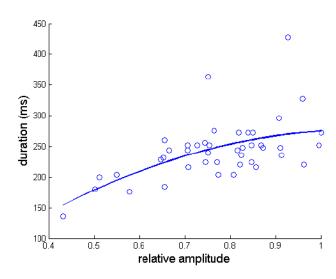
# Chapter 3 Overdetermined linear systems



# 3.1 Fitting Functions to Data Overdetermined linear systems

- In many situations, we want to put a simple curve through data
- We discussed interpolating data previously, but there would be relatively little data for this.
- For interpolating a quadratic curve, with three constants to find, we would need  $(x_i,y_i)$  for j=1,2,3
- We would then have the right number of equations (3) to find the coefficients for  $f(x) = a_1x^2 + a_2x + a_3$  to pass through the data
- In that case, we would have to solve  $y_j = f(x_j)$  for j=1,2,3 for the  $a_j$

• The system is of the following form, with n=m=3:

$$\begin{bmatrix} t_1^{n-1} & t_1^{n-2} & \cdots & t_1 & 1 \\ t_2^{n-1} & t_2^{n-2} & \cdots & t_2 & 1 \\ t_3^{n-1} & t_3^{n-2} & \cdots & t_3 & 1 \\ \vdots & \vdots & & \vdots & \vdots \\ t_n^{n-1} & t_n^{n-2} & \cdots & t_n & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

 But, there are many cases where there is too much data to interpolate because the oscillation of polynomials would be a poor model

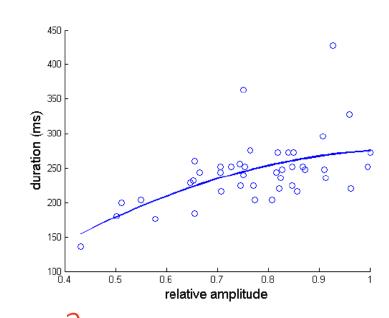
- When there is more data, we have n < m, and sometimes n << m
- The system is still of the form:

$$\begin{bmatrix} t_1^{n-1} & t_1^{n-2} & \cdots & t_1 & 1 \\ t_2^{n-1} & t_2^{n-2} & \cdots & t_2 & 1 \\ t_3^{n-1} & t_3^{n-2} & \cdots & t_3 & 1 \\ \vdots & \vdots & & \vdots & \vdots \\ t_n^{n-1} & t_n^{n-2} & \cdots & t_n & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

• How to solve? Find the  $a_j$  to minimize the distance from the data to the curve:

$$\min_{a} \sum_{i=1}^{n} [y_i - (a_1 x_i^2 + a_2 x_i + a_3)]^2$$

- Example: eye blink durations  $(y_j)$  and amplitudes  $(x_j)$  with m=43 blinks
- We want to put a quadratic through the data
- Solving the equation and plotting the quadratic and data gives plot at right
- One could rightly wonder if a different function could fit the data better here



How to solve these problems?

$$\min_{a} \sum_{i=1}^{n} [y_i - (a_1 x_i^2 + a_2 x_i + a_3)]^2$$

- For this minimization problem, we could compute the partial derivative with respect to each a\_j and set the derivative equal to zero.
- Solving those equations would produce the coefficients and thus the function we seek.
- Linear least squares are often approached this way.
- We want to focus on a more linear algebra oriented approach

# Overdetermined systems

More generally, we can seek linear combos of functions for fitting

$$f(t) = c_1 f_1(t) + \dots + c_n f_n(t)$$

• For this minimization problem, we consider the residual

$$R(c_1,\ldots,c_n) = \sum_{i=1}^m [y_i - f(t_i)]^2$$

• From linear algebra,  $R = \mathbf{r}^T \mathbf{r}$ , and we can write the following...

#### Overdetermined systems

More generally, we can seek linear combos of functions for fitting

$$\mathbf{r} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{m-1} \\ y_m \end{bmatrix} - \begin{bmatrix} f_1(t_1) & f_2(t_1) & \cdots & f_n(t_1) \\ f_1(t_2) & f_2(t_2) & \cdots & f_n(t_2) \\ \vdots \\ f_1(t_{m-1}) & f_2(t_{m-1}) & \cdots & f_n(t_{m-1}) \\ f_1(t_m) & f_2(t_m) & \cdots & f_n(t_m) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$$

- Now  $\mathbf{r}^T\mathbf{r} = \|\mathbf{r}\|_2^2$  so that, for  $A = \mathbb{R}^{m \times n}$ , we solve  $\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{b} \mathbf{A}\mathbf{x}\|_2^2$
- The unknows **x** are the coefficients we seek
- Let's see how to do this...



