TW776 Asst 4 - short answers

Least squares, GS, Householder

(a)

$$a + bx_1 + cy_1 = z_1$$
$$a + bx_2 + cy_2 = z_2$$
$$\vdots$$
$$a + bx_m + cy_m = z_m$$

$$\Rightarrow \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \vdots & & \\ 1 & x & \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{bmatrix}$$

(b)

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ -2 \\ 0 \end{bmatrix} \qquad (A\underline{x} = \underline{b})$$

NEs:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ -2 \\ 0 \end{bmatrix}$$

Normal Equations:

$$\begin{bmatrix} 4 & 4 & 2 \\ 4 & 6 & 3 \\ 2 & 3 & 2 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -2 \end{bmatrix} \qquad (A^T A \underline{x} = A^T \underline{b})$$

Solve: $a = -1/4, \quad b = \frac{3}{2}, \quad c = -3$

$$\underline{r} = \begin{bmatrix} 1/4 \\ -1/4 \\ -1/4 \\ 1/4 \end{bmatrix}, \quad \|\underline{r}\|_2 = \frac{1}{2}.$$

(b) Gram-S: $\underset{4\times 3}{A} = \underset{4\times 3}{Q}\,\underset{3\times 3}{R}$

$$[\underline{a}_1 \ \underline{a}_2 \ \underline{a}_3] = [\underline{q}_1 \ \underline{q}_2 \ \underline{q}_3]\begin{bmatrix} r_{11} & r_{12} & r_{13} \\ & r_{22} & r_{23} \\ & & r_{33} \end{bmatrix}$$

Compare col 1:

$$\underline{a}_1 = r_{11}\underline{q}_1$$

$$r_{11} = \|\underline{a}_1\| = 2, \quad \underline{q}_1 = \frac{1}{2}\underline{a}_1 = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$$

Compare col 2:

$$\underline{a}_2 = r_{12}\underline{q}_1 + r_{22}\underline{q}_2$$

$*\ q_1^T$:

$$\underline{q}_1^T \cdot \underline{a}_2 = r_{12}\underbrace{\underline{q}_1^T\underline{q}_1}_{1} + r_{22}\cancelto{0}{\underline{q}_1^T\underline{q}_2}$$

$$r_{12} = \underline{q}_1^T \cdot \underline{a}_2 = 2$$

$$\underline{a}_2 - 2\underline{q}_1 = r_{22}\underline{q}_2.$$

$$\begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = r_{22}\,q_2$$

$$r_{22} = \| \quad \|_2 = \sqrt{2}$$

$$\underline{q}_2 = \begin{bmatrix} -1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix}$$

Compare col 3: $\underline{a}_3 = r_{13}\underline{q}_1 + r_{23}\underline{q}_2 + r_{33}\underline{q}_3$

$* \ \underline{q}_1^T$: $\underline{q}_1^T\underline{a}_3 = r_{13}\underbrace{\underline{q}_1^T\underline{q}_1}_{1} + r_{23}\cancel{\underline{q}_1^T\underline{q}_2}^{0} + r_{33}\cancel{\underline{q}_1^T\underline{q}_3}^{0}$

$$r_{13} = \underline{q}_1^T\underline{a}_3 = 1$$

$* \ \underline{q}_2^T$ $\underline{q}_2^T\underline{a}_3 = r_{13}\cancel{\underline{q}_2^T\underline{q}_1}^{0} + r_{23}\underbrace{\underline{q}_2^T\underline{q}_2}_{1} + r_{33}\cancel{\underline{q}_2^T\underline{q}_3}^{0}$

$$r_{23} = \underline{q}_2^T \cdot \underline{a}_3 = 1/\sqrt{2}$$

$$\underline{a}_3 - r_{13}\underline{q}_1 - r_{23}\underline{q}_2 = r_{33}\underline{q}_3$$

$$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} - \begin{bmatrix} -1/2 \\ 0 \\ 0 \\ +1/2 \end{bmatrix} = r_{33}\underline{q}_3$$

