

## Another example

assume 3-digit decimal arithmetic.

$$\begin{bmatrix} .780 & .563 \\ .913 & .659 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} .217 \\ .254 \end{bmatrix}$$

If we compute the solution with pivoting, we obtain

$$x = \begin{bmatrix} -.443 \\ 1.000 \end{bmatrix}, \quad r = \begin{bmatrix} -.000460 \\ -.000541 \end{bmatrix}$$

$$x_{true} = \begin{bmatrix} 1.000 \\ -1.000 \end{bmatrix}$$

- Solution has small residual but very large error
- In fact signs of the solution are opposite!

# Condition Number of a Matrix

The first problem is **well-conditioned**; small changes in the data produce small changes in the answer.

The second problem is **ill-conditioned**; small changes in the data can produce large changes in the answer.

A measure of how close a matrix is to singular

$$\begin{aligned}\text{cond}(A) &= \kappa(A) = \|A\| \cdot \|A^{-1}\| \\ &= \frac{\text{maximum stretch}}{\text{maximum shrink}} = \frac{\max_i |\lambda_i|}{\min_i |\lambda_i|}\end{aligned}$$

- $\text{cond}(I) = 1$
- $\text{cond}(\text{singular matrix}) = \infty$

# Properties of the condition number

Some properties:

- $\kappa(A) \geq 1$  for all matrices.
- $\kappa(A) = \infty$  for singular matrices.
- $\kappa(cA) = \kappa(A)$  for any nonzero scalar  $c$ .
- $\kappa(D) = \max |d_{ii}| / \min |d_{ii}|$  if  $D$  is diagonal.
- $\kappa$  measures closeness to singularity better than the determinant.

# Relation between condition number and error

$$Ax_{true} = b \rightarrow \|b\| = \|Ax_{true}\| \leq \|A\| \|x_{true}\|$$

$$\|x_{true}\| \geq \frac{\|b\|}{\|A\|} \rightarrow \frac{\mathbf{1}}{\|\mathbf{x}_{true}\|} \leq \frac{\|\mathbf{A}\|}{\|\mathbf{b}\|}$$

$$Ax = b - r \rightarrow A(x_{true} - x) = r$$

$$(x_{true} - x) = A^{-1}r \rightarrow \|\mathbf{x}_{true} - \mathbf{x}\| \leq \|\mathbf{A}^{-1}\| \|r\|$$

$$\frac{\|\mathbf{x}_{true} - \mathbf{x}\|}{\|\mathbf{x}_{true}\|} \leq \frac{\|r\|}{\|\mathbf{b}\|} \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$$

$$= \frac{\|r\|}{\|b\|} \kappa(A).$$

- In words: relative error is smaller than norm of residual divided by norm of rhs times condition number
- So larger condition number means larger error

# Closing remarks

- Never compute matrix inverse
- Use a stable algorithm
- Check residual and condition number of problem
- If condition number is large, do not trust solution
  - Can problem be reformulated somehow?

# LU code

```
%LU Triangular factorization
% [L,U,p] = lutx(A) produces a unit lower triangular
% matrix L, an upper triangular matrix U, and a
% permutation vector p, so that L*U = A(p,:).
```

- Initialize

- Matrix size `[n,n] = size(A);`
- Permutation vector `p = (1:n)'`

- Second output argument to max is index of max element

```
for k = 1:n-1
    % Find largest element below diagonal in k-th column
    [r,m] = max(abs(A(k:n,k)));
    m = m+k-1;
```

- If max element is zero then we need not eliminate

```
% Skip elimination if column is zero
if (A(m,k) ~= 0)
```

- Exchange rows

- update permutation vector

```
% Swap pivot row
if (m ~= k)
    A([k m],:) = A([m k],:);
    p([k m]) = p([m k]);
end
```

# Look at LU code

- Multipliers for each row below diagonal
  - Note multipliers are stored in the lower triangular part of A
- Vectorized update
  - $A(i,k) \cdot A(k,j)$  multiplies column vector by row vector to produce a square, rank 1 matrix of order  $n-k$ .
  - matrix is then subtracted from the submatrix of the same size in the bottom right corner of A.
  - In a programming language without vector and matrix operations, this update of a portion of A would be done with doubly nested loops on i and j.
  - Cost is  $n^2$  and done n times for a total cost of  $n^3$
- Computes decomposition in the matrix A itself
- Here they are separated, but when memory is important it can be left there

```
% Compute multipliers
i = k+1:n;
A(i,k) = A(i,k)/A(k,k);

% Update the remainder of the matrix
j = k+1:n;
A(i,j) = A(i,j) - A(i,k)*A(k,j);

end

end

% Separate result
L = tril(A,-1) + eye(n,n);
U = triu(A);
```

