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One of the fundamental tenets of numerical linear algebra is to exploit matrix factorizations. Doing so has numerous benefits, ranging from allowing clearer analysis and deeper understanding to simplifying the efficient implementation of algorithms. Textbooks in numerical analysis and matrix analysis nowadays maximize the use of matrix factorizations, but this was not so in the first half of the 20th century. Golub has done as much as anyone to promulgate the benefits of matrix factorization, particularly the QR factorization and the singular value decomposition, and especially through his book *Matrix Computations* with Van Loan [28]. The five papers in this section illustrate several different facets of the matrix factorization paradigm.

On direct methods for solving Poisson's equations, by Buzbee, Golub, and Nielson [9]

Cyclic reduction is a recurring topic in numerical analysis. In the context of solving a tridiagonal linear system of order $2^n - 1$, the idea is to eliminate the odd-numbered unknowns, thus halving the size of the system, and to continue this procedure recursively until a single equation remains. One unknown can now be solved for and the rest are obtained by substitution. Cyclic odd-even reduction—to give it its full name—is thus a particular instance of the divide and conquer principle. The method was derived by Golub when he was a PhD student, but it became widely known only through Hockney's paper on solving the Poisson equation [32], in which he acknowledges the help of Golub.

This paper presents cyclic reduction for block tridiagonal systems arising in the discretization of Poisson's equation on a rectangle or L-shaped region with Dirichlet, Neumann, or periodic boundary conditions. The required properties of the coefficient matrix are essentially that it be symmetric block tridiagonal and block Toeplitz, with commuting blocks. Two variants of cyclic reduction are described. The first, more straightforward one (Section 3), is found to be "virtually useless" for practical computation, because of numerical instability, the nature of which is analyzed in Section 10. The second variant,

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suggested by Buneman, is shown to be mathematically equivalent to the first (Section 11), and to be numerically stable (Section 13).

At the time this work was done, iterative methods were prevalent for solving linear systems arising in the discretization of partial differential equations. The development of cyclic reduction and of methods exploiting the fast Fourier transform represented a shift back to direct methods and created the research topic of "fast Poisson solvers". Indeed Hockney [32] was able to solve Poisson's equation on a 48×48 mesh in 0.9 seconds on an IBM 7090, claiming a factor of 10 improvement in speed over the best iterative solvers of the time.

A flurry of papers followed this one, generalizing the method to irregular regions and to different equations. See Swartztrauber [43] for a list of references. Swartztrauber also gives a detailed analysis of the FACR(ℓ) method. This method, originally suggested by Hockney, carries out ℓ steps of cyclic reduction and then uses the fast Fourier transform to diagonalize the blocks of the reduced matrix (exploiting the fact that the blocks have the Fourier matrix as their eigenvector matrix), thereby producing a number of independent tridiagonal systems. He shows that by a suitable choice of ℓ, an operation count of $O(mn \log\log n)$ can be achieved, where the original matrix is block $n \times n$ tridiagonal with $m \times m$ blocks. This operation count beats the $O(mn \log n)$ count for cyclic reduction itself and is close to linear in the dimension of the matrix.

Cyclic reduction for a tridiagonal system $Ax = b$ is equivalent to Gaussian elimination on $(PAP^T)Px = Pb$, where P is a certain permutation matrix [31]. This connection has proved useful in some more recent error analyses of the method [1], [45].

Interest in cyclic reduction was rekindled by the advent of parallel computers, since the method produces smaller, independent "eliminated" systems that can be solved in parallel [33]. More recently, cyclic reduction has been applied to infinite block tridiagonal linear systems arising in the numerical solution of Markov chains, in which context it is called logarithmic reduction; for details and references see Bini, Latouche, and Meini [6, Chap. 7].

This is one of Golub's most highly cited papers. In 1992 it was deemed a Citation Classic by the Institute for Scientific Information, who collate the Science Citation Index. Buzbee wrote an article explaining the background to the paper [10]. The collaboration began when Golub visited Los Alamos National Laboratory and the three authors tried to understand a program written by Buneman for solving the Poisson equation "at a speed and accuracy that far exceeded established techniques such as relaxation and alternating directions". Understanding the numerical stability properties of the two variants of block cyclic reduction, and showing that they were mathematically equivalent, took some time. Buzbee notes that "Over a period of about 18 months, with no small amount of mathematical sleuthhounding, we completed this now-*Classic* paper. During that 18 months, we were tempted on several occasions to publish intermediate results. However, we continued to hold out for a full understanding, and, in the end, we were especially pleased that we waited until we had a comprehensive report."