$$\begin{bmatrix} 0 \\ -1/2 \\ 1/2 \\ 0 \end{bmatrix} = r_{33}\underline{q}_3$$

$$r_{33} = \| \quad \|_2 = 1/\sqrt{2}$$

$$\underline{q}_3 = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}$$

$$Q = \begin{bmatrix} 1/2 & -1/\sqrt{2} & 0 \\ 1/2 & 0 & -1/\sqrt{2} \\ 1/2 & 0 & 1/\sqrt{2} \\ 1/2 & 1/\sqrt{2} & 0 \end{bmatrix}, \quad R = \begin{bmatrix} 2 & 2 & 1 \\ 0 & \sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$$

$$A\underline{x} = \underline{b} \Rightarrow A^T A \underline{x} = A^T \underline{b}$$

$$A = QR, \ A^T = R^T Q^T \Rightarrow R^T R \underline{x} = R^T Q^T \underline{b}$$

$$\underline{x} = (R^T R)^{-1} R^T Q^T \underline{b} = R^{-1} \underbrace{(R^T)^{-1} R^T}_{I} Q^T \underline{b}$$

$$R\underline{x} = Q^T \underline{b}$$

$$\begin{bmatrix} 2 & 2 & 1 \\ 0 & \sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} -1/2 \\ 0 \\ -3/\sqrt{2} \end{bmatrix}$$

Back-substitution : $c = -3$, $b = 3/2$, $a = -1/4$ $\longrightarrow$

Householder:

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ +1 \\ -2 \\ 0 \end{bmatrix}$$

$\uparrow$
$\underline{z}$

$\alpha = \pm\|z\|_2 = \pm 2$; $\quad \underline{z} - \alpha \underline{e}_1 = \begin{bmatrix} +3 \\ 1 \\ 1 \\ 1 \end{bmatrix}$

For hand calculation it does not matter which sign; for floating pt implementation we'd choose the minus here since $z_1 = 1 > 0$

$$\underline{u} = \frac{1}{\sqrt{12}} \begin{bmatrix} 3 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$P_1 = \underset{4\times 4}{\underset{\sim}{I}} - 2\underline{u}\,\underline{u}^T$$

$$P_1 A \underline{x} = P_1 \underline{b}$$

$$\begin{bmatrix} -2 & -2 & -1 \\ 0 & \frac{1}{3} & -\frac{1}{3} \\ 0 & \frac{1}{3} & \frac{2}{3} \\ 0 & \frac{4}{3} & \frac{2}{3} \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ \frac{7}{6} \\ -\frac{11}{6} \\ \frac{1}{6} \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{4}{3} \end{bmatrix}}_{z}$$

$$\underline{z} = \frac{1}{3}\begin{bmatrix} 1 \\ 1 \\ 4 \end{bmatrix}, \quad \alpha = \pm \frac{\sqrt{18}}{3} = \pm\sqrt{2}$$

$-$ sign

$$\underline{z} - \alpha \underline{e}_1 = \begin{bmatrix} \frac{1}{3} + \sqrt{2} \\ \frac{1}{3} \\ \frac{4}{3} \end{bmatrix}$$

$$\underline{u} = \frac{z}{\|z\|} = \begin{bmatrix} 0.7860 \\ 0.1499 \\ 0.5997 \end{bmatrix}$$

$$P_2 = \left[\begin{array}{c|c} 1 & \\ \hline & \underbrace{I}_{3\times 3} - 2uu^T \end{array}\right]$$

$$P_2 \, P_1 \, A \, \underline{x} = P_2 \, P_1 \, \underline{b}$$

$$\begin{bmatrix} -2 & -2 & -1 \\ & -\sqrt{2} & -\frac{1}{\sqrt{2}} \\ & & 0.5984 \\ & & 0.3815 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ 0 \\ -2.0559 \\ -0.7235 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} 0.5984 \\ 0.3815 \end{bmatrix}}_{z}$$

$$\alpha = \pm \|z\|_2 = \pm\sqrt{2}, \quad \underline{z} - \alpha \underline{e}_1 = \begin{bmatrix} 1.3025 \\ 0.3815 \end{bmatrix}$$