# Code to solve linear system using LU

- In Matlab the backslash operator can be used to solve linear systems.
- For square matrices it employs LU or special variants
  - Lower triangular
  - Upper triangular
  - symmetric
- Symmetric LU is called Cholesky decomposition
  - $A=LL^T$
  - Upper and lower triangular are equal (transposes)
  - If matrix not positive-definite go to regular solution

```
function x = bslashtx(A,b)
% BSLASHTX Solve linear system (backslash)
% x = bslashtx(A,b) solves A*x = b

[n,n] = size(A);
if isequal(triu(A,1),zeros(n,n))
    % Lower triangular
    x = forward(A,b);
    return
elseif isequal(tril(A,-1),zeros(n,n))
    % Upper triangular
    x = backsubs(A,b);
    return
elseif isequal(A,A')
    [R,fail] = chol(A);
    if ~fail
        % Positive definite
        y = forward(R',b);
        x = backsubs(R,y);
        return
    end
end
end
```



# Code continues

```
% Triangular factorization
```

```
[L,U,p] = lutx(A);
```

- Call LU

- Solve  $y=Lb$

```
% Permutation and forward elimination
```

```
y = forward(L,b(p));
```

- Solve  $x=Uy$

```
x = backsubs(U,y);
```

```
function x = forward(L,x)
```

```
% FORWARD. Forward elimination.
```

```
% For lower triangular L, x = forward(L,b) solves  $L*x = b$ .
```

```
[n,n] = size(L);
```

```
for k = 1:n
```

```
    j = 1:k-1;
```

```
    x(k) = (x(k) - L(k,j)*x(j))/L(k,k);
```

```
end
```

```
function x = backsubs(U,x)
```

```
% BACKSUBS. Back substitution.
```

```
% For upper triangular U, x = backsubs(U,b) solves  $U*x = b$ .
```

```
[n,n] = size(U);
```

```
for k = n:-1:1
```

```
    j = k+1:n;
```

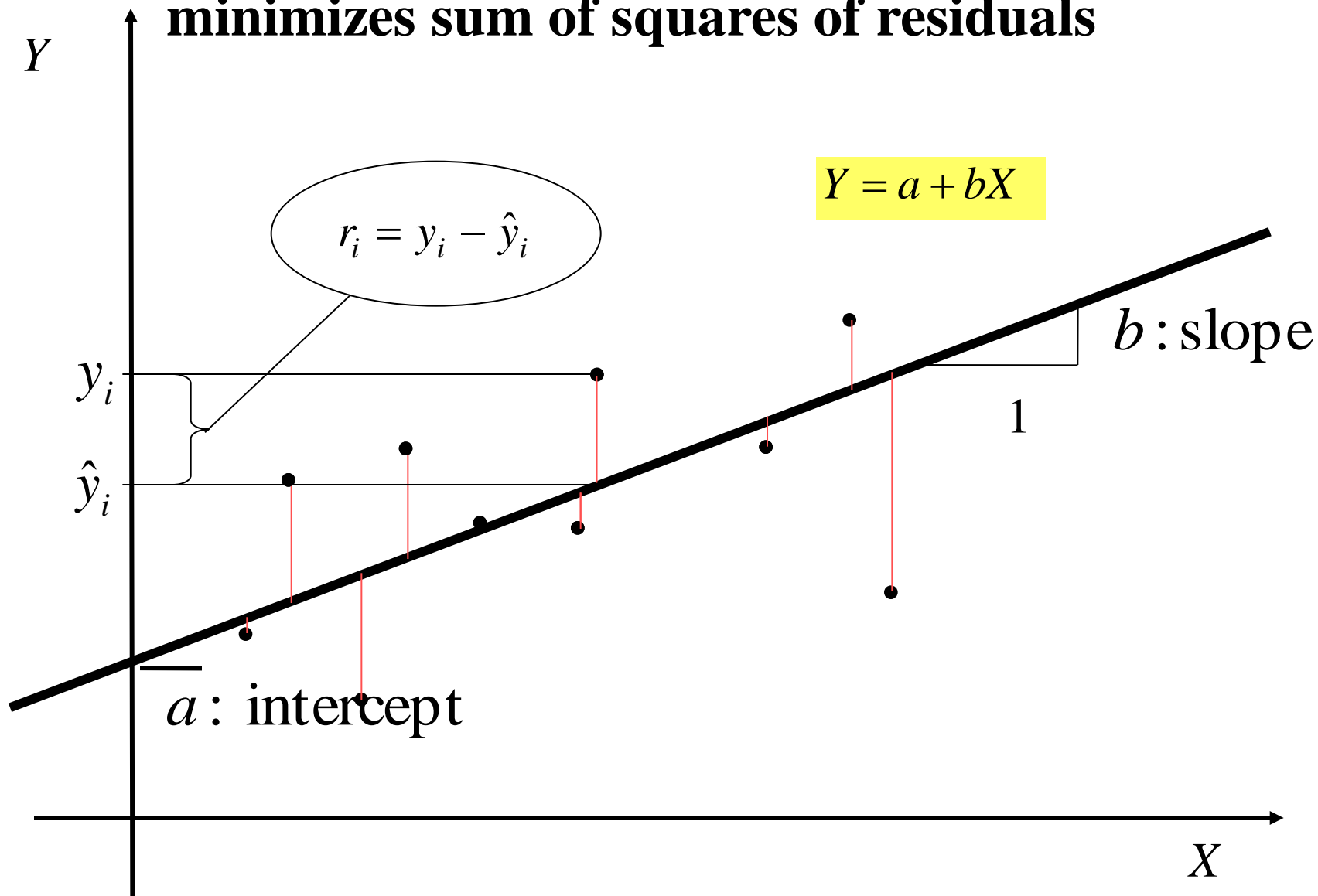
```
    x(k) = (x(k) - U(k,j)*x(j))/U(k,k);
```

```
end
```