# Overdetermined systems: The Normal Equations

- Let's take a linear algebraic view of the minimization problem
- To see how to solve the minimization problem consider Theorem 3.1: If x satisfies  $A^T(Ax b) = 0$ , then x solves the least squares problem  $\min_{x} ||b Ax||_2$

$$\begin{aligned} \|\mathbf{A}(\mathbf{x} + \mathbf{y}) - \mathbf{b}\|_{2}^{2} &= [(\mathbf{A}\mathbf{x} - \mathbf{b}) + (\mathbf{A}\mathbf{y})]^{T} [(\mathbf{A}\mathbf{x} - \mathbf{b}) + (\mathbf{A}\mathbf{y})] \\ &= (\mathbf{A}\mathbf{x} - \mathbf{b})^{T} (\mathbf{A}\mathbf{x} - \mathbf{b}) + 2(\mathbf{A}\mathbf{y})^{T} (\mathbf{A}\mathbf{x} - \mathbf{b}) + (\mathbf{A}\mathbf{y})^{T} (\mathbf{A}\mathbf{y}) \\ &= \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_{2}^{2} + 2\mathbf{y}^{T} \mathbf{A}^{T} (\mathbf{A}\mathbf{x} - \mathbf{b}) + \|\mathbf{A}\mathbf{y}\|_{2}^{2} \\ &= \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_{2}^{2} + \|\mathbf{A}\mathbf{y}\|_{2}^{2} \ge \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_{2}^{2}. \end{aligned}$$

- To make this work, we needed  $A^{T}(Ax b) = 0$ , or  $A^{T}Ax = A^{T}b$
- ullet These are the "normal equations": solve them for  $oldsymbol{x}$

- The normal equations  $A^TAx = A^Tb$  are a square linear system for x
- The theoretical solution is  $\mathbf{x} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}$
- We could write  $x = A^+b$ , where  $A^+ = (A^TA)^{-1}A^T$
- A<sup>+</sup> is the "pseudoinverse" of A
  - In MATLAB, it may be obtained from pinv(A)
  - Some properties of  $A^TA$  are important...

• Some properties of  $A^TA$  are important...

**Theorem 3.2.** For any real  $m \times n$  matrix **A** with  $m \ge n$ , the following are true:

- 1.  $A^T A$  is symmetric.
- 2.  $A^T A$  is singular if and only if the columns of A are linearly dependent. (Equivalently, we say that A is rank deficient, which means that the rank of A is less than n.)
- 3. If  $A^TA$  is nonsingular, then it is positive definite.
  - For 2, if  $A^TA$  is singular, then  $A^TAz = 0$  for nonzero z; we need to show that this happens only if A is singular. If we premultiply by  $z^T$ , then  $0 = z^TA^TAz = \left| |Az| \right|_2^2$ . This can only happen if Az = 0; if that happens, A is singular.

- To use the normal equations to solve the least squares problem, do the following:
  - 1. Compute  $N = A^T A$
  - 2. Compute  $z = A^T b$
  - 3. Solve the  $n \times n$  linear system Nx = z for x
- The computation is easy, but the conditioning is poor.
- In the homework, you are asked to prove that  $\kappa(A^TA) = \kappa(A)^2$ , so that the magnification of the residual may be large.

• Example: do a cubic fit to some data as follows

```
>> t = [1; 2; 3; 4; 5; 6];
>> y = [1.5; 3.9; 6; 13; 27; 30];
>> A = [t.^3 t.^2 t ones(size(t))];
>> N = A'*A
N =
       67171
                   12201
                                2275
                                             441
                                 441
                                              91
       12201
                    2275
        2275
                   441
                                  91
                                              21
         441
                      91
                                  21
```

• The columns of A are powers of t (a Vandermonde matrix).