The simplex method of linear programming using LU decomposition, by Bartels and Golub [4]

In the simplex method for linear programming, the basis matrix changes one column at a time, and some linear systems involving each new basis matrix are solved to determine the next basis change. By 1957, implementations were using sparse LU factors of an initial basis B_0 [35] and updating the factors a number of times before factorizing the current basis directly. The updates were in product form: $B_0 = LU$, $B_k = LUE_1E_2 \dots E_k$, where each E_k differs from the identity in only one column. (Most authors thought they were updating the *inverse* of each basis matrix, but the updates they used involved the same numbers as in the product form given here.) Bartels and Golub recognized that the product-form update is potentially unstable. They focused the linear programming community on the importance of maintaining numerical stability and the possibility of achieving it by updating the LU factors directly. Their method replaces the old column by the new column, effectively creating a "column spike" in the U factor, then cyclically permutes the spike to make it the last column of U, which becomes upper Hessenberg. Row operations, with row interchanges for stability, are performed to restore the upper triangular form. The L factor is updated in product form, but U is maintained as an explicit triangle.

Various LU updates were proposed by subsequent authors, most of whom were concerned with sparse problems. Forrest and Tomlin [15] store U column-wise and update it by deleting a column and row of U and adding a new column at the end, while generating a triangular matrix E_j^T (differing from the identity in only one row) to update L in product-form. This was soon recognized to be equivalent to the Bartels–Golub update but without any row interchanges for stability. (See Nocedal and Wright [37, Sec. 13.4] for an illustrated comparison of the methods.) Reid [40] stores U row-wise and applies the cyclic permutation to both the rows and columns of U, creating a "row spike" that tends to be sparse. Row operations are applied with row interchanges for stability, thus achieving a sparse form of the Bartels–Golub update with reasonable efficiency. Fletcher and Matthews [14] show how to update explicit LU factors in a stable way (keeping both L and U triangular), but sparsity cannot be preserved. Sparse forms of the Bartels–Golub update are in use today in Reid's code LA15 [39] and in LUSOL [19] (and hence in MINOS [36] and SNOPT [20]), but commercial linear programming codes flirt with instability by using the Forrest-Tomlin update because of an overriding desire for speed. Fortunately the Bartels–Golub viewpoint suggests a way to avoid significant instability: test if any element of E_j above is large, and if so refactorize rather than update.

A curious feature of the Bartels and Golub paper is that it does not describe the LU factorization updating that is proposed. Details of that are given in an earlier paper of the same authors on Chebyshev solution of overdetermined systems (the first paper in their reference list) and by Bartels [2], who gives a detailed error analysis of it. The present paper accompanies CACM Algorithm 250, an Algol 60 code that appears a few pages later in the same issue of the journal [3]. The Bartels–Golub method has comparable numerical stability properties to Gaussian elimination with partial pivoting, and so can in rare cases suffer from exponential error growth. A detailed analysis of this phenomenon is given by Powell [38], who constructs pathological examples for both the Bartels–Golub and the Fletcher–Matthews approaches.

Calculating the singular values and pseudo-inverse of a matrix, by Golub and Kahan [22]

The singular value decomposition (SVD) is today so widely used and ubiquitous that it is hard to imagine the computational scene in the early 1960s, when the SVD was relatively little known, its utility for solving a wide range of problems was unrecognized, and no satisfactory way of computing it was available. This paper helped bring the SVD to prominence by explaining two of its major applications, pointing out pitfalls in the more obvious methods of computation, and developing a strategy for a numerically stable SVD algorithm.

The paper begins by recalling the role of the pseudo-inverse in providing the minimum-norm solution to a linear least squares problem. The necessity and the difficulty of determining the rank when the matrix is (nearly) rank deficient are then pointed out, by arguments and examples that are now standard, but were only just beginning to be recognized. The use of the SVD to determine the pseudo-inverse and thereby to solve the rank-deficient least squares problem is advocated, along with the now standard device, motivated by the Eckart–Young theorem, of setting to zero any computed singular values that are negligible.

