# STAT 309: MATHEMATICAL COMPUTATIONS I
# FALL 2022
# PROBLEM SET 3

**1.** Given a symmetric $A \in \mathbb{R}^{n\times n}$, $\mathbf{0} \neq \mathbf{x} \in \mathbb{R}^n$, and $\mathbf{b} \in \mathbb{R}^n$. Let

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

Consider the QR decomposition

$$[\mathbf{x}, \mathbf{r}] = QR$$

and observe that if $E\mathbf{x} = \mathbf{r}$, then

$$(Q^{\mathsf{T}} E Q)(Q^{\mathsf{T}}\mathbf{x}) = Q^{\mathsf{T}}\mathbf{r}.$$

Show how to compute a symmetric $E \in \mathbb{R}^{n\times n}$ so that it attains

$$\min_{(A+E)\mathbf{x}=\mathbf{b}} \|E\|_F,$$

where the minimum is taken over all symmetric $E$ (Note: The point here is that one must usually take into account that errors occurring in symmetric matrices must also be symmetric).

**2.** Let $A \in \mathbb{R}^{m\times n}$ and suppose its complete orthogonal decomposition is given by

$$A = Q_1 \begin{bmatrix} L & 0 \\ 0 & 0 \end{bmatrix} Q_2^{\mathsf{T}},$$

where $Q_1$ and $Q_2$ are orthogonal, and $L$ is an nonsingular lower triangular matrix. Recall that $X \in \mathbb{R}^{n\times m}$ is the unique pseudo-inverse of $A$ if the following Moore–Penrose conditions hold:
(i) $AXA = A$,
(ii) $XAX = X$,
(iii) $(AX)^{\mathsf{T}} = AX$,
(iv) $(XA)^{\mathsf{T}} = XA$
and in which case we write $X = A^{\dagger}$.
(a) Let

$$A^{-} = Q_2 \begin{bmatrix} L^{-1} & Y \\ 0 & 0 \end{bmatrix} Q_1^{\mathsf{T}}, \qquad Y \neq 0.$$

Which of the four conditions (i)–(iv) are satisfied?
(b) Prove that

$$A^{\dagger} = Q_2 \begin{bmatrix} L^{-1} & 0 \\ 0 & 0 \end{bmatrix} Q_1^{\mathsf{T}}$$

by letting

$$A^{\dagger} = Q_2 \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} Q_1^{\mathsf{T}}$$

and by completing the following steps:
- Using (i), prove that $X_{11} = L^{-1}$.
- Using the symmetry conditions (iii) and (iv), prove that $X_{12} = 0$ and $X_{21} = 0$.
- Using (ii), prove that $X_{22} = 0$.

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**3.** Let $A \in \mathbb{R}^{m\times n}$, $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{c} \in \mathbb{R}^n$. We are interested in the least squares problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|A\mathbf{x} - \mathbf{b}\|_2^2. \tag{3.1}$$

(a) Show that $\mathbf{x}$ is a solution to (3.1) if and only if $\mathbf{x}$ is a solution to the *augmented system*

$$\begin{bmatrix} I & A \\ A^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{r} \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}. \tag{3.2}$$

(b) Show that the $(m+n)\times(m+n)$ matrix in (3.2) is nonsingular if and only if $A$ has full column rank.

(c) Suppose $A$ has full column rank and the QR decomposition of $A$ is

$$A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}.$$

Show that the solution to the augmented system

$$\begin{bmatrix} I & A \\ A^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{c} \end{bmatrix}$$

can be computed from

$$\mathbf{z} = R^{-\mathsf{T}}\mathbf{c}, \qquad \begin{bmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \end{bmatrix} = Q^{\mathsf{T}}\mathbf{b},$$

and

$$\mathbf{x} = R^{-1}(\mathbf{d}_1 - \mathbf{z}), \qquad \mathbf{y} = Q \begin{bmatrix} \mathbf{z} \\ \mathbf{d}_2 \end{bmatrix}.$$

(d) Hence deduce that if $A$ has full column rank, then

$$A^{\dagger} = R^{-1}Q_1^{\mathsf{T}}$$

where $Q = [Q_1, Q_2]$ with $Q_1 \in \mathbb{R}^{m\times n}$ and $Q_2 \in \mathbb{R}^{m\times(m-n)}$. Check that this agrees with the general formula derived for a rank-retaining factorization $A = GH$ in the lectures.