# Fitting data to a model

- Practical science involves lots of fitting of data to models
- Tasks arise commonly in science
  - Fit straight lines and curves to data
  - More generally fit a parametric model to data
- Parametric: Model contains parameters
  - Job of fitting is to estimate the parameters that “best” make the model fit the data
  - “best” → define best
  - For this section, best is least square error
- Simplest example of model fitting problem
  - Linear regression

**Want to estimate Regression Line that  
minimizes sum of squares of residuals**



# How do we find $a$ and $b$ ?

Find  $a$  and  $b$  by minimizing sum of squares of individual point residuals, with respect to  $a$  and  $b$

$$E(a,b)=\sum_{i=1}^N (r_i)^2 = \sum_{i=1}^N (y_i - [bx_i + a])^2$$

- Differentiate cost function with respect to  $b$  and  $a$  and get two equations in two unknowns

$$\frac{\partial E}{\partial a} = -\sum_{i=1}^n 2(y_i - (a + bx_i)) \frac{\partial(a + bx_i)}{\partial a} = 0$$

$$n a + b \sum_{i=1}^n x_i = \sum_{i=1}^n y_i$$

$$\frac{\partial E}{\partial b} = -\sum_{i=1}^n 2(y_i - (a + bx_i)) \frac{\partial(a + bx_i)}{\partial b} = 0$$

$$a \sum_{i=1}^n x_i + b \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i.$$

# Least Squares for more unknowns

- Suppose we wish to solve

$$\mathbf{A}\mathbf{c}=\mathbf{y}$$

$\mathbf{A}$  is a  $m \times n$  matrix,  $\mathbf{c}$  is a  $n$  vector, and  $\mathbf{y}$  is a  $m$  vector

- Look for solution  $\mathbf{c}$  that minimizes same cost function, the sum of squares of residuals  $r_i$  at each data point  $x_i$

$$F(\mathbf{c})=\|\mathbf{A}\mathbf{c} - \mathbf{y}\|_2^2$$

$$F(\mathbf{c}) = \sum_{i=1}^m r_i^2 = \sum_{i=1}^m \left( \sum_{j=1}^n A_{ij} c_j - y_i \right)^2 = \sum_{i=1}^m \left( \sum_{j=1}^n A_{ij} c_j - y_i \right) \left( \sum_{k=1}^n A_{ik} c_k - y_i \right)$$

Differentiate with respect to the unknowns  $c_l$  and set to zero

$$\frac{\partial F}{\partial c_l} = \sum_{i=1}^m \left[ \left( \sum_{j=1}^n A_{ij} \frac{\partial c_j}{\partial c_l} \right) \left( \sum_{k=1}^n A_{ik} c_k - y_i \right) + \left( \sum_{j=1}^n A_{ij} c_j - y_i \right) \left( \sum_{k=1}^n A_{ik} \frac{\partial c_k}{\partial c_l} \right) \right] = 0$$

