MATH 571 Numerical Methods for Scientific Computing I Winter 2006

Assignment #4 due: Friday, March 10

page 62 (Gram-Schmidt orthogonalization) 8.2

page 76 (Householder QR factorization) 10.2 (reduced, not full), 10.3

1. Consider the overdetermined linear system: $x - y = 1,\ x + y = 0,\ x = 1$. Sketch the lines in the xy-plane. Find and plot the least squares solution.

2. The molecular weights of six nitric oxides (N_aO_b) were measured experimentally, yielding the results below. Using this data, perform a least squares fit to estimate the atomic weights of nitrogen and oxygen. You may use any method to solve the least squares problem.

NO (30.006), N_2O (44.013), NO_2 (46.006), N_2O_3 (76.012), N_2O_4 (92.011), N_2O_5 (108.010)

3. Prove.

a) $\kappa(A) \geq 1$ for any induced matrix norm

b) If U is unitary, then $\kappa_2(U) = 1,\ \kappa_2(UA) = \kappa_2(AU) = \kappa_2(A)$.

c) $\kappa_2(A) = \sigma_{\max}/\sigma_{\min}$

d) If A is hermitian, then $\kappa_2(A) = |\lambda|_{\max}/|\lambda|_{\min}$.

e) If $Ax = b$ and $(A + \delta A)(x + \delta x) = b$, then $\dfrac{||\delta x||/||x + \delta x||}{||\delta A||/||A||} \leq \kappa(A)$.

f) Consider the following example of $Ax = b,\ (A + \delta A)(x + \delta x) = b$.

$$\begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}, \quad \begin{pmatrix} 10 & 7 & 8.1 & 7.2 \\ 7.08 & 5.04 & 6 & 5 \\ 8 & 5.98 & 9.89 & 9 \\ 6.99 & 4.99 & 9 & 9.98 \end{pmatrix} \begin{pmatrix} -81 \\ 137 \\ -34 \\ 22 \end{pmatrix} = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$

Verify the arithmetic. Compute $\dfrac{||\delta x||_\infty/||x + \delta x||_\infty}{||\delta A||_\infty/||A||_\infty}$, $\kappa_\infty(A)$.

4. Consider the problem $f(x_1, x_2, x_3) = (x_1 + x_2) \times x_3$, evaluated by the algorithm $\widetilde{f}(x_1, x_2, x_3) = (\mathrm{fl}(x_1) \oplus \mathrm{fl}(x_2)) \otimes \mathrm{fl}(x_3)$. Show that the algorithm is backward stable. In deriving this result, you may assume that each individual floating point operation is backward stable, as shown in class. (More generally, it can be shown that the composition of two backward stable algorithms is backward stable.)

5. a) Repeat the steps on page 42 of the course lecture notes, illustrating the backward stability of Householder's algorithm for QR factorization using Matlab's `qr` command. Give the six numerical answers. Do your results agree with the results in the notes? Explain.

b) Repeat part (a) replacing Householder's algorithm by modified Gram-Schmidt using the function `mgs` created in exercise 8.2 above. Give the six numerical answers. Explain the similarities and differences in comparison with your results from part (a).

announcement: The midterm exam is on Monday, March 13, in class. It will cover the material from chapters 1-19 in the text (i.e. everything before Gaussian elimination). You may use one page of notes (one side). Calculators are not allowed (nor will they be needed).