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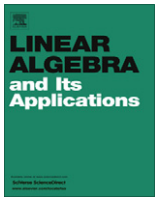

Preface

A mathematical biography of Danny C. Sorensen

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ABSTRACT

On the occasion of his 65th birthday, we briefly recount Dan Sorensen's profound contributions to optimization, numerical linear algebra, and model order reduction for dynamical systems.

1. Introduction

This special issue of *Linear Algebra and its Applications* is dedicated to Dan Sorensen in celebration of his 65th birthday. Dan has played a central role in the development of theory, algorithms, and software for numerical linear algebra, especially eigenvalue problems. He has also made fundamental contributions to optimization and, most recently, to model reduction for dynamical systems. Beyond his professional activities, Dan has served as a role model for many of us, inspiring many younger numerical analysts to be thoughtful and sober, and instilling an admirable work ethic.

Dan has made important contributions to many prominent algorithms, including trust region methods [39,48,50], the symmetric divide-and-conquer algorithm [13,22], the implicitly restarted Arnoldi method [49], Lyapunov equation solvers [31], and model reduction for linear and nonlinear systems [15,29]. Dan has also contributed to the major mathematical software projects LAPACK [2] and ARPACK [36], and co-authored several books on high performance linear algebra [19,21]. Throughout his career, Dan has shown a penchant for designing timely, elegant algorithms that lead to efficient, stable software implementations.

The papers in this issue reflect many of Dan's interests. In accordance with his current research emphasis, a third of the papers in this issue relate to model reduction. "Inexact solves in interpolatory model reduction" by Beattie, Gugercin, and Wyatt analyzes the effect of iteratively solving linear systems within an interpolatory model reduction framework. The question of how this affects the interpolation properties of the reduced-order model is considered. "A structured quasi-Arnoldi procedure for model order reduction of second-order systems" by Bai, Lin, Li, and Su deals with a model reduction approach for second-order dynamical systems that arise, e.g., in (micro-electrical-)mechanical systems. Their approach allows the computation of a reduced-order second-order model without explicit projection, while preserving Hermite interpolation conditions (i.e., moment-matching) as in the Padé-via-Lanczos framework for first-order systems [26]. The interpolatory model reduction framework is applied to two-dimensional systems, i.e., linear systems containing a free parameter (in addition to

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the time/frequency variable) in the paper "On two-variable rational interpolation" by Antoulas, Ionita, and Lefteriu. In this work, the Loewner matrix approach gives a realization of a 2D system from measured input/output data. A major advantage of model reduction based on balanced truncation is the availability of an *a priori* bound for the approximation error. Antoulas has derived an expression for the $\mathcal{H}_2$-norm of the error system of continuous-time system approximations, which can provide *a posteriori* error estimates, in [4]. This idea is extended to discrete-time systems in Chahlaoui's "A posteriori error bounds for discrete balanced truncation". Though not directly a paper on model reduction, "A low-rank Krylov squared Smith method for large-scale discrete-time Lyapunov equations" by Sadkane has its main application in this field, as the computational bottleneck of balanced truncation methods for discrete-time systems (as treated in Chahlaoui's paper) is the numerical solution of a dual pair of Stein equations (i.e., discrete-time Lyapunov equations).

A second category of papers is related to eigenvalue computation. Hochstenbach, Muhič, and Plestenjak discuss the transformation of a quadratic two-parameter eigenvalue problem to a linear multi-parametric eigenvalue problem in "On linearizations of the quadratic two-parameter eigenvalue problems". In electronic structure calculations, one is often interested in minimizing certain energy functionals. Yang and Meza consider "Minimizing the Kohn-Sham Total Energy for Periodic Systems". Though from its title this might not appear to be a paper about eigenvalues, the usual solution approaches in this area are based on computing certain eigenfunctions of the corresponding single-particle Hamiltonian, which, after discretization, leads to an algebraic eigenvalue problem. This problem is at the core of the constrained minimization algorithm employed by the authors to solve the energy minimization problem. Meerbergen and Vandebril return to one of Dan's most influential contributions, the implicitly restarted Arnoldi algorithm. They propose a novel method for computing eigenvalues near a vertical line, an essential problem in linear stability analysis, in "A reflection on the implicitly restarted Arnoldi method for computing eigenvalues near a vertical line". The method transforms a generalized eigenvalue problem into a Lyapunov eigenvalue problem [38], which is ripe for solution via the implicitly restarted Arnoldi method, nicely bridging Dan's contribution to both eigenvalue computations and Lyapunov solvers. The recent trend to exploit advanced linear algebra techniques in learning theory is reflected in "Eigenvalue bounds for an alignment matrix in manifold learning" by Ye and Zhi.

