

Chap 3 Overdetermined Linear System

- Motivation
 - The least square problems
 - Solutions
 - Optimizing via LA & calculus
 - Normal equations
 - QR method for Least squares
 - Householder for QR
-] Mathematical viewpoints
-] Numerical viewpoints

- From linear system to least squares problem

$$A \mathbf{x} = \mathbf{b}$$

$$\min \| \mathbf{b} - A \mathbf{x} \|_2^2$$

To minimize the sum of
the squares of the residual

square linear system ($m=n$)

$$\boxed{\quad} = \boxed{\quad}$$

$$\| \boxed{\quad} - \boxed{\quad} \|_2^2 = \mathbf{x}$$

overdetermined linear system ($m > n$)

- Three views

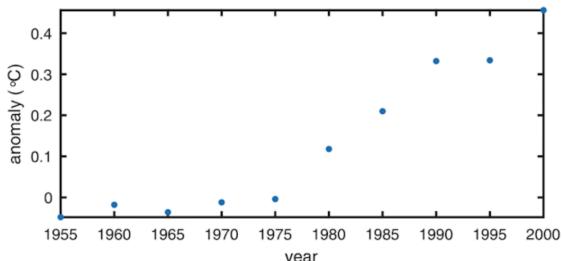
- Math: to minimize the inner product ($\|x\|_2^2 = (x^\top \cdot x)$)
- Stat: maximum likelihood
- Physics: 2-norm coincide energy, minimize in natural systems

§ 3.1 Fitting functions to data

- Example 3.1.1

Here are 5-year averages of the worldwide temperature anomaly as compared to the 1951–1980 average (source: NASA).

```
t = (1955:5:2000)';
y = [-0.0480; -0.0180; -0.0360; -0.0120; -0.0040;
     0.1180; 0.2100; 0.3320; 0.3340; 0.4560];
plot(t,y, '.')
```



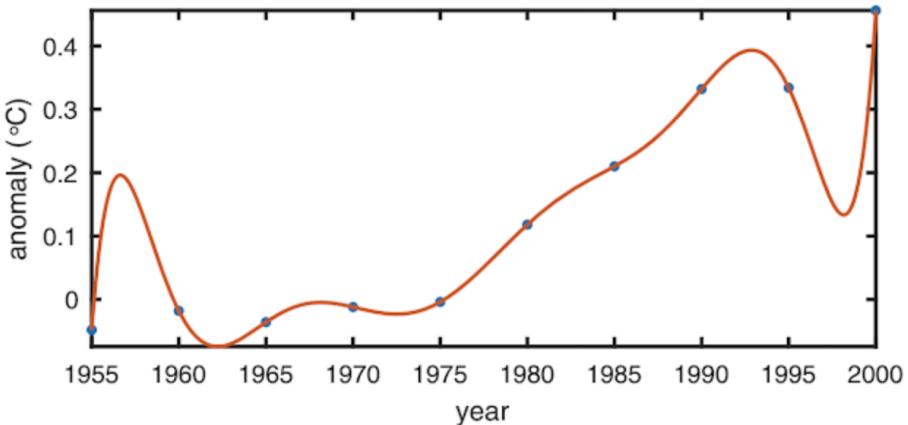
```

t = (t-1950)/10;
V = t.^0; % vector of ones
n = length(t);
for j = 1:n-1
    V(:, j+1) = t.*V(:, j);
end
c = V\y;
p = @(x) polyval(flipud(c), (x-1950)/10);
hold on, fplot(p,[1955 2000])

```

CHW] : To improve the condition [3
number of the matrix

To construct the Vandermonde matrix



Overfitting!

Try too hard to
reproduce the
data exactly.

- Sensitivity of higher order polynomial fitting

[Think] How to fix the overfitting problem?

