TW776: Assignment 4 — For Thursday, 7 April

Assignment Guidelines

- Write a short report to illustrate your work. Use full sentences and include code snippets where applicable.
- Reports are to be handed in during the lecture on the due date.
- Feel free to discuss the work with your classmates, but write your own computer codes, generate your own figures, devise your own proofs and examples, and write your own report.
- It is acceptable to consult the library or internet on any problem. But if you do, it is important that you rewrite the material in your own words and cite your source.
- Unless told otherwise, use built-in functions in MATLAB or Python as far as possible. Do not write your own. This is not a course in programming.

Least Squares, Gram-Schmidt, Householder

In Ascher & Greif, Exercise 6.2 (p. 173) linear regression was discussed. The same technique can be used to fit a plane $z = a + bx + cy$ to a set of data (x_k, y_k, z_k), $k = 1, 2, \ldots, m$, where $m > 3$.

(a) Show that the problem can be formulated as the overdetermined system

$$\begin{pmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ \vdots & \vdots & \vdots \\ 1 & x_m & y_m \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{pmatrix}$$

(b) For the special set of data

x	0	1	1	2
y	0	0	1	1
z	0	1	-2	0

write down the overdetermined system. Also write down the normal equations, and use software to solve them to obtain estimates for a, b and c. Then compute the residual, $\boldsymbol{r}$, as well as $\|\boldsymbol{r}\|_2$.

(c) Apply the Gram-Schmidt procedure (by hand) to the matrix of part (b) to factor it into QR, where Q is 4×3 with orthogonal columns, and R is 3×3 and upper-triangular. Use this QR factorisation to solve the least squares problem, and confirm that the same result as in part (b) is obtained.

(d) Also apply Householder reflections (by hand) to solve the least squares problem directly (no need to factor into Q and R).

(e) Use the built-in least squares solver in your software system to solve the problem for the data

x	0	1.2	2.1	3.4	4.0	4.2	5.6	5.8	6.9
y	0	0.5	6.0	0.5	5.1	3.2	1.3	7.4	10.2
z	1.2	3.4	-4.6	9.9	2.4	7.2	14.3	3.5	1.3

Give the values of a, b, c and $\|\boldsymbol{r}\|_2$. Now use the graphics capabilities of your software to plot the data points in xyz-space, and on the same set of axes the least squares fit $z = a + bx + cy$.

Least Squares Methods for Square Systems

In Chapter 6, least squares methods were applied to the overdetermined system $A\boldsymbol{x} = \boldsymbol{b}$, where A is $m \times n$ and $m > n$. In principle nothing prevents one from applying Gram-Schmidt, MGS, or Householder to square linear systems $A\boldsymbol{x} = \boldsymbol{b}$, where A is $n \times n$. So instead of factoring A into LU it is factored into QR, and then

$$A\boldsymbol{x} = \boldsymbol{b} \qquad \Longrightarrow \qquad QR\boldsymbol{x} = \boldsymbol{b} \qquad \Longrightarrow \qquad R\boldsymbol{x} = Q^T\boldsymbol{b}.$$

The system on the right is then solved by back substitution. This is often the preferred approach if numerical stability is of prime importance, which is what we investigate here.

To investigate the stability of this method, use the built-in QR factorisation of your software system to implement the above procedure. Apply it to the Wilkinson matrix of Assignment 3, with the same right-hand side as was defined there. Calculate the ℓ_∞-error in the computed values of $\boldsymbol{x}$, for $n = 10, 20, 30, 40, 50, 60$. List the errors in a table, as well as in a log-linear plot (error vs n). How do these errors compare to those of GEPP and GECP? On the other hand, how does the theoretical operation count of this QR method compare to the $\sim \frac{2}{3}n^3$ of GE? Discuss. *Hint:* The operation count for the QR factorisation is given at the bottom of p. 165 in Ascher & Greif.