Closely related to eigenvalue problems is the task of computing singular values and vectors of matrices, due to its intimate relation to the symmetric eigenvalue problem. In "A Krylov–Schur approach to the truncated SVD", Stoll applies implicit restarting using Krylov–Schur factorizations to the large-scale singular value problem. An optimization-based approach to computing a truncated SVD is discussed by Baker, Gallivan, and Van Dooren in "Low-rank incremental methods for computing dominant singular subspaces".

Finally, the paper "Large-scale Tikhonov regularization via reduction by orthogonal projection" by Lampe, Reichel, and Voss presents a sequential Krylov projection method to compute an approximate solution of Tikhonov-regularized large-scale ill-posed least-squares problems.

In the following sections, we discuss Dan's contributions to the main fields of his research: Section 2 deals with the trust region subproblem arising in optimization algorithms. His work on eigenvalue problems is discussed in Section 3. Many of his algorithms have lead to mathematical software, often implemented by Dan himself and his students. This is briefly considered in Section 4, while his most recent interest in model reduction is reflected in Section 5.

2. The trust region subproblem

For 30 years Dan has worked on the trust region subproblem (TRSP) in optimization. The TRSP is a constrained quadratic minimization problem

$$\min g^T x + \frac{1}{2} x^T A x$$

for a given vector g and symmetric matrix A, subject to the constraint $\|x\|_2 \leq \Delta$. The TRSP arises in optimization algorithms when the initial iterate is not near a local minimizer, and is also equivalent

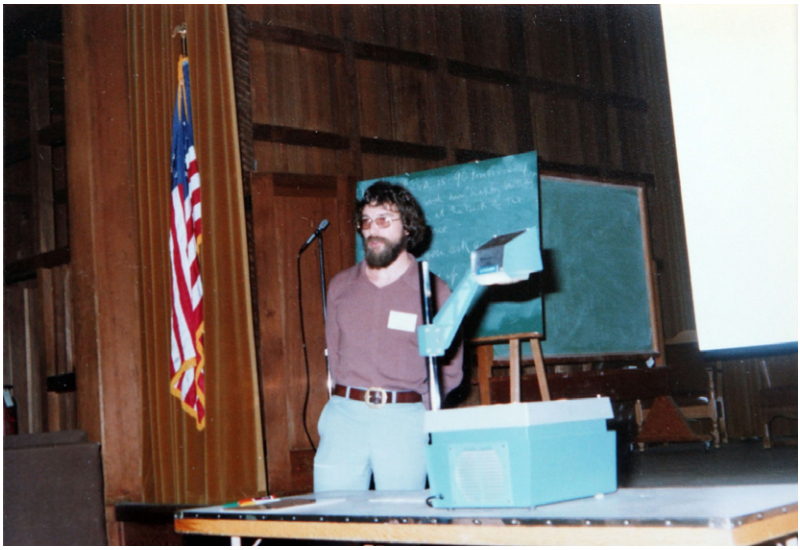

Fig. 1. Dan Sorensen speaking on "Updating the decomposition of a symmetric indefinite matrix" at the Gatlinburg VII Conference on Numerical Algebra, held in Asilomar, California, in 1977. (Photograph by courtesy of Walter Gander.)

to Tikhonov regularization for ill-posed linear least squares problems. In the case of optimization, for example, trust region methods allow one to use the Hessian of an objective function even when the Hessian has negative eigenvalues. The subproblem is difficult, and Dan's work has played a major role in the development of these algorithms.

Dan's work on the TRSP began in the late 1970s. We will focus on two papers from that period [39,48]. These papers represent pioneering work on the structure of the trust region subproblem, efficient direct methods for its solution, and the application of these methods in unconstrained optimization. The paper [48] suggested several symmetric factorization approaches, and showed that the solution had the form $(A+\lambda I)x = -g$, where $A+\lambda I$ is positive semidefinite. This characterization was used in the paper [39] with Moré to base an algorithm for unconstrained optimization on careful management of λ. This paper represented a real advance in the treatment of the *hard case*, where $(A+\lambda I)x = -g$ can only hold if $-\lambda$ is an eigenvalue of A. Hard case or nearly hard case problems arise frequently in regularization of ill-posed problems [44].

More recently, Dan has worked on large scale problems, where one must use iterative methods because factorization of $A - \lambda I$ is impossible due to the scale of the problem or the unavailability of a matrix representation for the linear transformation A. The most recent papers [34,42–44,50] reformulate the TRSP as a parameter-dependent eigenvalue problem, use a Lanczos method to solve that problem, and thereby drive an iterative method for the optimal value of the parameter. The resulting scalar *secular equation* for the parameter is solved using a rational interpolating model of the nonlinear function [44]. This work hearkens back to Dan's earliest work on eigenvalue problems. Most recently, Dan has tackled the solution of large scale trust region subproblems via a nonlinear Arnoldi method [34] (see Fig. 1).