- Derivative is 1 for  $j=l$  (or  $k=l$ ), otherwise zero. Define

$$\frac{\partial c_k}{\partial c_l} = \delta_{kl} = \begin{cases} 1 & \text{if } k = l \\ 0 & \text{otherwise} \end{cases}$$

- Also called Kronecker Delta
- This yields the following equation for each  $l$

$$\sum_{i=1}^m \left[ \left( \sum_{k=1}^n A_{il} A_{ik} c_k - A_{il} y_i \right) + \left( \sum_{j=1}^n A_{ij} A_{il} c_j - A_{il} y_i \right) \right] = 0$$

$$2 \left( \sum_{i=1}^m \sum_{k=1}^n A_{il} A_{ik} c_k - \sum_{i=1}^m A_{il} y_i \right) = 0$$

- Can recognize these as the following equation

$$2(\mathbf{A}^t \mathbf{A} \mathbf{c} - \mathbf{A}^t \mathbf{y}) = 0 \quad \text{or} \quad \mathbf{A}^t \mathbf{A} \mathbf{c} = \mathbf{A}^t \mathbf{y}$$

## Normal equations $\mathbf{A}^t \mathbf{A} \mathbf{c} = \mathbf{A}^t \mathbf{y}$

- For  $\mathbf{A}$  size  $m \times n$  and  $\mathbf{c}$  of size  $n$  and  $\mathbf{y}$  of size  $m$  what are the dimensions of the normal equations?
  - $n \times n$
- Have converted it to a regular system that we know how to solve
- Solve via LU decomposition
- Solution accurate if the matrix  $\mathbf{A}^t \mathbf{A}$  is well conditioned
- Cost of solving normal equations
  - Matrix product  $n^2 m$  operations.
  - Matrix vector product  $nm$  operations
  - LU decomposition  $n^3/3$  operations

# More on Normal Equations

- Normal equations are only important theoretically
- In practice least squares solved via a different process
  - QR decomposition
- Why?
  - Somewhat expensive as we have to form  $A^t A$
  - involves matrix multiplication and then solution
  - More importantly it is poorly conditioned
  - $\text{cond}(A^t A) = (\text{cond}(A))^2$
- Would like a method whose errors are closer to the condition number of  $A$



# Look at the fitting matrix in more detail

- Instead
  - Look for methods that can directly operate on  $\mathbf{A}$  to get the solution
  - Recall in LU we did a set of transformations to  $\mathbf{A}$  and the r.h.s. to find  $\mathbf{c}$
  - Today we will look at the QR algorithm
- Goal in least squares is to find the coordinates of the vector in the *column space of matrix* that *best approximates* the right hand side in a *least squares sense*
- *Matrix vector product*
  - *Produces a vector that is a combination of column vectors of matrix*

# Key Ideas

- Column space of a matrix: the vector space formed by the collection of column vectors in a matrix
- Every matrix vector product results in a vector formed by linear combination of vectors in the column space
- A  $m \times n$  rectangular matrix  $\mathbf{A}$  takes  $n$  vectors into  $m$  vectors
- Let the least squares problem be  $\mathbf{A}\mathbf{c}=\mathbf{f}$
- Let the solution which minimizes the residual be  $\mathbf{c}_*$
- Then  $\mathbf{c}_*$  creates on matrix vector product a rhs  $\mathbf{f}_*$  that is in the column space of  $\mathbf{A}$
- We want that  $\mathbf{c}_*$  minimizes  $\mathbf{r}=\|\mathbf{f}-\mathbf{f}_*\|$

$$\begin{bmatrix} 1 & 8 & 13 & 12 \\ 14 & 11 & 2 & 7 \\ 4 & 5 & 16 & 9 \\ 15 & 10 & 3 & 6 \end{bmatrix}$$

# Null Space of A

- Not all  $m$  vectors will be reachable even if we supply arbitrary  $n$  vectors
- *Range* of A: the part of the space of  $m$  vectors that are reachable

$$\text{Range}(A) = \{\mathbf{y} \in R^m : \mathbf{y} = \mathbf{A}\mathbf{x} \text{ for some } \mathbf{x} \in R^n\}$$

- *The range of A contains all those vectors that can be made up using the columns of A*
- *Rank(A)* is the dimension of the range of A
- Null space of A: those vectors  $\mathbf{x}$ , for which  $\mathbf{A}\mathbf{x}$  is zero

$$\text{Null}(\mathbf{A}) = \{\mathbf{x} \in R^n : \mathbf{A}\mathbf{x} = \mathbf{0}\}$$

$$\text{Dim}(\text{Null}(\mathbf{A})) + \text{Rank}(\mathbf{A}) = n$$

- Key idea: Minimize the error in the part that can be reached

# QR decomposition

- Suppose we can write

$$\mathbf{A} = \mathbf{Q}' \mathbf{R}'$$

- $\mathbf{Q}'$  is an orthonormal matrix of dimension  $m \times m$
- $\mathbf{R}'$  is a  $m \times n$  matrix that can be written as  $\begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$

$\mathbf{R}$  is a triangular  $n \times n$  matrix and  $\mathbf{0}$  is a matrix of zeroes of size  $m-n \times n$

$\mathbf{Q}'$  can also be partitioned as  $[\mathbf{Q} \ \mathbf{Q}^{\sim}]$  with  $\mathbf{Q}$  containing  $n$  orthonormal columns of size  $m$  and  $\mathbf{Q}^{\sim}$   $m-n$  orthonormal columns

- If  $\mathbf{Ax} = \mathbf{b}$  then  $(\mathbf{Q}' \mathbf{R}')\mathbf{x} = \mathbf{b}$  or  $\mathbf{Q}'(\mathbf{R}'\mathbf{x}) = \mathbf{b}$  or  $\mathbf{Q}'\mathbf{y} = \mathbf{b}$ 
  - So if  $\mathbf{b}$  is in  $\text{range}(\mathbf{A})$ , it is also in  $\text{range}(\mathbf{Q}')$
  - Similarly if  $\mathbf{Q}'\mathbf{y} = \mathbf{b}$ ; then  $\mathbf{b} = \mathbf{Ax}$  with  $\mathbf{x} = \mathbf{R}^{-1}\mathbf{y}$
  - Columns of  $\mathbf{Q}$  form an orthonormal basis for  $\text{range}(\mathbf{A})$

# Orthogonal Matrices

- Orthogonal matrices are square matrices that have their columns orthonormal to each other
  - dot product of different column vectors is zero, while of the same column is one
  - Denoted  $\mathbf{Q}$
  - Most trivial orthogonal matrix is the identity matrix
  - $\mathbf{Q}^t \mathbf{Q} = \mathbf{I}$
  - For an orthonormal matrix
  - $\mathbf{Q}^t \mathbf{Q} = \mathbf{I}$
  - So  $\mathbf{Q}^{-1} = \mathbf{Q}^T$

generalization: a complex matrix is *Hermitian* iff  $\mathbf{Q}^{-1} = \mathbf{Q}^H$   
where superscript  $^H$  denotes complex conjugate transpose

# Orthogonal matrix facts

- Suppose  $\mathbf{Q}$  is an orthonormal matrix
- Then for any vector  $\mathbf{r}$  the Euclidean norm is preserved in an orthonormal transformation
- Proof

$$\|\mathbf{Q}\mathbf{r}\|^2 = (\mathbf{Q}\mathbf{r})^t (\mathbf{Q}\mathbf{r}) = \mathbf{r}^t \mathbf{Q}^t \mathbf{Q} \mathbf{r} = \mathbf{r}^t (\mathbf{Q}^t \mathbf{Q}) \mathbf{r} = \mathbf{r}^t \mathbf{r} = \|\mathbf{r}\|^2$$

- If  $\mathbf{Q}$  is an orthonormal matrix  
so is the extended matrix  $\mathbf{Q}_e$
- Easy to show from definition that

$$\mathbf{Q}_e = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix}$$

$$\mathbf{Q}_e^t \mathbf{Q}_e = \mathbf{I}$$

# Solving least squares with QR

- $A=Q'R'$
- Let  $r = y - Ac$        $b = Q'^t y$
- Goal of least squares find the  $c$  that minimizes squared error (residue)
- Partition  $b$  in to two pieces
  - $b_1$  of dimension  $n$
  - $b_2$  of dimension  $m-n$
  - $\|r\|^2 = \|y - Ac\|^2 = \|y - Q' R' c\|^2$
  - Length is not changed by multiplication with orthogonal matrix
  - So  $\|r\|^2 = \|Q'^t r\|^2 = \|Q'^t [y - Q' R' c]\|^2$   
 $= \|b_1 - R c\|^2 + \|b_2 - 0c\|^2$

So no matter what  $c$  is the second term remains unchanged

If we minimize  $\|r\|^2$  the best we can do is minimize first term

# Solving LS via QR

- How do we minimize  $\|c_1 - R x\|^2$ 
  - If  $R$  is full rank set solve  $Rx=c$  then we have done the best we can
  - (if  $R$  is rank deficient solve in least squares sense)
  - Recall  $R$  is triangular so this equation can be easily solved
- Algorithm
  - Compute QR factorization of  $A=Q'R'$
  - Form  $c_1=Q^t b$
  - Solve  $Rx=c_1$
  - If  $R$  is full rank and  $Q^~$  is available then the norm of the residual is  $\|Q^{~t} b\|$ . Else  $r = b - A x$ .



# Computing the QR factorization

- In LU: Converted matrix  $A$  to triangular matrix  $U$  by adding multiples of other rows
  - Elements below a given column were zeroed out
  - The multipliers were stored in  $L$  which gave us  $A=LU$
- Here want to zero out entries below the diagonal and convert to triangular matrix  $R$  but do it with orthogonal matrices
- Two strategies
- Zero out a column at a time using a matrix  $Q_1$  so that  $Q_1^t A$  gives us all entries below a certain one in a column as zero
  - Householder transformations
  - Result  $Q_n^t \dots Q_2^t Q_1^t A = R$  or  $A = Q_1 \dots Q_{n-1} Q_n R = Q R$
- Zero out one specific entry of a column at a time
  - Givens rotations
- Product of orthogonal matrices is orthogonal

# To compute QR

- Perform a sequence of orthogonal transformations that zero out elements
- Orthogonal transformations can be rotations or reflections or combinations

- Givens Rotation:

$$G = \begin{bmatrix} c & s \\ s & -c \end{bmatrix}$$

- Givens matrix has elements

- $c^2 + s^2 = 1$

- How do we use a rotation to zero out an element?

- Let  $z = [z_1 \ z_2]^t$

$$Gz = \begin{bmatrix} cz_1 + sz_2 \\ sz_1 - cz_2 \end{bmatrix} = xe_1$$

- We want

- Eliminate  $z_2$   $(c^2 + s^2)z_1 = cx$ ,  $c = z_1/x$ .

- Similarly we get  $s = z_2/x$ , and  $z_1^2 + z_2^2 = x^2$

# Givens QR

- To apply idea to larger matrix, embed the Givens matrix in identity matrix. We will use the notation  $G_{ij}$  to denote an  $n \times n$  identity matrix with its  $i$ th and  $j$ th rows modified to include the Givens rotation: for example, if  $n = 6$ , then

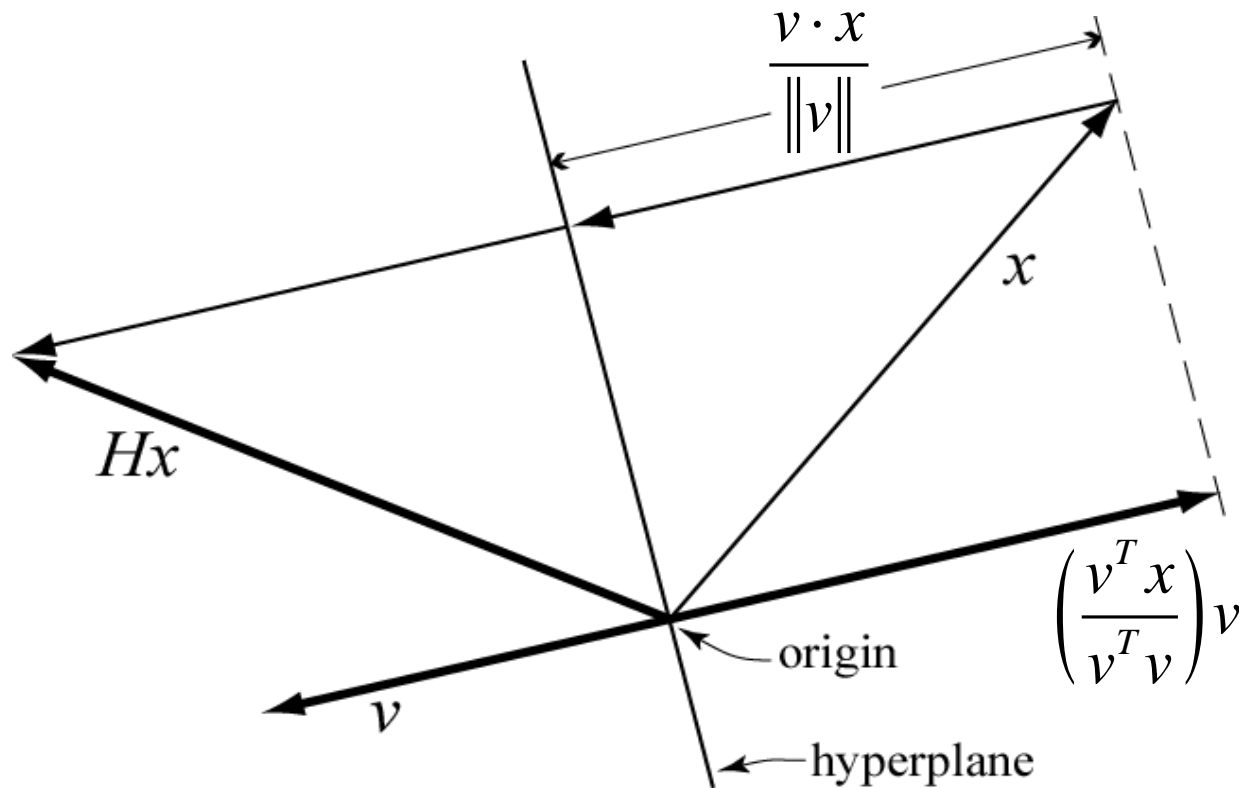
$$G_{25} = \begin{bmatrix} \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{c} & 0 & 0 & \mathbf{s} & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & \mathbf{s} & 0 & 0 & -\mathbf{c} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{bmatrix},$$