- Example: do a cubic fit to some data
- The condition number for N is fairly large for only a  $4 \times 4$  matrix
- ullet Solving manually for the coefficients  $oldsymbol{a}$  is shown
- The residual for this approach is about 1e-11
- Using a=pinv(A)\*y, one gets a residual of about 3e-11, very similar
- Our error could be as bad as 1e6 larger

```
>> cond(N)
ans =
   2.1515e+06
>> cond(A)
ans =
   1.4668e+03
>> a = N \setminus (A'*y)
a =
   -0.4370
    5.4925
  -13.9276
   11.1333
 >> norm(A'*y-N*a)
 ans =
```

9.1803e-12

#### Normal Equations: better

- We can do a little bit better by using Cholesky factorization because  $A^TA$  is SPD
- We do less work finding only the single upper triangular matrix R

```
function x = lsnormal(A,b)
  % LSNORMAL Solve linear least squares by normal equations.
  % Input:
4 % A coefficient matrix (m by n, m>n)
5 % b right-hand side (m by 1)
6 % Output:
  % x minimizer of || b-Ax ||
  N = A'*A; z = A'*b;
10 R = chol(N);
11 	 w = forwardsub(R',z);
                                         % solve R'z=c
12 x = backsub(R,w);
                                         % solve Rx=z
```

- For polynomial fits, we need a Vandermonde matrix
- The columns are powers of t
- It's poorly conditioned whether using Cholesky factorization or not
- The underlying problem is that the columns are less different as *n* or the degree increases: try it.

```
n = [10:10:100]';
 condA 2 = zeros(size(n));
for k=1:length(n)
    t=[1:n(k)]';
    A=[t.^2 t ones(size(t))];
    condA 2(k) = cond(A, 2);
 end
 format short
 table(n,condA 2)
```

#### Overdetermined systems: better

- We need a better way to compute a least squares fit for many problems.
- We can make use of a factorization that creates a matrix with orthonormal columns (an ONC matrix).
- First, consider why an ONC matrix is good.
- If we make orthonormal columns, the conditioning is the best we can do
- In comparison, the Vandermonde matrix is poorly conditioned, but we convert it into something much better

- Consider a set of vectors  $q_1$ , ...,  $q_k$ .
- Orthogonal if  $q_i^T q_i = 0$ , if  $i \neq j$ , and nonzero if i = j
- Orthonormal if  $q_i^T q_i = 1$ , for all i = 1, ..., k
- Consider square of difference of two vectors:

$$\|\mathbf{q}_1 - \mathbf{q}_2\|^2 = (\mathbf{q}_1 - \mathbf{q}_2)^T (\mathbf{q}_1 - \mathbf{q}_2)$$
  
=  $\mathbf{q}_1^T \mathbf{q}_1 - 2\mathbf{q}_1^T \mathbf{q}_2 + \mathbf{q}_2^T \mathbf{q}_2 = \|\mathbf{q}_1\|^2 + \|\mathbf{q}_2\|^2$ .

• The difference term drops out: this avoids subtractive cancellation where the difference term becomes negligible

• Now make a  $k \times k$  matrix Q with ONCs:  $q_1, ..., q_k$ .

$$\mathbf{Q}^{T}\mathbf{Q} = \begin{bmatrix} \mathbf{q}_{1}^{T} \\ \mathbf{q}_{2}^{T} \\ \vdots \\ \mathbf{q}_{k}^{T} \end{bmatrix} \begin{bmatrix} \mathbf{q}_{1} & \mathbf{q}_{2} & \cdots & \mathbf{q}_{k} \end{bmatrix} = \begin{bmatrix} \mathbf{q}_{1}^{T}\mathbf{q}_{1} & \mathbf{q}_{1}^{T}\mathbf{q}_{2} & \cdots & \mathbf{q}_{1}^{T}\mathbf{q}_{k} \\ \mathbf{q}_{2}^{T}\mathbf{q}_{1} & \mathbf{q}_{2}^{T}\mathbf{q}_{2} & \cdots & \mathbf{q}_{2}^{T}\mathbf{q}_{k} \\ \vdots & \vdots & & \vdots \\ \mathbf{q}_{k}^{T}\mathbf{q}_{1} & \mathbf{q}_{k}^{T}\mathbf{q}_{2} & \cdots & \mathbf{q}_{k}^{T}\mathbf{q}_{k} \end{bmatrix}$$

- The resulting matrix is a  $k \times k$  identity matrix because only diagonal terms are non zero
- Inverse of ONC matrix is easy:  $\boldsymbol{Q}^{-1} = \boldsymbol{Q}^T$ !!