**4.** Let $A \in \mathbb{R}^{m\times n}$. Suppose we apply QR with column pivoting to obtain the decomposition

$$A = Q \begin{bmatrix} R & S \\ 0 & 0 \end{bmatrix} \Pi^{\mathsf{T}}$$

where $Q$ is orthogonal and $R$ is upper triangular and invertible. Let $\mathbf{x}_B$ be the *basic solution*, i.e.,

$$\mathbf{x}_B = \Pi \begin{bmatrix} R^{-1} & 0 \\ 0 & 0 \end{bmatrix} Q^{\mathsf{T}}\mathbf{b},$$

and let $\hat{\mathbf{x}} = A^{\dagger}\mathbf{b}$. Show that

$$\frac{\|\mathbf{x}_B - \hat{\mathbf{x}}\|_2}{\|\hat{\mathbf{x}}\|_2} \le \|R^{-1}S\|_2.$$

(*Hint*: If

$$\Pi^{\mathsf{T}}\mathbf{x} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} \quad \text{and} \quad Q^{\mathsf{T}}\mathbf{b} = \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix},$$

consider the associated linearly constrained least-squares problem

$$\min \|\mathbf{u}\|_2^2 + \|\mathbf{v}\|_2^2 \quad \text{s.t. } R\mathbf{u} + S\mathbf{v} = \mathbf{c}$$

and write down the augmented system for the constrained problem).

**5.** Let $\mathbf{u} \in \mathbb{R}^n$, $\mathbf{u} \neq \mathbf{0}$. A *Householder* matrix $H_{\mathbf{u}} \in \mathbb{R}^{n\times n}$ is defined by

$$H_{\mathbf{u}} = I - \frac{2\mathbf{u}\mathbf{u}^{\mathsf{T}}}{\|\mathbf{u}\|_2^2}.$$

(a) Show that $H_{\mathbf{u}}$ is both symmetric and orthogonal.
(b) Show that for any $\alpha \in \mathbb{R}$, $\alpha \neq 0$,

$$H_{\alpha\mathbf{u}} = H_{\mathbf{u}}.$$

In other words, $H_{\mathbf{u}}$ only depends on the 'direction' of $\mathbf{u}$ and not on its 'magnitude'.
(c) In general, given a matrix $M \in \mathbb{R}^{n\times n}$ and a vector $\mathbf{x} \in \mathbb{R}^n$, computing the matrix-vector product $M\mathbf{x}$ requires $n$ inner products — one for each row of $M$ with $\mathbf{x}$. Show that $H_{\mathbf{u}}\mathbf{x}$ can be computed using only two inner products.
(d) Given $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$ where $\mathbf{a} \neq \mathbf{b}$ and $\|\mathbf{a}\|_2 = \|\mathbf{b}\|_2$. Find $\mathbf{u} \in \mathbb{R}^n$, $\mathbf{u} \neq \mathbf{0}$ such that

$$H_{\mathbf{u}}\mathbf{a} = \mathbf{b}.$$

(e) Show that $\mathbf{u}$ is an eigenvector of $H_{\mathbf{u}}$. What is the corresponding eigenvalue?
(f) Show that every $\mathbf{v} \in \operatorname{span}\{\mathbf{u}\}^{\perp}$ (cf. orthogonal complement in Homework **1**) is an eigenvector of $H_{\mathbf{u}}$. What are the corresponding eigenvalues? What is $\dim(\operatorname{span}\{\mathbf{u}\}^{\perp})$?
(g) Find the eigenvalue decomposition of $H_{\mathbf{u}}$, i.e., find an orthogonal matrix $Q$ and a diagonal matrix $\Lambda$ such that

$$H_{\mathbf{u}} = Q\Lambda Q^{\mathsf{T}}.$$

**6.** In this exercise, we will implement and compare Gram–Schmidt and Householder QR. Your implementation should be tailored to the program you are using for efficiency (e.g. vectorize your code in Matlab/Octave/Scilab). Assume in the following that the input is a matrix $A \in \mathbb{R}^{m\times n}$ with $\operatorname{rank}(A) = n \leq m$ and we want to find its full QR decomposition $A = QR$ where $Q \in \mathrm{O}(m)$ and $R \in \mathbb{R}^{m\times n}$ is upper-triangular.
(a) Implement the (classical) Gram–Schmidt algorithm to obtain $Q$ and $R$.
(b) Implement the Householder QR algorithm to obtain $Q$ and $R$. You should (i) store $Q$ implicitly, taking advantage of the fact that it can be uniquely specified by a sequence of vectors of decreasing dimensions; (ii) choose $\alpha$ in your Householder matrices to have the opposite sign of $x_1$ to avoid cancellation in $v_1$ (cf. notations in lecture notes).
(c) Implement an algorithm for forming the product $Q\mathbf{x}$ and another for forming the product $Q^{\mathsf{T}}\mathbf{y}$ when $Q$ is stored implicitly as in (b).
(d) For increasing values of $n$, generate an upper triangular $R \in \mathbb{R}^{n\times n}$ and a $B \in \mathbb{R}^{n\times n}$, both with random standard normal entries. Use your program's built-in function for QR factorization to obtain a random[1] $Q \in \mathrm{O}(n)$ from the QR factorization of $B$. Now form $A = QR$ and apply your algorithms in (a) and (b) to find the QR factors of $A$ — let these be $\widehat{Q}$ and $\widehat{R}$. Tabulate (using graphs with appropriate scales) the relative errors

$$\frac{\|R - \widehat{R}\|_F}{\|R\|_F}, \quad \frac{\|Q - \widehat{Q}\|_F}{\|Q\|_F}, \quad \frac{\|A - \widehat{Q}\widehat{R}\|_F}{\|A\|_F}, \quad \frac{\|I - \widehat{Q}^{\mathsf{T}}\widehat{Q}\|_F}{\|I\|_F}$$

for various values of $n$ and for each method. Scale $Q, R, \widehat{Q}, \widehat{R}$ appropriately so that $R$ and $\widehat{R}$ have positive diagonal elements. Note that the denominators $\|Q\|_F = \|I\|_F = \sqrt{n}$ cannot be omitted since they depend on $n$.
(i) Comment on the relative errors in $\widehat{Q}$ and $\widehat{R}$ (these are called forward errors) versus the relative error in $\widehat{Q}\widehat{R}$ and $\widehat{Q}^{\mathsf{T}}\widehat{Q}$ (these are called backward error; note that the latter measures a loss of orthogonality).
(ii) Comment on the relative error in $\widehat{Q}\widehat{R}$ and $\widehat{Q}^{\mathsf{T}}\widehat{Q}$ computed with Gram–Schmidt versus that computed with Householder QR.

[1] This is usually how one would generate a random orthogonal matrix.

(e) Generate a *Vandermonde matrix* and a vector,

$$A = \begin{bmatrix} 1 & \alpha_0 & \alpha_0^2 & \dots & \alpha_0^{n-1} \\ 1 & \alpha_1 & \alpha_1^2 & \dots & \alpha_1^{n-1} \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_{m-1} & \alpha_{m-1}^2 & \dots & \alpha_{m-1}^{n-1} \end{bmatrix} \in \mathbb{R}^{m\times n}, \quad \mathbf{b} = \begin{bmatrix} \exp(\sin 4\alpha_0) \\ \exp(\sin 4\alpha_1) \\ \exp(\sin 4\alpha_2) \\ \vdots \\ \exp(\sin 4\alpha_{m-1}) \end{bmatrix} \in \mathbb{R}^m,$$

where $\alpha_i = i/(m-1)$, $i = 0, 1, \dots, m-1$. This arises when we try to do polynomial fitting

$$e^{\sin 4x} \approx c_0 + c_1 x + c_2 x^2 + \cdots + c_{n-1} x^{n-1}$$

over the interval $[0, 1]$ at discrete points $x = 0, \frac{1}{m-1}, \frac{2}{m-1}, \dots, \frac{m-2}{m-1}, 1$. For $n = 15$ and $m = 100$, solve the least squares problem $\min\|A\mathbf{x} - \mathbf{b}\|_2$ and state your value of $c_{14}$ using each of the following methods:

(i) Applying QR factorization to $A$.

(ii) Applying QR factorization to the augmented matrix $[A, \mathbf{b}] \in \mathbb{R}^{m\times(n+1)}$.

(iii) Solving the normal equations $A^{\mathsf{T}} A\mathbf{x} = A^{\mathsf{T}}\mathbf{b}$.

For (i) and (ii), your code should show how the respective QR factors are used in obtaining a solution of the least squares problem. You are free to use your program's built-in functions (e.g., `A\b` in Matlab/Octave/Scilab) for solving linear systems but for other things, use what you have implemented in (a), (b), (c). The true value of $c_{14}$ is $2006.787453080206\dots$. Comment on the accuracy of each method and algorithm.