and multiplication of a vector by this matrix leaves all but rows 2 and 5 of the vector unchanged.

- Algorithm
  - for  $i=1, \dots, n$ 
    - for  $j=i+1, \dots, m$ 
      - Find Givens matrix  $G_{ij}$  to zero out  $j,i$  element of  $A$  using the value at position  $(i,i)$
      - $A = G_{ij}A$
  - end
- end

# Householder Geometry

- $Hx$  is  $x$  reflected through the hyperplane perpendicular to  $v$  ( $p : p^T v = 0$ )



# Householder Transformations

The *Householder transformation* determined by vector  $v$  is:

$$H = I - 2 \frac{vv^T}{v^T v}$$

outer product,  $n \times n$  matrix

inner product, scalar

To apply it to a vector  $x$ , compute:

$$Hx = \left( I - 2 \frac{vv^T}{v^T v} \right) x = x - 2 \frac{v(v^T x)}{v^T v}$$

$$Hx = x - \left( 2 \frac{v^T x}{v^T v} \right) v$$

scalar

# Householder Properties

- $H$  is symmetric, since

$$H^T = \left( I - 2 \frac{vv^T}{v^T v} \right)^T = I^T - 2 \frac{(vv^T)^T}{v^T v} = I - 2 \frac{v^{TT} v^T}{v^T v} = H$$

- $H$  is orthogonal, since

$$\begin{aligned} H^T H &= HH = \left( I - 2 \frac{vv^T}{v^T v} \right) \left( I - 2 \frac{vv^T}{v^T v} \right) \\ &= I - 4 \frac{vv^T}{v^T v} + 4 \frac{v(v^T v)v^T}{(v^T v)^2} = I - 4 \frac{vv^T}{v^T v} + 4 \frac{vv^T}{v^T v} = I \end{aligned}$$

and  $H^T H = I$  implies  $H^T = H^{-1}$

# Householder to Zero Matrix Elements

We'll use Householder transformations to zero subdiagonal elements of a matrix.

Given any vector  $a$ , find the  $v$  that determines an  $H$  such that,

$$Ha = \alpha e_1 = \alpha[1, 0, 0, \dots, 0]^T$$

Now solve for  $v$ :

$$Ha = a - \left( 2 \frac{v^T a}{v^T v} \right) v = a - \mu v = \alpha e_1$$

where  $\mu$  is parenthesized scalar, related to length of  $v$

$$\Rightarrow v = (a - \alpha e_1) / \mu$$

We're free to choose  $\mu = 1$ , since  $\|v\|$  does not affect  $H$

# Choosing the Vector $v$

So  $v = a - \alpha e_1$  for some scalar  $\alpha$ .

But  $\|Ha\|_2 = \|a\|_2$

(prove this by expanding  $\|Ha\|_2^2 = (Ha)^T Ha$ )

and  $\|Ha\|_2 = |\alpha|$  by design, so  $\alpha = \pm\|a\|_2$

(either sign will work).