• For real-valued  $n \times k$  matrix  $\boldsymbol{Q}$  with ONCs, Theorem 3.3:

1. 
$$\mathbf{Q}^T \mathbf{Q} = \mathbf{I} (k \times k \text{ identity})$$

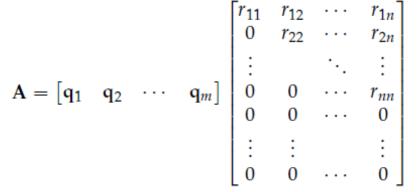
- 2.  $\|\mathbf{Q}\mathbf{x}\|_2 = \|\mathbf{x}\|_2$  for all k-vectors  $\mathbf{x}$ .
- 3.  $\|\mathbf{Q}\|_2 = 1$ .
- For part 2: using 2 norm,

$$\|\mathbf{Q}\mathbf{x}\|_{2}^{2} = (\mathbf{Q}\mathbf{x})^{T}(\mathbf{Q}\mathbf{x}) = \mathbf{x}^{T}\mathbf{Q}^{T}\mathbf{Q}\mathbf{x} = \mathbf{x}^{T}\mathbf{I}\mathbf{x} = \|\mathbf{x}\|_{2}^{2}.$$

- For real-valued  $n \times n$  matrix Q with ONCs, Theorem 3.4:
  - 1.  $\mathbf{Q}^T$  is also an orthogonal matrix.
  - 2.  $\kappa(\mathbf{Q}) = 1$  in the 2-norm.
  - 3. For any other  $n \times n$  matrix  $\mathbf{A}$ ,  $\|\mathbf{AQ}\|_2 = \|\mathbf{A}\|_2$ .
  - 4. If U is another  $n \times n$  orthogonal matrix, then QU is also orthogonal.
- Doesn't change the norm of a matrix either, and keeps a matrix orthogonal if it started that way

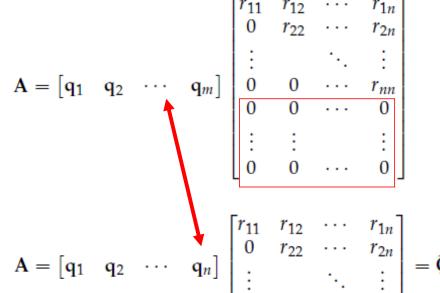
# Factoring A into QR

- Theorem 3.5: Every real-valued  $m \times n$  matrix A, with m > n, can be written as A=QR, where:
  - Q is an  $m \times m$  orthogonal matrix and
  - R is an  $m \times n$  upper triangular matrix
- The result has m orthonormal columns in Q and n nonzero rows for m>n



# Factoring *A* into *QR*

- When  $m \gg n$ , those zero rows in  $\mathbf{R}$ , and the last n+1: m columns in  $\mathbf{Q}$  are a waste
- A compressed version drops those rows of *R* and columns of *Q*
- The compressed form is used for solving the overdetermined system



# QR for overdetermined system

- Apply QR factorization to A in rectangular system
- Use compressed form

# Factoring *A* into *QR*

- Try what happens with different methods
- Start with vdmonde\_cond.m and vdmonde\_solns.m

```
% solution methods
% N = A'*A; z = A'*b; x comp = N\z;
% res sol(k) = norm(z-N*x comp,2);
x comp = lsnormal(A,b);
R = chol(A'*A);
 res sol(k) = norm(A'*b-(R'*R)*x comp,2);
% x comp = A b;
% res sol(k) = norm(b-A*x comp,2);
% x comp=lsqrfact(A,b);
% res sol(k) = norm(b-A*x comp,2);
```

#### How to compute the QR factorization?

- The underlying idea is simple. We want to build R by zeroing out each column below the diagonal.
- That part is like constructing U in the LU factorization.
- However, instead of L, we will build an orthogonal matrix Q instead.
- And, we have to be able to do this with rectangular matrices.
- Start with this idea: Can we create an orthogonal matrix that zeros the first column of the matrix A below  $A_{11}$ ?
- We want the norm of the original column to replace  $A_{11}$  too