The paper makes two main algorithmic contributions. The first is the algorithm for bidiagonalizing a matrix by Householder transformations, given in Section 2. This provides a numerically stable reduction of the SVD problem to that of computing the SVD of a bidiagonal matrix. The second contribution builds on an observation of Lanczos [34, Sec. 3.7] that the eigenvalues of $C = \left[\begin{smallmatrix} 0 & A \\ A^* & 0 \end{smallmatrix}\right]$ are plus and minus the singular values of A. With A an upper bidiagonal matrix, Golub and Kahan note that C can be symmetrically permuted into a tridiagonal matrix by the operation (in MATLAB notation) $C(p, p)$, where $p = [n + 1,\ 1,\ n + 2,\ 2,\ \ldots,\ 2n,\ n]$. The available machinery for solving the symmetric tridiagonal eigenvalue problem is then applicable, and the last part of Section 3, and Section 4, concentrate on describing and adapting appropriate techniques (Sturm sequences and deflation). Here is where there is a surprise: the paper makes no mention at all of the QR algorithm. Yet a number of papers and textbooks state that this paper derives the complete SVD algorithm! In fact, how to adapt the Francis QR algorithm [16], [17] to the bidiagonal SVD was shown later by Golub in a less easily accessed paper [21], and the fine details were published in a Fortran code [8] and subsequently in [25].

Along with the Householder reduction to bidiagonal form, the use of the Lanczos method is mentioned at the end of Section 2, anticipating later work such as that in [23], where the Lanczos method would be developed for large-scale SVD computations.

Numerical methods for computing angles between linear subspaces, by Björck and Golub [7]

Björck and Golub's paper treats the problem of computing the principal angles between subspaces, along with associated principal vectors. This work is particularly aimed at the case where the subspaces are the ranges of given rectangular matrices. The key observation (Theorem 1) is that the cosines of the angles and the principal vectors are the singular values and transformed singular vectors of the matrix product $Q_1^* Q_2$, where the columns of Q_i form an orthonormal basis for the ith subspace. The authors propose computing the required orthonormal bases by Householder QR factorization or modified Gram–Schmidt.

The cosines of the angles are called canonical correlations in the statistics literature, and prior to this work they were computed via a "normal equations" eigenproblem. This paper is illustrative of the theme in Golub's work that orthogonalization methods should generally preferred because of their excellent numerical stability properties.

Björck and Golub go on to analyze the sensitivity of the problem, obtaining a perturbation bound for the errors in the angles that is proportional to the sum of the condition numbers of the two rectangular matrices. Armed with this information, they show via rounding error analysis that the numerical method produces results with forward error consistent with the perturbation bound. Special attention is given to the computation of small angles, since obtaining them via their cosines is not numerically reliable. The case of rank deficient matrices is also analyzed.

This is a remarkably thorough paper giving a beautiful, and relatively early, example of the power of the QR factorization and the SVD. It has hardly aged in the more than thirty years since publication. Only a few subsequent papers have attempted to improve upon or extend it. Golub and Zha [29] give a more detailed perturbation analysis, while in [30] they discuss equivalent characterizations of the principal angles and algorithms for large sparse or structured matrices. Drmač [13] shows that the Björck–Golub algorithm is mixed forward–backward stable: the computed singular values approximate with small relative error the exact cosines of the principal angles between the ranges of slight perturbations of the original two matrices.

Methods for modifying matrix factorizations, by Gill, Golub, Murray, and Saunders [18]

This paper treats the updating of the Cholesky factorization and the complete orthogonal decomposition after a rank-1 change, as well as (in the last section) updating of a QR factorization after the addition or deletion of rows or columns. Such changes are common in many applications, including in data fitting and signal processing problems, in which the data may be generated in real time. This paper was the first to emphasize the use of orthogonal transformations—particularly Givens transformations, which it uses extensively—and to give careful attention to the numerical stability of updating formulae. As such it has been very influential, as indicated by its being in Golub's top 10 most cited papers.

For Cholesky updating the rank-1 perturbation is allowed to be positive or negative semidefinite, but the perturbed matrix is assumed still to be positive definite. The case of a negative semidefinite perturbation can be tricky numerically, and in addition to the five different methods given here other methods have subsequently been proposed and analyzed, including ones based on hyperbolic transformations, which originate in an observation of Golub [26]. For an overview, see Stewart [41, Sec. 4.3].

It is tempting for the reader to skip over Section 2 of the paper, thinking that this is now standard material. However, Lemma 1 is not well known and new applications of it have recently been discovered. The lemma essentially says that the orthogonal QR factor of a tridiagonal matrix T has semiseparable structure—a property that can be exploited in computing trace(T^{-1}), for example [5].

Summary

This section has reviewed just five of Golub's contributions on matrix factorizations. Others include [11], [12], [24], [27], [44]. Golub and Van Loan [28] remains a standard reference for all aspects of matrix factorizations, including for what Stewart [42] calls the "big six" matrix factorizations.

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