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CAAM 550
HW 7
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Problem 1
part i
See Jupyter notebook for code and results.

part ii
The condition number of the normal equation (from Theorem 5.4.1) is $\kappa_2(A^TA) = (\sigma_1/\sigma_n)^2$. The condition number of the least squares problem using QR decomposition (from theorem 7.6.2) is $\kappa_2(A) = \sigma_1/\sigma_n$. In the charts, the condition number of each method is presented and it is clear that as t_0 increases, the condition number of both methods increase, but the condition number of the Normal equation increases much quicker than the condition number of the QR decomposition method. As a result the error of the normal solution method also grows quicker than the error when using the QR decomposition as t_0 increases.

Problem 2
part i
Multiplying out the given matrices produces the linear set of equations

$$\begin{aligned} r + Ax &= b \\ A^Tr &= 0 \end{aligned}$$

From the first equation then it is clear that $r = b - Ax$, so substituting into the second yields

$$\begin{aligned} A^T(b - Ax) &= 0 \\ A^Tb - A^TAx &= 0 \\ A^Tb &= A^TAx \end{aligned}$$

which is the normal equation. The solution to the normal equation is also the solution to the linear least squares problem

$$\min_x ||Ax - b||_2^2$$

so therefore these 2 problems are equivalent.

part ii
Multiplying out the given matrices produces the linear set of equations

$$\begin{aligned} r + Ax &= b \\ A^Tr &= 0 \end{aligned}$$

Using the first equation above,

$$\begin{aligned}
r + Ax &= b \\
r &= b - APP^{-1}x \\
r &= QQ^Tb - Q\begin{pmatrix} R \\ 0 \end{pmatrix} P^{-1}x \\
r &= Q[Q^Tb - \begin{pmatrix} R \\ 0 \end{pmatrix} P^{-1}x] \\
Q^Tr &= Q^Tb - \begin{pmatrix} R \\ 0 \end{pmatrix} P^{-1}x
\end{aligned}$$

Let $y = P^{-1}x \in \mathbb{R}^n$, and $(Q^Tr)_1, (Q^Tb)_1 \in \mathbb{R}^n$ be the upper n rows of Q^Tr and Q^Tb respectively, and similarly $(Q^Tr)_2, (Q^Tb)_2 \in \mathbb{R}^{m-n}$ be the last $m-n$ rows of Q^Tr and Q^Tb respectively. Then

$$\begin{bmatrix} (Q^Tr)_1 \\ (Q^Tr)_2 \end{bmatrix} = \begin{bmatrix} (Q^Tb)_1 \\ (Q^Tb)_2 \end{bmatrix} - \begin{pmatrix} Ry \\ 0 \end{pmatrix}$$

The top half of this equation can then be solved for y using back substitution:

$$Ry = (Q^Tb)_1 - (Q^Tr)_1$$

The solution x can then be found as

$$x = Py$$

part iii
Multiplying out the given matrices produces the linear set of equations

$$\begin{aligned}
r + Ax &= b \\
A^Tr &= 0
\end{aligned}$$

Using the first equation above,

$$\begin{aligned}
r + Ax &= b \\
r &= UU^Tb - U\Sigma V^Tx \\
r &= U(U^Tb - \Sigma V^Tx)
\end{aligned}$$

Let $z = V^Tx$, then

$$\begin{aligned}
U^Tr &= U^Tb - \Sigma z \\
\Sigma z &= U^Tb - U^Tr
\end{aligned}$$

Because Σ is a diagonal matrix, the components of z can be found as

$$z_i = (U^Tb - U^Tr)_i$$

Then the solution x can be found by calculating

$$x = Vz$$

Problem 3
part i
In the original problem,

$$A \in \mathbb{R}^{m\times 2} = \begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{pmatrix}$$

$$x \in \mathbb{R}^2 = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$b \in \mathbb{R}^m = \begin{pmatrix} b(t_1) \\ b(t_2) \\ \vdots \\ b(t_m) \end{pmatrix}$$

In the quadratic fit least squares,

$$\tilde{A} \in \mathbb{R}^{m\times 3} = \begin{pmatrix} 1 & t_1 & t_1^2 \\ 1 & t_2 & t_2^2 \\ \vdots & \vdots & \vdots \\ 1 & t_m & t_m^2 \end{pmatrix}$$

$$\tilde{x} \in \mathbb{R}^3 = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\tilde{b} \in \mathbb{R}^m = \begin{pmatrix} b(t_1) \\ b(t_2) \\ \vdots \\ b(t_m) \end{pmatrix}$$

Therefore it is plain that the first 2 columns of $\tilde{A}$, $\tilde{A}_{1,2} = A$, and $\tilde{b} = b$.

part ii
Because the Householder Reflectors are computed using the columns of A from left to right, the matrices Q_1 and Q_2 computed for A are identical to the matrices $\tilde{Q}_1$ and $\tilde{Q}_2$ computed for $\tilde{A}$ and can be reused in the QR Decomposition of $\tilde{A}$. Therefore only one additional Householder rotation is required to be calculated.

part iii
See Jupyter notebook for code and results.

Problem 4
part i
See Jupyter notebook for code and results.

part ii
Define $A \in \mathbb{R}^{mk,n}$ as the block matrix

$$A = \begin{bmatrix} H\exp(Bt_1) \\ H\exp(Bt_1) \\ \vdots \\ H\exp(Bt_m) \end{bmatrix}$$

Then let b be the stack of z vectors

$$b = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{pmatrix}$$

Then the solution x of the least squares problem

$$\min_x ||Ax - b||_2$$

is the best estimate of x_0.

part iii
See Jupyter notebook for code and results.

part iv
See Jupyter notebook for code and results.

part v
(See Jupyter notebook for calculations.) The largest singular value for the matrix A is $\sigma_1 \approx 1.29$, and the smallest non-zero singular value is $sigma_{44} \approx 1.84 \times 10^{-14}$. This leads to a very large conditioning number, $\kappa_2 \approx 6.99 \times 10^{12}$, which means that even a small error in the measurement data can lead to a very large error in the solution.