18.335 Midterm, Spring 2015

Problem 1: (10+(10+10) points)

- (a) Suppose you have a forwards-stable algorithm \tilde{f} to compute $f(x) \in \mathbb{R}$ for $x \in \mathbb{R}$, i.e. $\|\tilde{f}(x) f(x)\| = \|f\|O(\varepsilon_{\text{mach}})$. Suppose f is bounded below and analytic (has a convergent Taylor series) everywhere; suppose it has some global minimum $f_{\min} > 0$ at x_{\min} . Suppose that we compute x_{\min} in floating-point arithmetic by exhaustive search: we just evaluate \tilde{f} for all $x \in \mathbb{F}$ and return the x where \tilde{f} is smallest. Is this procedure stable or unstable? Why? (Hint: look at a Taylor series of f.)
- (b) Consider the function f(x) = Ax where $A \in \mathbb{C}^{m \times n}$ is an $m \times n$ matrix.
 - (i) In class, we proved that naive summation (by the obvious in-order loop) is stable, and in the book it was similarly proved that the function $g(x) = b^T x$ (dot products of x with \bar{b}) is backwards stable for $x \in \mathbb{C}^n$ when computed in the obvious loop \tilde{g} [that is: for each x there exists an \tilde{x} such that $\tilde{g}(x) = g(\tilde{x}) \text{ and } ||\tilde{x} - x|| = ||x|| O(\varepsilon_{\text{mach}})].$ Your friend Simplicio points out that each component f_i of f(x) is simply a dot product $f_i(x) = a_i^T x$ (where a_i^T is the *i*-th row of A)—so, he argues, since each component of f is backwards stable, f(x) must be backwards stable (when computed by the same obvious dot-product loop for each component). What is wrong with this argument (assuming m > 1)?
 - (ii) Give an example A for which f(x) is definitely *not* backwards stable for the obvious \tilde{f} algorithm.

Problem 2: (10+10+10 points)

In figure 1 are shown, from class, the classical/modified Gram–Schmidt (CGS/MGS) and Householder algorithms to compute the QR factorization $A = \hat{Q}\hat{R}$ (reduced: \hat{Q} is $m \times n$) or A = QR (Q is $m \times m$) respectively of an $m \times n$ matrix A. Recall that, using the QR factorization, we can solve the least-squares problem $\min ||Ax - b||_2$ by $\hat{R}\hat{x} = \hat{Q}^*b$. Recall that we can compute the right-hand side \hat{Q}^*b by forming an augmented $m \times (n+1)$ matrix $\check{A} = (A,b)$, finding its QR factorization $\check{A} = \check{Q}\check{R}$ and obtaining \hat{Q}^*b from the last column of $\check{R} = \check{Q}^*\check{A}$.

Classical/Modified Gram-Schmidt

$$\begin{aligned} &\text{for } j = 1 \text{ to } n \\ &v_j = a_j \\ &\text{for } i = 1 \text{ to } j - 1 \\ &\left\{ \begin{array}{l} r_{ij} = q_i^* \pmb{a_j} & \text{(CGS)} \\ r_{ij} = q_i^* \pmb{v_j} & \text{(MGS)} \\ v_j = v_j - r_{ij} q_i \\ r_{jj} = \|v_j\|_2 \\ q_j = v_j / r_{jj} \end{aligned} \right. \end{aligned}$$

Algorithm: Householder QR Factorization

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for k=1 to n x=A_{k:m,k} v_k=\mathrm{sign}(x_1)\|x\|_2e_1+x v_k=v_k/\|v_k\|_2 A_{k:m,k:n}=A_{k:m,k:n}-2v_k(v_k^*A_{k:m,k:n})
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Figure 1: Left: Classical/Modified Gram-Schmidt algorithm. Right: Householder QR algorithm. (Figures borrowed from Per Persson's 18.335 slides.)

Explain whether this procedure is better than computing \hat{Q}^*b directly for:

- (a) Classical Gram-Schmidt.
- (b) Modified Gram-Schmidt.
- (c) Householder QR. (Recall that, for Householder QR, we don't actually compute Q explicitly, but instead store the reflectors v_k and re-use them as needed to multiply by Q or Q^* .)

That is, each of the above three algorithms computes the QR factorization of A—for each of the three algorithms is it an improvement to compute \hat{Q}^*b via that algorithm on \check{A} compared with computing \hat{Q} (or its equivalent) by that algorithm and then performing the \hat{Q}^*b multiplication?

Problem 3: (10+20+10 points)

Suppose A and B are $m \times m$ matrices, $A = A^*$, $B = B^*$, and B is positive-definite. Consider the "generalized" eigenproblem of finding solutions $x \neq 0$ and λ to $Ax = \lambda Bx$, or equivalently solve the ordinary eigenproblem $B^{-1}Ax = \lambda x$. (In general, $B^{-1}A$ is *not*

Hermitian.) Suppose that there are m distinct eigenvalues $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_m|$ and corresponding eigenvectors x_1, \ldots, x_m .

- (a) Show that the λ_k are real and that $x_i^*Bx_j = 0$ for $i \neq j$. (Hint: multiply both sides of $Ax = \lambda Bx$ by x^* , similar to the derivation for Hermitian problems in class.)
- (b) Explain how to generalize the modified Gram–Schmidt algorithm (figure 1) to compute an "SR" factorization $B^{-1}A = SR$ where $S^*BS = I$. (That is, the columns s_k of S form a basis for the columns of $B^{-1}A$ as in QR, but orthogonalized so that $s_i^*Bs_j = 0$ for $i \neq j$ and = 1 for i = j.) Make sure your algorithm still requires $\Theta(m^3)$ operations!
- (c) In exact arithmetic, what would S in the SR factorization of $(B^{-1}A)^k$ converge to as $k \to \infty$, and why? (Assume the "generic" case where none of the eigenvectors happen to be orthogonal to the columns of B.)