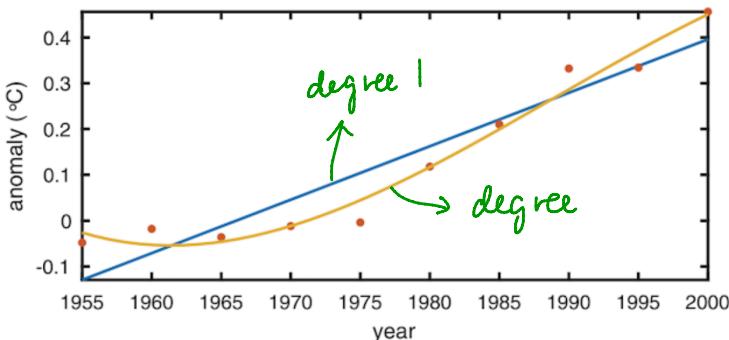
[Idea]: Smaller n (lower degree)

$$y \approx f(t) = c_1 + c_2 t + \cdots + c_{n-1} t^{n-2} + c_n t^{n-1}, \quad (3.1.1)$$

with $n < m$. Just as in (2.1.2), we can express a vector of f values by a matrix-vector multiplication:

$$\begin{bmatrix} f(t_1) \\ f(t_2) \\ f(t_3) \\ \vdots \\ f(t_m) \end{bmatrix} = \begin{bmatrix} 1 & t_1 & \cdots & t_1^{n-1} \\ 1 & t_2 & \cdots & t_2^{n-1} \\ 1 & t_3 & \cdots & t_3^{n-1} \\ \vdots & \vdots & & \vdots \\ 1 & t_m & \cdots & t_m^{n-1} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix}. \quad (3.1.2)$$

```
V = [ t.^0 t t.^2 t.^3]; % Vandermonde-ish matrix
c = V\y;
f = @(x) polyval(c(end:-1:1),x-1955);
fplot(f,[1955 2000])
```



$$m \begin{array}{|c|} \hline \end{array} = m \begin{array}{|c|c|} \hline n & n \\ \hline \end{array}$$

$$y = Vc$$

$$\Rightarrow y \approx Vc$$

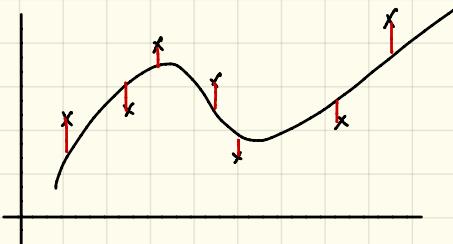
- The linear least squares formulation

$$f(t) = c_1 f_1(t) + c_2 f_2(t) + \dots + c_n f_n(t)$$

- Example : $f_1(t) = 1, f_2(t) = t, \dots, f_n(t) = t^{n-1}$
- The fit, $f(t)$, depends on the unknown parameters (c_1, \dots, c_n) linearly
- Nonlinear example : $f(t) = c_1 + c_2 e^{c_3 t}$

- Optimization : To minimize $R(c_1, \dots, c_n) = \sum_{i=1}^m [y_i - f(t_i)]^2$

Geometric :

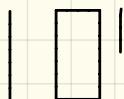


- [HW] Why not $|y_i - f(t_i)|$?

Matrix

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

$$\Rightarrow \underset{x \in \mathbb{R}^n}{\operatorname{argmin}} \|b - Ax\|_2^2$$



- Note: If $m = n$,
to solve $Ax = b \equiv$
 $\operatorname{argmin}_x \|b - Ax\|_2^2$

$$\because \|b - Ax\|_2^2 \geq 0$$

- Change of variables

$$- g(t) = a_1 e^{a_2 t} \Rightarrow \log y \approx \log g(t) = (\log a_1) + a_2 t$$

$$\Rightarrow \hat{y} = c_1 + c_2 t$$

$$- h(t) = a_1 t^a \Rightarrow \log y \approx \log h(t) = \log(a_1) + a_2 \log t$$

