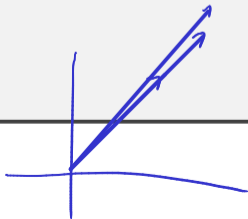
$$\text{cond}_2(A) = \sigma_1 / \sigma_n$$

$$N(A) = \text{span}(v_{k+1}, \dots, v_n)$$

$$N(\epsilon) = \text{span}\left(\underbrace{(0 \dots 0 | 0 \ 0 \ 0)^T}_{k+1}, \dots, (0 \dots 0)^T\right)$$

$$\text{rank}(A) = k$$

$$\text{num-rank}(A, \epsilon) = \#\{\sigma_i \geq \epsilon\}$$



SVD: What's this thing good for? (II)

► Low-rank Approximation

Theorem (Eckart-Young-Mirsky)

If $k < r = \text{rank}(A)$ and

$$A_k = \sum_{i=1}^k \sigma_i u_i v_i^T, \quad \text{then}$$

$$\min_{\text{rank}(B) \leq k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1},$$

$$\min_{\text{rank}(B) \leq k} \|A - B\|_F = \|A - A_k\|_F = \sqrt{\sum_{j=k+1}^n \sigma_j^2}.$$

SVD: What's this thing good for? (III)

- ▶ The minimum norm solution to $Ax \cong b$:

$$A = U\Sigma V^T = \sum_{i=1}^n \sigma_i u_i v_i^T$$

$$Ax \cong b \Leftrightarrow \Sigma \underline{V^T x} \cong U^T b \quad y = V^T x$$

$$\Sigma y \cong \underline{U^T b} = c$$

$$\Sigma = \begin{bmatrix} \sigma_1 & & & & & & \\ & \sigma_2 & & & & & \\ & & \dots & & & & \\ & & & \sigma_r & & & \\ & & & & 0 & \dots & 0 \\ & & & & & \dots & 0 \end{bmatrix}$$

$$\Sigma^+ = \begin{bmatrix} \sigma_1^{-1} & & & & & & \\ & \dots & & & & & \\ & & \sigma_2^{-1} & & & & \\ & & & & 0 & & \\ & & & & & \dots & \\ & & & & & & 0 \dots \end{bmatrix}$$

$$\|\Sigma y - c\|_2^2 = \sum_{i=1}^r (\sigma_i y_i - c_i)^2 + \underbrace{\sum_{i=r+1}^n c_i^2}_{\text{purple underline}}$$

$$\|y\|_2^2 = \sum_{i=1}^r y_i^2 + \sum_{i=r+1}^n y_i^2$$

SVD: Minimum-Norm, Pseudoinverse

What is the minimum 2-norm solution to $Ax \cong b$ and why?

$$y = \Sigma^+ U^T b \text{ is the minimum norm solution.}$$
$$\rightarrow \Sigma y \cong U^T b. \quad x = Vy = \underbrace{V \Sigma^+ U^T}_{\text{pseudoinverse}} b$$

Generalize the pseudoinverse to the case of a rank-deficient matrix.

$$\text{when } A \text{ full rank, } V \Sigma^+ U^T = (A^T A)^{-1} A$$

Comparing the Methods

Methods to solve least squares with A an $m \times n$ matrix:

① normal eqn.

$A^T A$, solve. $n^2 m / 2 + n^3 / 6$

② QR with Householder dr.
 $mn^2 - n^3 / 3$

③ SVD: $mn^2 + n^3$

$\rangle O(mn^2 + n^3)$

Demo: Relative cost of matrix factorizations [cleared]

In-Class Activity: Householder, Givens, SVD

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Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Properties and Transformations

Sensitivity

Computing Eigenvalues

Krylov Space Methods

Nonlinear Equations

Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Additional Topics

Eigenvalue Problems: Setup/Math Recap

A is an $n \times n$ matrix.

- ▶ $\mathbf{x} \neq 0$ is called an *eigenvector* of A if there exists a λ so that

$$A\mathbf{x} = \lambda\mathbf{x}.$$

- ▶ In that case, λ is called an *eigenvalue*.
- ▶ The set of all eigenvalues $\lambda(A)$ is called the *spectrum*.
- ▶ The *spectral radius* is the magnitude of the biggest eigenvalue:

$$\rho(A) = \max \{|\lambda| : \lambda \in \lambda(A)\}$$

Finding Eigenvalues

How do you find eigenvalues?

$$\begin{aligned} A\mathbf{x} = \lambda\mathbf{x} &\Leftrightarrow (A - \lambda I)\mathbf{x} = 0 \\ &\Leftrightarrow A - \lambda I \text{ singular} \Leftrightarrow \det(A - \lambda I) = 0 \end{aligned}$$

$\det(A - \lambda I)$ is called the *characteristic polynomial*, which has degree n , and therefore n (potentially complex) roots.

Does that help algorithmically? Abel-Ruffini theorem: for $n \geq 5$ is no general formula for roots of polynomial. IOW: no.

- ▶ For LU and QR, we obtain *exact* answers (except rounding).
- ▶ For eigenvalue problems: not possible—must *approximate*.

[Demo: Rounding in characteristic polynomial using SymPy \[cleared\]](#)

Multiplicity

$$\det(A - \lambda I) = (\lambda - 5)^2 (\lambda - 3)^4$$

What is the *multiplicity* of an eigenvalue?

Actually, there are two notions called multiplicity:

- ▶ *Algebraic Multiplicity*: multiplicity of the root of the characteristic polynomial
- ▶ *Geometric Multiplicity*: # of lin. indep. eigenvectors

In general: $AM \geq GM$.

If $AM > GM$, the matrix is called *defective*.

An Example

Give characteristic polynomial, eigenvalues, eigenvectors of

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

$$|\lambda I - A| = (\lambda - 1)^2$$

$$AM = 2$$

$$GM = 1 < AM.$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 1 \cdot \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\Rightarrow \begin{aligned} x + y &= x & \Rightarrow & y = 0 \\ y &= y \end{aligned}$$

$$\begin{bmatrix} x \\ 0 \end{bmatrix}$$

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