• If we can do this with a matrix, say 
$$Q_1$$
, then we have changed  $A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} = [a_1 \ a_2 \ a_3]$ 

into (red is changed):

$$\mathbf{Q}_1 \mathbf{A} = \begin{bmatrix} ||\mathbf{a}_1|| & A_{12} & A_{13} \\ 0 & A_{22} & A_{23} \\ 0 & A_{32} & A_{33} \end{bmatrix}$$

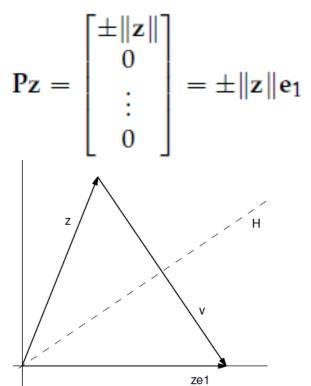
• For this discussion,  $\|a\| = \|a\|_2$  (norms are 2-norms)

• If we can do this for one column, then we could operate on the second column with, say  $Q_2$ , such that

second column with, say 
$$\mathbf{Q}_2$$
, such that 
$$\mathbf{Q}_2(\mathbf{Q}_1\mathbf{A}) = \begin{bmatrix} |\mathbf{a}_1|| & A_{12} & A_{13} \\ 0 & ||\widehat{\mathbf{a}}_2|| & A_{23} \\ 0 & 0 & A_{33} \end{bmatrix}$$

- For this small matrix, this would be **R**.
- In this case, we only operate on the red 2x2 submatrix, so that we don't mess up what we did with the first column.
- For larger matrices, we can do the same thing, and string more of the  $Q_j$  together; these are like the  $L_j$  in LU factorization

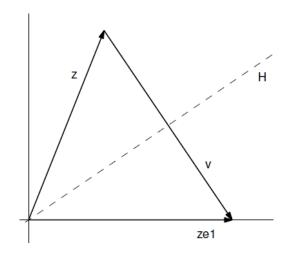
- Let's figure out how to do this for a single vector first.
- We want to find P to get the +/the norm of the vector times  $e_1$
- The vector z is given; define  $v = ||z||e_1 z$
- In terms of vectors, v connects z, the given vector, to what we want, which is  $\|z\|e_1$



- ullet H is a sketch of the orthogonal subspace to  $oldsymbol{v}$
- To get from z to  $||z||e_1$ , we are reflecting about H
- The matrix that does this is

$$P = I - 2 \frac{vv^T}{v^T v}, v \neq 0$$

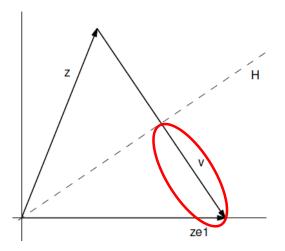
- Or P=I, v=0
- Note:  $\boldsymbol{v}\boldsymbol{v}^T$  is a matrix,  $\boldsymbol{v}^T\boldsymbol{v}$  scalar



- How does P work? (i.e., proof)
- First compute Pz
- The matrix that does this is

$$Pz = z - 2\frac{vv^{T}}{v^{T}v}z = z - 2\frac{z^{T}v}{v^{T}v}v$$

- But, the last term is twice the vector component of z in the v direction!
- So, by eye, this works great...



- This process is called a Householder reflection
- ullet The reflection is about the subspace H that is orthogonal to  $oldsymbol{v}$
- The reflection matrix P is both symmetric ( $P = P^T$ ) and orthogonal ( $P^T = P^{-1}$ )
- The size of P depends on the size of z: if  $z \in \mathbb{R}^{m \times 1}$  then  $P \in \mathbb{R}^{m \times m}$

• Proving it now, we need

$$\mathbf{v}^T \mathbf{v} = \|\mathbf{z}\|^2 - 2\|\mathbf{z}\|z_1 + \mathbf{z}^T \mathbf{z} = 2\|\mathbf{z}\|(\|\mathbf{z}\| - z_1),$$
  
 $\mathbf{v}^T \mathbf{z} = \|\mathbf{z}\|z_1 - \mathbf{z}^T \mathbf{z} = -\|\mathbf{z}\|(\|\mathbf{z}\| - z_1),$ 

Then we find

$$Pz = z - 2 \cdot \frac{-\|z\|(\|z\| - z_1)}{2\|z\|(\|z\| - z_1)}v = z + v = \|z\|e_1.$$

Just what we needed!