$$\Rightarrow \hat{y} = c_1 + c_2 \hat{t}$$

- MATLAB: semi log y, log log

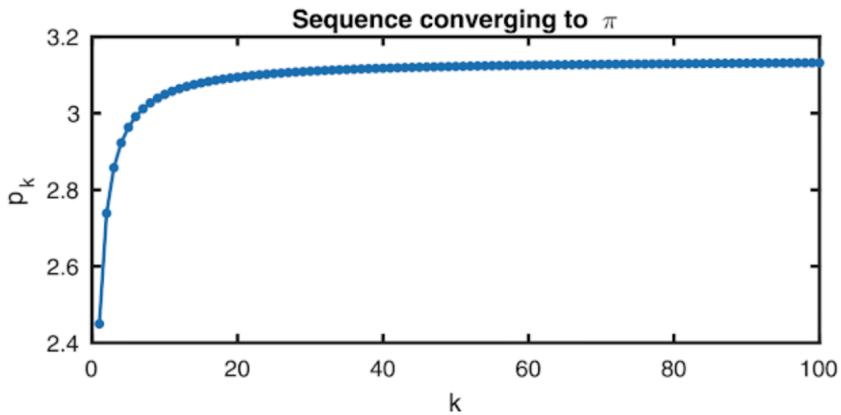
Example 3.1.3

Finding numerical approximations to π has fascinated people for millennia. One famous formula is

$$\frac{\pi^2}{6} = 1 + \frac{1}{2^2} + \frac{1}{3^2} + \dots$$

Say s_k is the sum of the first k terms of the series above, and $p_k = \sqrt{6s_k}$. Here is a fancy way to compute these sequences in a compact code.

```
k = (1:100)';
s = cumsum( 1./k.^2 ); % cumulative summation
p = sqrt(6*s);
plot(k,p,'.-')
xlabel('k'), ylabel('p_k')
title('Sequence converging to \pi')
```



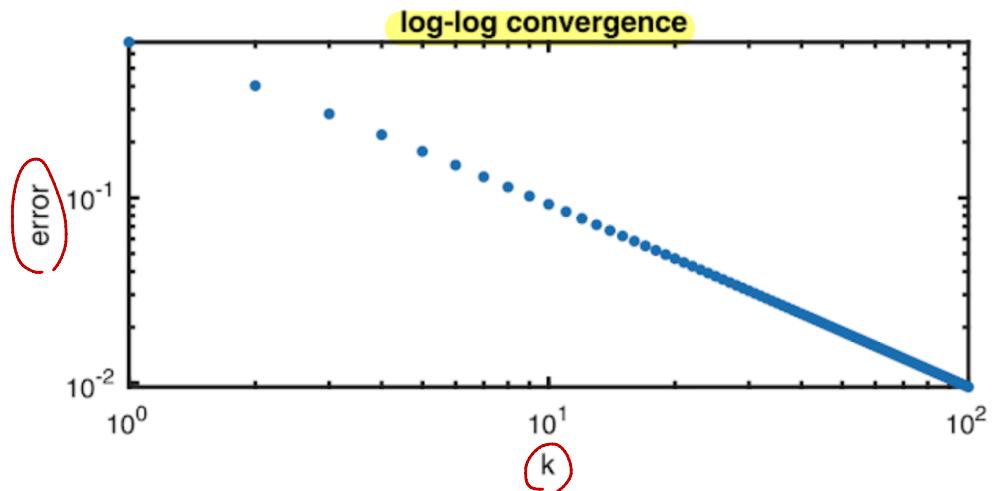
$$\pi^2 \approx 6 \left[1 + \dots + \frac{1}{k^2} \right]$$

$$\Rightarrow \pi \approx \underbrace{\sqrt{6 s_k}}_{P_k}$$

P_k : estimate π
by k terms

This graph suggests that $p_k \rightarrow \pi$ but doesn't give much information about the rate of convergence. Let $\epsilon_k = |\pi - p_k|$ be the sequence of errors. By plotting the error sequence on a log-log scale, we can see a nearly linear relationship.

```
ep = abs(pi-p); % error sequence
loglog(k,ep,'.'), title('log-log convergence')
xlabel('k'), ylabel('error'), axis tight
```



This suggests a power-law relationship where $\epsilon_k \approx ak^b$, or $\log \epsilon_k \approx b(\log k) + \log a$.

