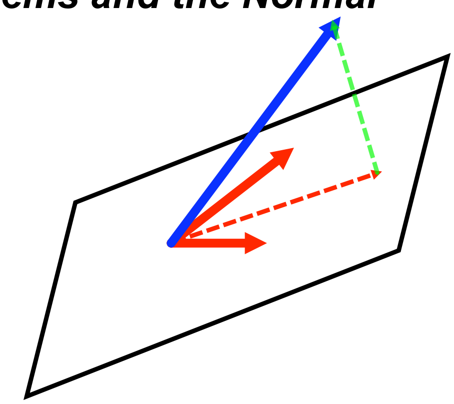
Lecture 19: Numerical Linear Algebra #3
Direct methods for solving Linear Least Squares problems

Outline

1) Quick Review: Linear Least Squares Problems and $A^TAx=A^Tb$
2) Issues with solving the Normal Equations
3) Orthogonalization, the QR Factorization and Least Squares
   A) Introduction
   B) QR by modified Gram-Schmidt $A \rightarrow Q$
   C) QR by Householder Transformation $A \rightarrow R$ (similarity to LU factorization)

Review: Linear Least-squares problems and the Normal Equations.



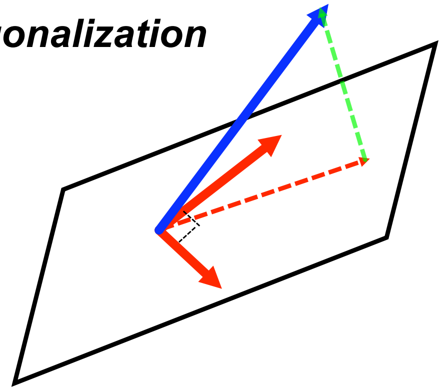
Normal Equations and Condition number squaring

The SVD and the $cond(A)_2$

Normal Equations and Condition number squaring

Example: A= [1 a 0; 1 0 a]', b=[1 1 1]

Solution of Least Squares by Orthogonalization (QR factorization)



Solution of Least Squares by Orthogonalization (QR factorization)

Theorem: Every mxn full-column rank Matrix A can be factored as A=QR where Q is mxn and contains an orthonormal basis for C(A) and R is nxn upper-triangular and invertible. (Proof by construction/Gram-Schmidt).

Solution of Least Squares by Orthogonalization (QR factorization)

Theorem: if A=QR, the solution of the normal Equations $A^T A \hat{\underline{x}} = A^T \underline{b}$, is the solution of $R\hat{\underline{x}} = Q^T \underline{b}$

QR Factorization Algorithms: #1 Modified Gram-Schmidt Orthogonalization

Idea: Take A → Q by repeated projections, get $R=Q^T A$

QR Factorization Algorithms: #1 Modified Gram-Schmidt Orthogonalization

Example: A= [1 2 2 ; 1 1 0]

QR Factorization Algorithms: #1 Modified Gram-Schmidt Orthogonalization

Algorithm:

QR Factorization Algorithms:
#2 Orthogonalization by Householder transformation

Idea: Take A → R directly by repeated applications of Q matrices
(similar algorithm to LU factorization)

QR Factorization Algorithms:
#2 Orthogonalization by Householder transformation

The Householder Reflection Matrix $H = I - 2vv^T/v^Tv$

Properties:

1) Symmetric matrix

2) Q matrix

3) Reflects a vector around the hyperplane orthogonal to $\underline{v}$

QR Factorization Algorithms: #2 Orthogonalization by Householder transformation

Example: Find H to transform a=[1 2 2]' to [c 0 0]'

QR Factorization Algorithms: #2 Orthogonalization by Householder transformation

General Idea:

QR Factorization Algorithms: #2 Orthogonalization by Householder transformation

Example: A= [1 2 2 ; 1 1 0]

QR Factorization Algorithms: #2 Orthogonalization by Householder transformation

Algorithm: (quick and dirty)

```
[m,n]=size(A);  % get size of A

for k=1:n   % loop over columns
    i=k:m;   j=k:n; % sub-block indices

    % calculate the reflection vector v
    v=A(i,k); % extract subcolumn k
    v(1)=v(1)+sign(v (1))*norm(v); % modify first component by alpha
    v=v/norm(v); % normalize v

    % Multiply by Qk to transform sublock
    A(i,j) = A(i,j)-2*v*(v'*A(i,j)) ;
end
```

QR Factorization Algorithms:
#2 Orthogonalization by Householder transformation

Operation Counts: