STAT 309: MATHEMATICAL COMPUTATIONS I
FALL 2017
PROBLEM SET 3

1. 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 Λ such that

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

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

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

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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 $X_{22} = 0$.

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. 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

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

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).

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 $\operatorname{rank}(A) = n \le m$ 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 α 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

$$\frac{\|R - \widehat{R}\|_F}{\|R\|_F}, \quad \|Q - \widehat{Q}\|_F, \quad \frac{\|A - \widehat{Q}\widehat{R}\|_F}{\|A\|_F},$$

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.

(i) Comment on the relative errors in $\widehat{Q}$ and $\widehat{R}$ (these are called forward errors) versus the relative error in $\widehat{Q}\widehat{R}$ (this is called backward error).

(ii) Comment on the relative error in $\widehat{Q}\widehat{R}$ 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,

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

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 . . . . Comment on the accuracy of each method and algorithm.