$-$ sign

$$\underline{u} = \begin{bmatrix} 0.9597 \\ 0.2811 \end{bmatrix}$$

$$P_3 = \left[\begin{array}{cc|c} 1 & & \\ & 1 & \\ \hline & & I - 2uu^T \end{array}\right]$$

$$P_3 P_2 P_1 A \underline{x}_1 = P_3 P_2 P_1 \underline{b}$$

$$\left[\begin{array}{ccc} -2 & -2 & -1 \\ & -\sqrt{2} & -\frac{1}{\sqrt{2}} \\ & & -\sqrt{2} \\ \hline & & \end{array}\right] \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \left[\begin{array}{c} +\frac{1}{2} \\ 0 \\ \frac{3}{\sqrt{2}} \\ \hline \frac{1}{2} \end{array}\right] \begin{array}{l} \left.\right\} \text{Solve by back substit.} \\ c = -3,\ b = \frac{3}{2},\ a = -\frac{1}{4} \\ \text{— } \min \|\underline{r}\|_2 \end{array}$$

(e) For MATLAB output see next page

Least Squares, Gram-Schmidt, Householder

(e) Use the built-in least squares solver in your software system to solve the problem for the data

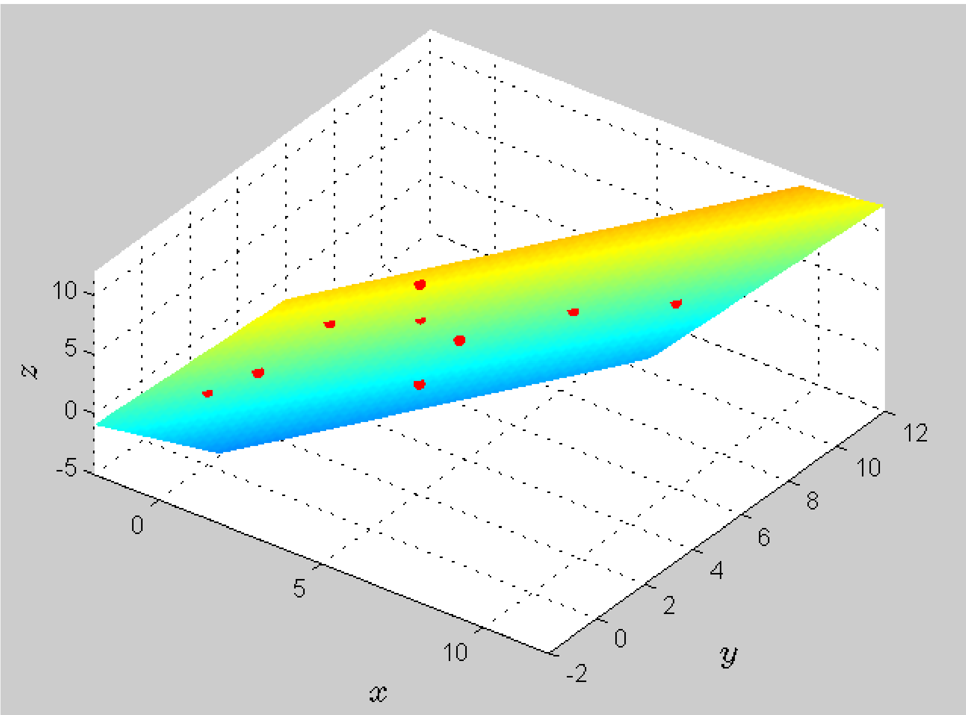
x	0	1.2	2.1	3.4	4.0	4.2	5.6	5.8	6.9
y	0	0.5	6.0	0.5	5.1	3.2	1.3	7.4	10.2
z	1.2	3.4	-4.6	9.9	2.4	7.2	14.3	3.5	1.3

