Lecture 7
Least Squares Problems

MIT 18.335J / 6.337J

Introduction to Numerical Methods

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September 28, 2006

The Linear Least Squares Problem

- In general, $Ax = b$ with $m > n$ has no solution
- Instead, try to minimize the *residual* $r = b - Ax$
- With the 2-norm we obtain the linear *least squares problem* (LSP):

> Given $A \in \mathbb{C}^{m \times n}, m \geq n, b \in \mathbb{C}^m$,
> find $x \in \mathbb{C}^n$ such that $\|b - Ax\|_2$ is minimized

- The minimizer x is the solution to the *normal equations*

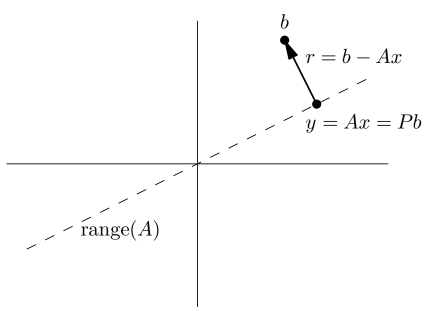
$$A^*Ax = A^*b$$

or, in terms of the *pseudoinverse* A^+:

$$x = A^+b, \qquad \text{where } A^+ = (A^*A)^{-1}A^* \in \mathbb{C}^{n,m}$$

Geometric Interpretation

- Find the point Ax in $\text{range}(A)$ closest to b
- This x will minimize the 2-norm of $r = b - Ax$
- $Ax = Pb$ where P is an orthogonal projector onto $\text{range}(A)$, so the residual must be orthogonal to $\text{range}(A)$



Solving the LSP – 1. Normal Equations

- If A has full rank, A^*A is square, hermitian positive definite system
- Solve by *Cholesky factorization* (Gaussian elimination)

Algorithm: Least Squares via Normal Equations

1. Form the matrix A^*A and the vector A^*b
2. Compute the Cholesky factorization $A^*A = R^*R$
3. Solve the lower-triangular system $R^*w = A^*b$ for w
4. Solve the upper-triangular system $Rx = w$ for x

- Work $\sim$ Forming A^*A + Cholesky $\sim mn^2 + n^3/3$ flops
- Fast, but sensitive to rounding errors

Solving the LSP – 2. QR Factorization

- Using $A = \hat{Q}\hat{R}$, b can be projected onto $\text{range}(A)$ by $P = \hat{Q}\hat{Q}^*$
- Insert into $Ax = b$ to get $\hat{Q}\hat{R}x = \hat{Q}\hat{Q}^*b$, or $\hat{R}x = \hat{Q}^*b$

Algorithm: Least Squares via QR Factorization

1. Compute the reduced QR factorization $A = \hat{Q}\hat{R}$
2. Compute the vector $\hat{Q}^*b$
3. Solve the upper-triangular system $\hat{R}x = \hat{Q}^*b$ for x

- Work $\sim$ QR Factorization $\sim 2mn^2 - 2n^3/3$ flops
- Good stability, relatively fast, used in MATLAB's "backslash" $\backslash$

Solving the LSP – 3. SVD

- Using $A = \hat{U}\hat{\Sigma}V^*$, b can be projected onto $\text{range}(A)$ by $P = \hat{U}\hat{U}^*$
- Insert into $Ax = b$ to get $\hat{U}\hat{\Sigma}V^*x = \hat{U}\hat{U}^*b$, or $\hat{\Sigma}V^*x = \hat{U}^*b$

Algorithm: Least Squares via SVD

1. Compute the reduced SVD $A = \hat{U}\hat{\Sigma}V^*$
2. Compute the vector $\hat{U}^*b$
3. Solve the diagonal system $\hat{\Sigma}w = \hat{U}^*b$ for w
4. Set $x = Vw$

- Work $\sim$ SVD $\sim 2mn^2 + 11n^3$ flops
- Very good stability properties, use if A is close to rank-deficient