\log \log

```
V = [ k.^0, log(k) ]; % fitting matrix
c = V \ log(ep); % coefficients of linear fit
```

```
c =
-0.1824
-0.9674
```

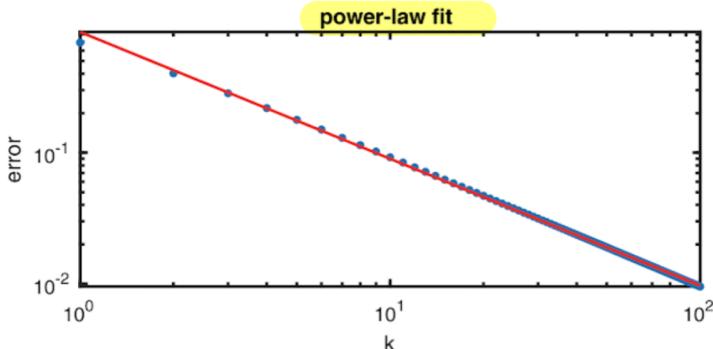
In terms of the parameters a and b used above, we have

```
a = exp(c(1)), b = c(2),
```

```
a =
0.8333
b =
-0.9674
```

It's tempting to conjecture that $b = -1$ asymptotically. Here is how the numerical fit compares to the original convergence curve.

```
hold on, loglog(k,a*k.^b,'r'), title('power-law fit')
```



Power-law fit

$$\varepsilon_k \approx a k^b$$

§ 3.2 The Normal Equations

- Matrix view

Theorem 3.2.1

If x satisfies $A^T(Ax - b) = 0$, then x solves the linear least squares problem, i.e., x minimizes $\|b - Ax\|_2$.

Proof. Let $y \in \mathbb{R}^n$ be any vector. Then $A(x + y) - b = Ax - b + Ay$, and

$$\begin{aligned}\|A(x + y) - b\|_2^2 &= [(Ax - b) + (Ay)]^T [(Ax - b) + (Ay)] \\ &= (Ax - b)^T (Ax - b) + 2(Ay)^T (Ax - b) + (Ay)^T (Ay) \\ &= \|Ax - b\|_2^2 + 2y^T A^T (Ax - b) + \|Ay\|_2^2 \\ &= \|Ax - b\|_2^2 + \|Ay\|_2^2 \\ &\geq \|Ax - b\|_2^2.\end{aligned}$$

□

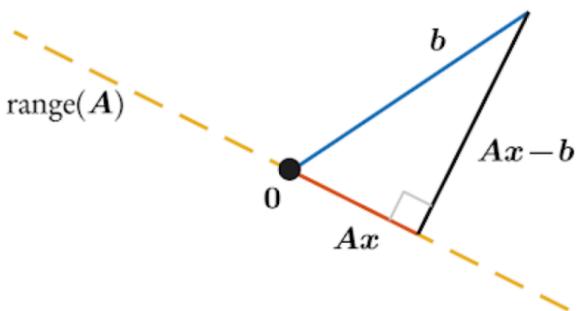
$$A^T(Ax - b) = 0$$

$$\Rightarrow \underbrace{A^T A x}_{\tilde{A} x} = \underbrace{A^T b}_{\tilde{b}}$$

$$\Rightarrow \tilde{A} x = \tilde{b}$$

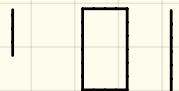
□ | |

- Geometric view



- **pseudoinverse:** $Ax \approx b \Rightarrow x = A^+b$

- MATLAB: $x = A \setminus b$ or $x = \text{pinv}(A) * b$



\uparrow

don't use! Just like $\text{inv}(A)$

Theorem 3.2.2

For any real $m \times n$ matrix A with $m \geq n$, 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, the rank of A is less than n .)
3. If $A^T A$ is nonsingular, then it is positive definite.