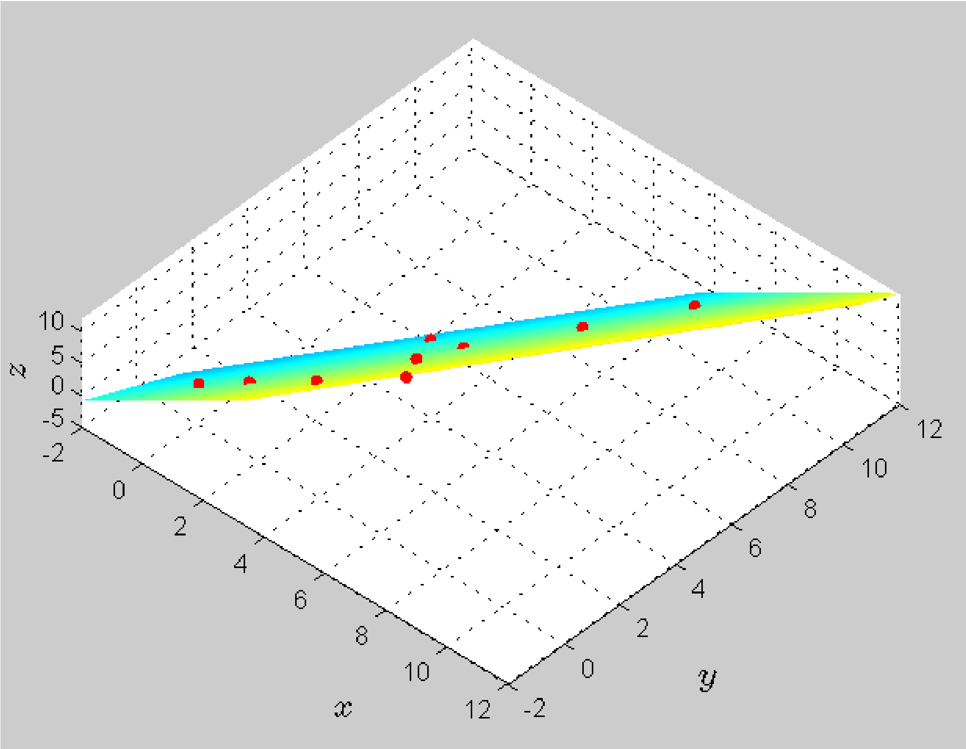
Give the values of a, b, c and $\|\boldsymbol{r}\|_2$. Now use the graphics capabilities of your software to plot the data points in xyz-space, and on the same set of axes the least squares fit $z = a + bx + cy$.

```
x = [0 1.2 2.1 3.4 4.0 4.2 5.6 5.8 6.9]';
y = [0 0.5 6.0 0.5 5.1 3.2 1.3 7.4 10.2]';
z = [1.2 3.4 -4.6 9.9 2.4 7.2 14.3 3.5 1.3]';
A = [ones(size(x)) x y];
sol = A\z; r = z-A*sol;
a = sol(1); b = sol(2); c = sol(3);
disp([a b c norm(r)])

  1.0399e+000   2.8530e+000 -1.9145e+000   5.6168e-001
```

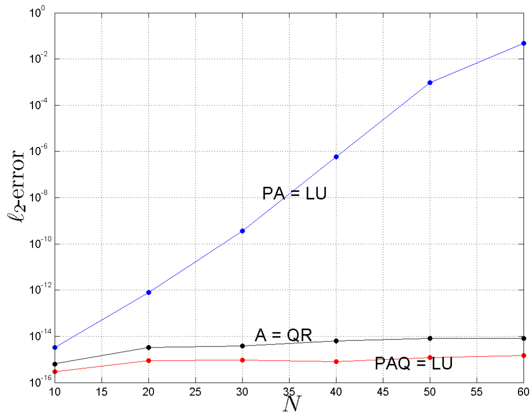
Two views (one from below the plane and the other from above)





Least Squares Methods for Square Systems

n	PA = LU	PAQ = LU	A = QR
10	3.2083e-015	2.9894e-016	6.4124e-016
20	7.7751e-013	9.0398e-016	3.2550e-015
30	3.6384e-010	9.5306e-016	3.7632e-015
40	5.7362e-007	8.0222e-016	6.4228e-015
50	9.3621e-004	1.2331e-015	8.1057e-015
60	4.7652e-002	1.5017e-015	8.0069e-015



From the above results it is clear that GE with partial pivoting is unstable for this matrix. GE with complete pivoting and QR are about equally stable. As for computational cost, the formula on p. 165 reduces to $\frac{4}{3}n^3$ if $m = n$, which means QR is about twice as expensive as GE. However, the operation count of $\frac{2}{3}n^3$ for GE did not include the cost of pivoting, which is not negligible in the case of complete pivoting. So in practice the speed of GE with complete pivoting and QR may not be very different.