Department of Mathematics, University of Utah
Analysis of Numerical Methods I
MTH6610 – Section 001 – Fall 2017

Lecture notes: Least-squares problems
Monday, September 18, 2017

These notes are not a substitute for class attendance. Their main purpose is to provide a lecture overview summarizing the topics covered.

Reading: Trefethen & Bau III, Lectures 11

We consider a popular problem in numerical analysis: least-squares problems. Let $A \in \mathbb{C}^{m \times n}$ with $m \geq n$, and for a given $b \in \mathbb{C}^m$ suppose we wish to find the solution x to

$$Ax = b.$$

Unless A is square and invertible, one cannot find x satisfying this equality for arbitrary b. However, we can hope to find a solution that makes the residual $b - Ax$ as small as possible, where we need to defive "small" in a certain metric. Using the familiar ℓ^2 norm, we seek to solve the problem

$$\text{Find } x \text{ that minimizes the function } \|b - Ax\|_2$$

We say that this is the least-squares solution to the system $Ax = b$.

Theorem 1. *Let $A \in \mathbb{C}^{m \times n}$, $m \geq n$, be full rank. Then there is a unique least-squares solution to $Ax = b$ given by*

$$A^* A x = b \qquad \Longrightarrow \qquad x = \left(A^* A\right)^{-1} A^* b$$

Furthermore, the residual $r = Ax - b$ is orthogonal to $\text{range}(P)$.

The formula $A^* A x = A^* b$ defining the least-squares solution is the set of so-called *normal equations.* If A is full rank, then the reduced SVD of A is

$$A = \widetilde{U} \widetilde{\Sigma} \widetilde{V}^*,$$

and thus an equivalent formula for the least-squares solution is

$$x = \widetilde{V} \widetilde{\Sigma}^{-1} \widetilde{U}^* b.$$

We also note that if $A = QR$ is the QR factorization of A, then yet another formula for the least-squares solution is

$$x = \left(R^* R\right)^{-1} A^* b$$

While the normal equations provide an explicit formula, using the QR decomposition to solve this problem is a more stable algorithm. Finally, we note that much of the above can be generalized to a weighted least-squares problem of the form

$$WAx = Wb,$$

where W is a diagonal $m \times m$ matrix.