Proof. The first part is left as an exercise (Exercise 3.2.3). For the second part, suppose that $A^T A z = \mathbf{0}$. Note that $A^T A$ is singular if and only if z may be nonzero. Left-multiplying by z^T , we find that

$$0 = z^T A^T A z = (Az)^T (Az) = \|Az\|_2^2,$$

which is equivalent to $Az = \mathbf{0}$. Then z may be nonzero if and only if the columns of A are linearly dependent.

Finally, we can repeat the manipulations above to show that for any nonzero n -vector v , $v^T (A^T A)v = \|Av\|_2^2 \geq 0$, and equality is not possible thanks to the second part of the theorem. \square

Function 3.2.1 (lsnormal) Solve linear least squares by normal equations.

```
1 function x = lsnormal(A,b)
2 % LSNORMAL    Solve linear least squares by normal equations.
3 % Input:
4 %   A      coefficient matrix (m by n, m>n)
5 %   b      right-hand side (m by 1)
6 % Output:
7 %   x      minimizer of || b-Ax ||
8
9 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
```

In summary, the steps for solving the linear least squares problem $Ax \approx b$ are as follows:

1. Compute $N = A^T A$.
2. Compute $z = A^T b$.
3. Solve the $n \times n$ linear system $Nx = z$ for x .

- Conditioning and stability

- To solve $Ax = b$, the condition number is $\kappa(A) = \|A\| \cdot \|A^{-1}\|$

- To solve the L.S.P., $\Rightarrow \kappa(A) = \|A\| \cdot \|A^+\|$

If $\text{rank}(A) < n \Rightarrow \kappa(A) = \infty$

- To solve the normal equations $(A^T A)x = (A^T b)$

$\Rightarrow \kappa(A^T A) = \kappa(A)^2$ (see exercise 7.3.8 for proof)

Cond. # \neq square!

① Example 3.2.1

Because the functions $\sin^2(t)$, $\cos^2(t)$, and 1 are linearly dependent, we should find that the following matrix is somewhat ill-conditioned.

```
t = linspace(0,3,400)';
A = [ sin(t).^2, cos((1+1e-7)*t).^2, t.^0 ];
kappa = cond(A)

kappa =
1.8253e+07
```

②

Now we set up an artificial linear least squares problem with a known exact solution that actually makes the residual zero.

```
x = [1;2;1];
b = A*x;
```

Using backslash to find the solution, we get a relative error that is about κ times machine epsilon.

```
x_BS = A\b;
observed_err = norm(x_BS-x)/norm(x)
max_err = kappa*eps
```

```
observed_err =
1.3116e-10
max_err =
4.0530e-09
```

