Notes of a Numerical Analyst

Square or Rectangular?

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These interlocking pairs are on my mind:

square or rectangular matrices,
interpolation or least-squares,
algebra or analysis.

I see these as different aspects of a trend that is taking a century to unfold.

No idea is more fundamental in mathematics than solving equations, the starting point of algebra. If there are n linear equations in n unknowns, this leads to $n \times n$ square matrices:

$$Ax = b. \tag{1}$$

If the problem comes from fitting data, you are doing interpolation.

Very often, however, it is possible to examine the fit at $m > n$ points. This offers the option of $m \times n$ rectangular matrices and least squares:

$$Ax \approx b. \tag{2}$$

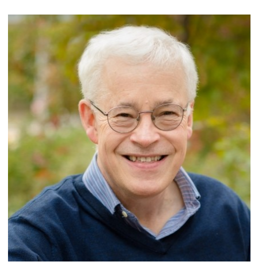
Now we are doing analysis, minimising an error norm. Many problems are capable of being generalised from square to rectangular, as in Eqs. (1) and (2). In my own work, an example has been the generalisation from eigenvalues (algebra) to pseudospectra (analysis).

Methods of algebra are often employed to solve problems of analysis (eigenvalues themselves are a giant example), but methods of analysis can be more robust. Just try interpolating equispaced function samples on an interval with polynomials. The result may be exponentially divergent, the 'Runge phenomenon'. Or try solving a discretised PDE by collocating in exactly n points; there is danger again. The scientific community has been decades slow to appreciate the easy robustness that comes with rectangular formulations. When Householder introduced his transformations in 1959, now the very hallmark of least-squares fitting, he presented them for $n \times n$ matrix inversion! Golub and others saw it better a few years later, but still, their definitions of QR factorisation and the singular value decomposition leaned on square factors rather than rectangular ones, leaving us successors to juggle expressions like 'skinny' and 'economy-sized' for the matrices we actually work with. As for me, it took me years to realise that the most natural setting of pseudospectra was rectangular, not square.

I have a theory about why we have been slow to embrace rectangular formulations. Since Gauss and Laplace, it has been known that least-squares fitting is a magical tool for dealing with noise, a discovery that helped launch the field of statistics. So that was the message we absorbed: least squares is about noise. We have been slow to see that the same robustness may be equally crucial when there is no noise. Least squares was used occasionally for scientific computing as early as the 1960s or 1970s, but not much. To this day, many people invite trouble by interpolating.

Cleve Moler, creator of backslash

And I have a hero to nominate. From the start in the late 1970s, Cleve Moler set up MATLAB so that `x = A\b` solves Eq. (1) if $m = n$ (by Gaussian elimination) and Eq. (2) if $m > n$ (by Householder reflectors). His introduction of the 'backslash' was one great move, and his silently giving it these two equal interpretations was another.



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