• Now, how to work with one column at a time in  $A \in \mathbb{R}^{m \times n}$ . m > n?

- There, the first column was  $a_1$ ; that replaces z, so that  $v = \|a_1\|e_1 a_1$
- And then, as before,

$$\boldsymbol{P}_1 = \boldsymbol{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}$$

• We define  $Q_1 = P_1$  now, so that the first column is  $||a_1||e_1$ , and in general all the other columns are modified.

- Let  $Q_1 A = A^{(1)}$ . For the second column, we choose to work with the  $m-1\times n-1$  submatrix  $A^{(1)}(2;m,2;n)$  (in Matlab notation)
- Then, we construct a new P, the column we work on is  $\hat{a}_2$

$$\widehat{\boldsymbol{a}}_2 = \boldsymbol{a}_2^{(1)}(2:m) = \boldsymbol{A}^{(1)}(2:m,2)$$

• This replaces z, so that

$$v = \|\widehat{a}_2\|e_1 - \widehat{a}_2$$

• And then, as before,

$$\boldsymbol{P}_2 = \boldsymbol{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}$$

• We define  $\mathbf{Q}_2 = \mathbf{I}_{m \times m}$  then set  $\mathbf{Q}_2(2:m,2:m) = \mathbf{P}_2$  now, so that the second column below  $A_{12}^{(1)}$  becomes  $\|\widehat{\boldsymbol{a}}_2\|\mathbf{e}_1$ , with the whole submatrix modified.

- Let  $Q_2Q_1A=A^{(2)}$ . For the third column (k=3), we choose to work with the  $m-2\times n-2$  submatrix  $A^{(2)}(3:m,3:n)$  (in Matlab notation)
- Then, we construct a new  $P = P_3$ , using  $v = \hat{a}_3$ , that is  $m 2 \times m 2$
- And then, as before,

$$\boldsymbol{P}_3 = \boldsymbol{I} - 2 \frac{\boldsymbol{v} \boldsymbol{v}^T}{\boldsymbol{v}^T \boldsymbol{v}}$$

• We keep going until we are done with the nth column, with  $\mathbf{Q}_k = \mathbf{I}_{m \times m}$  then set  $\mathbf{Q}_k(k; m, k; m) = \mathbf{P}_k$  until k = n is done

- Let  $Q_n \dots Q_2 Q_1 A = R$ .
- Then, the orthogonal matrix property is again very handy...
- Premultiplying by the transpose of each of those  $Q_{\underline{j}}$  and combining the product acting on R gives Q:

$$A = Q_1^T \dots Q_n^T R = QR, \qquad Q = Q_1^T \dots Q_n^T$$

- We can implement a simple version that constructs each of these matrices, but it is inefficient. Explore that first
- Matlab's qr function takes about  $(2mn^2 n^3)/3$  flops

```
Computing the QR factorization
```

```
Function
from text:
qrfact.m
```

```
2 % ORFACT OR factorization by Householder reflections.
3 % (demo only--not efficient)
4 % Input:
5 % A m-by-n matrix
  % Output:
   % Q,R A=QR, Q m-by-m orthogonal, R m-by-n upper triangular
  [m,n] = size(A):
10 Q = eye(m);
11 for k = 1:n
12 z = A(k:m,k);
  v = [-sign(z(1))*norm(z) - z(1); -z(2:end)];
14
  nrmv = norm(v):
15
    if nrmv < eps, continue, end % nothing is done in this iteration
16
    v = v / nrmv:
                                     % removes v'*v in other formulas
     % Apply the reflection to each relevant column of A and O
18
    for j = 1:n
19
     A(k:m,j) = A(k:m,j) - v*(2*(v'*A(k:m,j)));
20
     end
    for j = 1:m
     Q(k:m,j) = Q(k:m,j) - v*(2*(v'*Q(k:m,j)));
     end
24
   end
25
26
   0 = 0':
   R = triu(A);
                                      % enforce exact triangularity
```

1 function [0,R] = qrfact(A)

- Download grfact.m from Sakai (in files from book)
- Edit qrfact.m into a script or the function qrfactshow.m as in the handout you are given.
- Reproduce that example from qrfactshow.m
- If time permits, I will have additional data.