③

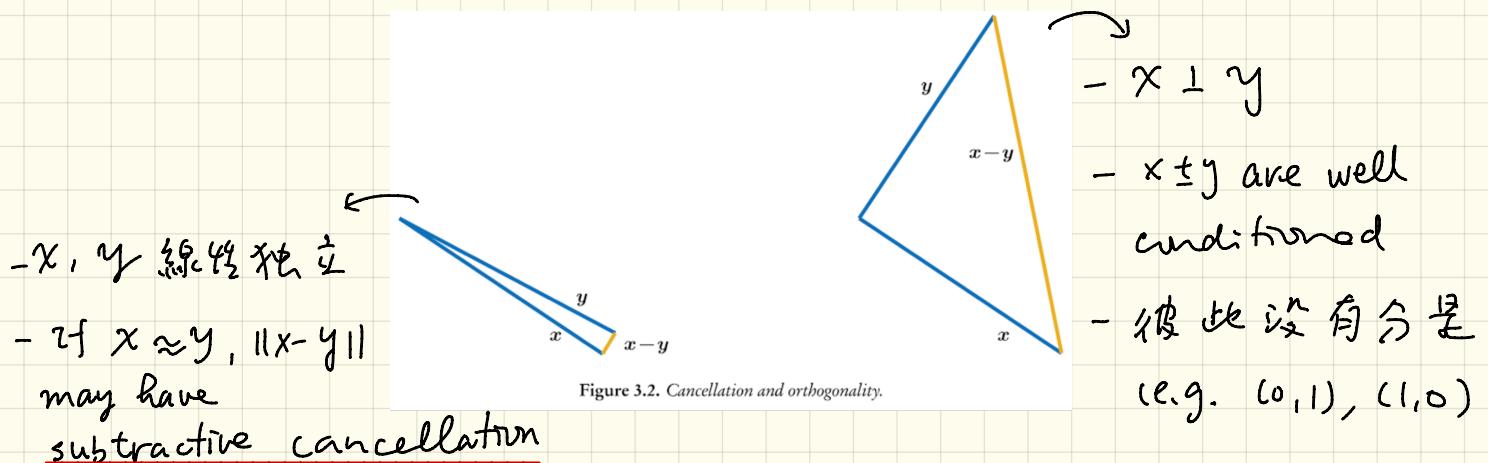
If we formulate and solve via the normal equations, we get a much larger relative error. With $\kappa^2 \approx 10^{14}$, we may not be left with more than about 2 accurate digits.

```
N = A'*A;
x_NE = N\ (A'*b);
observed_err = norm(x_NE-x)/norm(x)
digits = -log10(observed_err)
```

```
observed_err =
0.0150
digits =
1.8226
```

§ 3.3 QR factorization

- Orthogonal: $g_i^T g_j = 0, i \neq j$ (e.g. $U \perp V \Leftrightarrow U^T V = 0$)
- Orthonormal: $\begin{cases} g_i^T g_j = 0, \\ g_i^T g_i = 1 \text{ (i.e. } \|g_i\|_2 = 1) \end{cases}$



- Orthogonal matrix, orthonormal matrix

$$Q^T Q = \begin{bmatrix} q_1^T \\ q_2^T \\ \vdots \\ q_k^T \end{bmatrix} \begin{bmatrix} q_1 & q_2 & \cdots & q_k \end{bmatrix} = \begin{bmatrix} q_1^T q_1 & q_1^T q_2 & \cdots & q_1^T q_k \\ q_2^T q_1 & q_2^T q_2 & \cdots & q_2^T q_k \\ \vdots & \vdots & & \vdots \\ q_k^T q_1 & q_k^T q_2 & \cdots & q_k^T q_k \end{bmatrix} = \begin{bmatrix} \times & & & 0 \\ 0 & \times & \times & 0 \\ 0 & 0 & \ddots & \times \end{bmatrix}$$

Theorem 3.3.1

Suppose Q is a real $n \times k$ ONC matrix (matrix with orthonormal columns). Then

1. $Q^T Q = I$ ($k \times k$ identity);
2. $\|Qx\|_2 = \|x\|_2$ for all k -vectors x ; \Rightarrow 保長
3. $\|Q\|_2 = 1$.

Theorem 3.3.2

Suppose Q is an $n \times n$ real orthogonal matrix. Then

1. Q^T is also an orthogonal matrix;
2. $\kappa(Q) = 1$ in the 2-norm;
3. for any other $n \times n$ matrix A , $\|AQ\|_2 = \|A\|_2$;
4. if U is another $n \times n$ orthogonal matrix, then QU is also orthogonal.

Proof. The first part is derived above. The second part follows a pattern that has become well established by now:

$$\|Qx\|_2^2 = (Qx)^T (Qx) = x^T Q^T Q x = x^T I x = \|x\|_2^2.$$

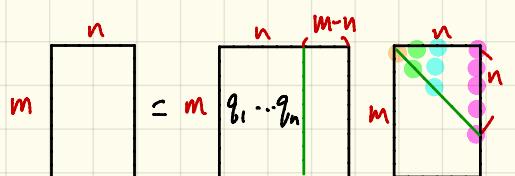
The last part of the theorem is left to the exercises. \square