To avoid  $v \approx 0$  we choose  $\alpha = -\text{sign}(a_1)\|a\|_2$ ,

so  $v = a + \text{sign}(a_1)\|a\|_2 e_1$  is our answer.



# Applying Householder Transforms

- Don't compute  $Hx$  explicitly, that costs  $3n^2$  flops.
- Instead use the formula given previously,

$$Hx = x - \left( 2 \frac{v^T x}{v^T v} \right) v$$

which costs  $4n$  flops (if you pre-compute  $v^T v$  or pre-normalize  $v^T v=2$ ).

- Typically, when using Householder transformations, you never compute the matrix  $H$ ; it's only used in derivation and analysis.

# Rank Revealing QR: $AP=QR$

- Crucial addition similar to pivoting

*for*  $k=1:N$

- Compute the norm of columns  $A(k:M, k:N)$
- If max norm of all columns is below threshold stop
- Swap column  $k$  of the matrix with the column with maximum norm
- Compute Householder transform using that column
- Apply to other columns

*end*

- Store column swaps in a permutation

# QR Decomposition

- Householder transformations are a good way to zero out subdiagonal elements of a matrix.
- $A$  is decomposed:

$$Q^T A = \begin{bmatrix} R \\ 0 \end{bmatrix} \quad \text{or} \quad Q Q^T A = A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$$

- where  $Q^T = H_n \dots H_2 H_1$  is the orthogonal product of Householders and  $R$  is upper triangular.
- Overdetermined system  $Ax=b$  is transformed into the easy-to-solve

$$\begin{bmatrix} R \\ 0 \end{bmatrix} x = Q^T b$$

# Other Norms

- Here we fit using the “least-squares” or  $L_2$  norm
- Could minimize the residual in other norms
- For example we may have more confidence in some data, and want to be sure that their residual is lower
  - Attach a weight to each residual
- Or we may like the 1-norm or infinity norm better

$$\|r\|_w^2 = \sum_1^m w_i r_i^2$$

$$\|r\|_1 = \sum_1^m |r_i| \qquad \|r\|_\infty = \max_i |r_i|$$

# SVD and Pseudo-Inverse

- $\mathbf{Ax}=\mathbf{b}$   $\mathbf{A}$  is  $m \times n$ ,  $\mathbf{x}$  is  $n \times 1$  and  $\mathbf{b}$  is  $m \times 1$ .
- $\mathbf{A}=\mathbf{USV}^t$  where  $\mathbf{U}$  is  $m \times m$ ,  $\mathbf{S}$  is  $m \times n$  and  $\mathbf{V}$  is  $n \times n$
- $\mathbf{USV}^t \mathbf{x}=\mathbf{b}$ . So  $\mathbf{SV}^t \mathbf{x}=\mathbf{U}^t \mathbf{b}$
- If  $\mathbf{A}$  has rank  $r$ , then  $r$  singular values are significant

$$\mathbf{V}^t \mathbf{x} = \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \mathbf{U}^t \mathbf{b}$$

$$\mathbf{x} = \mathbf{V} \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \mathbf{U}^t \mathbf{b}$$

$$\mathbf{x}_r = \sum_{i=1}^r \frac{\mathbf{u}_i^t \mathbf{b}}{\sigma_i} \mathbf{v}_i \quad \sigma_r > \varepsilon, \quad \sigma_{r+1} \leq \varepsilon$$

- Pseudoinverse  $\mathbf{A}^+ = \mathbf{V} \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \mathbf{U}^t$

–  $\mathbf{A}^+$  is a  $n \times m$  matrix.

– If  $\text{rank}(\mathbf{A}) = n$  then  $\mathbf{A}^+ = (\mathbf{A}^t \mathbf{A})^{-1} \mathbf{A}$

– If  $\mathbf{A}$  is square  $\mathbf{A}^+ = \mathbf{A}^{-1}$

## $Q^\sim$ forms Nullspace of $(A^t)$

- Choose  $z$  in nullspace of  $A^t$
- Let  $A^t z = 0$ 
  - $(Q'R')^t z = R'^t Q'^t z = 0$
  - So  $R^t y = 0$  for  $y = Q^t z$
  - If  $R$  is full rank this means  $y$  has to be the zero vector
  - So  $Q^t z = 0$
  - So  $z$  must be composed of the elements from  $Q^\sim$
  - So the columns of  $Q^\sim$  form an orthonormal basis for  $\text{nullspace}(A^t)$