- QR factorization

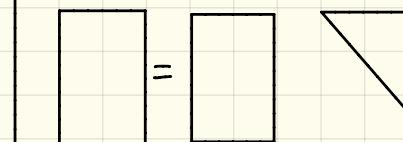
Theorem 3.3.3

Every real $m \times n$ matrix A ($m \geq n$) 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.

$$A = QR$$



$$A = \tilde{Q} \tilde{R} \quad (\text{Thin QR factorization})$$



- q_1, \dots, q_n 是 A 的 正交基底

$$a_1 \in \text{span}\{q_1\}$$

$$a_2 \in \text{span}\{q_1, q_2\}$$

⋮

$$a_n \in \text{span}\{q_1, q_2, \dots, q_n\}$$

係數：

係數：

係數：

[HW] How about LU?

Hint: L functions

總四步驟乙

基底

- Example 3.3.1

- | | | |
|-----------------|---------------------|----------|
| - Linear system | $Ax = b$ | $A = LU$ |
| least squares | $\min \ b - Ax\ _2$ | $A = QR$ |
- Normal equation: $A^T A x = A^T b$

① Cholesky factorization

$$(A^T A) = L L^T \quad \kappa(A^T A) = \kappa(A)^2$$

$$L L^T = \tilde{b}$$

② QR method

$$A = \hat{Q} \hat{R}$$

$$\cancel{\hat{R}^T} \cancel{\hat{Q}^T} \cdot \hat{Q} \hat{R} \cdot x = \cancel{\hat{R}^T} \cancel{\hat{Q}^T} b$$

$$\hat{R} x = \bar{b}$$

Function 3.3.1 (lsqrfact) Solve linear least squares by QR factorization.

```

1 function x = lsqrfact(A,b)
2 % LSQRFACT    Solve linear least squares by QR factorization.
3 % Input:
4 %   A      coefficient matrix (m by n, m>n)
5 %   b      right-hand side (m by 1)
6 % Output:
7 %   x      minimizer of || b-Ax ||
8
9 [Q,R] = qr(A,0);                      % compressed factorization
10 c = Q'*b;
11 x = backsub(R,c);

```

- Note : $x = A \setminus b$ solves the least squares problem

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- Note :

importantly, even though we derived (3.3.4) from the normal equations, *the solution of least squares problems via QR factorization does not suffer from the instability seen when the normal equations are solved directly using Cholesky factorization.*

§ 3.4 Computing QR factorization

- Hausholder reflection

P: orthogonal matrix

$$Px = \begin{bmatrix} \pm \|x\| \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \pm \|x\| \cdot e_1$$

外積, rank 1

$$P = I - 2 \frac{vv^\top}{v^\top v}, \text{ where } v = \|x\| e_1 - \underbrace{x}_{\text{normalization, } \|v\|_2^2}$$

- P is orthogonal

⇒ $\|x\|$

$$\|Px\|_2 = \|x\|_2$$

- Px 把 x "所有的重量" 集中在第一 $(1/2)$ component

I by rank-1 update

Theorem 3.4.1

Let $v = \|z\|e_1 - z$ and let P be given by (3.4.3). Then P is symmetric and orthogonal, and $Pz = \|z\|e_1$.

Proof. The case $v = 0$ is obvious. For $v \neq 0$, the proofs of symmetry and orthogonality are left to the exercises. As for the last fact, we simply compute

$$Pz = z - 2 \frac{vv^T z}{v^T v} = z - 2 \frac{v^T z}{v^T v} v, \quad (3.4.4)$$

and, since $e_1^T z = z_1$,

$$\begin{aligned} v^T v &= \|z\|^2 - 2\|z\|z_1 + z^T z = 2\|z\|(\|z\| - z_1), \\ v^T z &= \|z\|z_1 - z^T z = -\|z\|(\|z\| - z_1), \end{aligned}$$

leading finally to

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

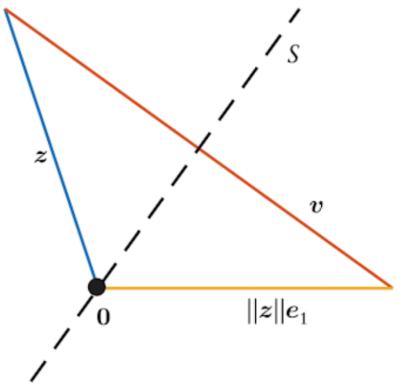


Figure 3.3. Action of a Householder reflector.

Step 1:

$$\left[P_1 \right] \left[\begin{array}{c|ccc} x & x & x \\ \hline x & x & x \\ x & x & x \\ \hline x & x & x \end{array} \right] = \left[\begin{array}{c|ccc} \bar{x} & \bar{x} & \bar{x} \\ \hline 0 & \bar{x} & \bar{x} \\ 0 & \bar{x} & \bar{x} \\ \hline 0 & \bar{x} & \bar{x} \end{array} \right]$$

Step 2 :

$$\left[\begin{array}{c|c} 1 & \\ \hline P_2 & \end{array} \right] \left[P_1 \right] \left[\begin{array}{c|ccc} x & x & x \\ \hline x & x & x \\ x & x & x \\ \hline x & x & x \end{array} \right] = \left[\begin{array}{c|c} 1 & \\ \hline P_2 & \end{array} \right] \left[\begin{array}{c|ccc} \bar{x} & \bar{x} & \bar{x} \\ \hline 0 & \bar{x} & \bar{x} \\ 0 & \bar{x} & \bar{x} \\ \hline 0 & \bar{x} & \bar{x} \end{array} \right]$$

$$= \left[\begin{array}{c|ccc} \bar{x} & \bar{x} & \bar{x} \\ \hline 0 & x' & x' \\ 0 & 0 & x' \\ 0 & 0 & x' \end{array} \right]$$

Step 3

$$= \begin{bmatrix} 1 & & \\ & 1 & \\ & & P_3 \end{bmatrix} \underbrace{\begin{bmatrix} 1 & & \\ & 1 & \\ & & P_2 \end{bmatrix}}_{\text{pink bracket}} \begin{bmatrix} & & \\ & P_1 & \\ & & \end{bmatrix} \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & \\ & 1 & \\ & & P_3 \end{bmatrix} \underbrace{\begin{bmatrix} \bar{x} & \bar{x} & \bar{x} \\ 0 & X' & X' \\ 0 & 0 & X' \\ 0 & 0 & X' \end{bmatrix}}_{\text{pink bracket}}$$

$$= \begin{bmatrix} \cancel{\bar{x}} & \cancel{\bar{x}} & \cancel{\bar{x}} \\ 0 & X' & X' \\ 0 & 0 & X'' \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} \cancel{\widehat{R}} \\ \underline{0} \end{bmatrix}$$

- $Q_{k|k} = \left[\begin{array}{c|c} I_{k-1} & 0 \\ \hline 0 & P_k \end{array} \right]$ is orthogonal!

$$Q_{k|k}^T Q_{k|k} = \left[\begin{array}{c|c} I_{k-1} & 0 \\ \hline 0 & P_k^T \end{array} \right] \left[\begin{array}{c|c} I_{k-1} & 0 \\ \hline 0 & P_k \end{array} \right] = \left[\begin{array}{c|c} I_{k-1} & 0 \\ \hline 0 & I_k \end{array} \right]$$

- $Q_3 Q_2 Q_1 A = \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}$

$$\underbrace{Q_1^T Q_2^T Q_3^T}_{\text{Q}} (Q_3 Q_2 Q_1) A = \underbrace{Q_1^T Q_2^T Q_3^T}_{\text{Q}} \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}$$

$Q^T Q = I$

$(Q_3 Q_2 Q_1) (Q_1^T Q_2^T Q_3^T) = I$

$$A = Q R$$

- Cost $\approx 2mn^2 - \frac{n^3}{3}$

Function 3.4.1 (qrfact) QR factorization by Householder reflections.