3. Eigenvalue problems

In his well-known 1973 paper on "Modified Matrix Eigenvalue Problems," Gene Golub posed the problem of computing all eigenvalues of a symmetric $n \times n$ matrix that is obtained from a rank-1 symmetric perturbation of another symmetric matrix whose eigendecomposition is known [28]. A determinant argument reduces the problem to finding all n roots of a rational equation, also known as a *secular equation*. Working with Bunch and Nielsen [13], in 1978 Dan proposed an efficient, stable

approach to this root-finding problem based on locally modeling the roots not with the linear equation of Newton's method, but rather with a rational equation. This technique formed the basis for Cuppen's "divide-and-conquer" algorithm for the symmetric eigenvalue problem [17]: a symmetric tridiagonal matrix can be viewed as a rank-one perturbation of the direct sum of two smaller tridiagonal matrices, which can in turn be independently diagonalized by reapplying the same idea. In a 1987 paper with Dongarra [22], Dan refined this approach with an eye toward contemporary high performance parallel computer architectures. However: "the surprising result is that the parallel algorithm, even when run in serial mode, is significantly faster than the previously best sequential algorithm on large problems" [22, p. s139]. While the computed eigenvalues were quite satisfactory, the orthogonality of computed eigenvectors posed a further challenge, to which Dan and others devoted attention [30,53]. The improved algorithm is now widely used via the LAPACK routine DSTEDC [1,45]. Dan's related work includes an adaptation of the divide-and-conquer method for singular value computation [32] and the development of block algorithms for reducing general matrices to condensed forms, the initial stage of dense eigenvalue calculations [23].

While suitable algorithms were available for the symmetric eigenvalue problem for both dense matrices (QR, or divide-and-conquer) and large, sparse matrices (Lanczos), during the mid-1980s there was considerable interest in developing robust algorithms to compute select eigenvalues of large-scale nonsymmetric matrices. As early as 1951, W.E. Arnoldi had introduced a variant of Lanczos's algorithm that would reduce a nonsymmetric matrix to upper Hessenberg form by a unitary similarity transformation [7]. In the years that followed, this method was viewed as a numerically-sensitive alternative to the now-standard approach based on Householder reflectors; see, e.g. [55]. Yousef Saad rehabilitated Arnoldi's method in 1980 [46], demonstrating how a *partial* reduction to Hessenberg form could provide expedient estimates to the eigenvalues of large nonsymmetric matrices. Saad's method orthogonally restricts the matrix to a lower-dimensional Krylov subspace, $\mathcal{K}_k(A, v) = \text{span}\{v, Av, \ldots, A^{k-1}v\}$; the eigenvalues of the small $k \times k$ matrix H_k that results from this restriction can be readily computed using dense methods. Unfortunately, for most practical problems this procedure converges slowly, requiring a growing amount of work and storage at each iteration. Thus Saad proposed restarting the method [46,47], replacing the original starting vector v with the updated vector $v_+ = \phi(A)v$ for some polynomial ϕ. By properly tuning ϕ, one aims to force a few eigenvalues of H_k to convergence. Though a major step forward, this restarted Arnoldi method suffered from three fundamental limitations: the need to automatically design an effective *polynomial filter* ϕ, numerical instabilities arising from the explicit application of that filter, and the loss of orthogonality of the numerically-computed Arnoldi vectors.

Upon moving to Rice University in 1989, Dan began teaching a widely-appreciated course on Numerical Linear Algebra. At this time he made a fundamental observation: essentially the same technology behind QR implicit shifts could be used to restart Arnoldi's method (viewed as a partial reduction to Hessenberg form). In his landmark 1992 article "Implicit application of polynomial filters in a k-step Arnoldi method" [49], Dan resolved the primary obstacles to the widespread adoption of the restarted Arnoldi algorithm with a trio of distinct but complementary ideas: (1) construct the filter polynomial p to have roots at the eigenvalues of H_k that least resemble the sought-after eigenvalues; (2) adapt the implicit shift technique from QR eigenvalue computations to apply any polynomial filter in a numerically stable fashion; (3) maintain strict numerical orthogonality of the Arnoldi basis vectors by exploiting the classical Gram-Schmidt algorithm with iterative refinement [18]. This work resulted in the implicitly restarted Arnoldi method.

4. Mathematical software

In addition to his algorithmic work, Dan was a contributor to the LAPACK software project [1,2]. The experience he gleaned from implementing linear algebra software on the cutting-edge hardware of the day resulted in two books published by SIAM with Dongarra, Duff, and van der Vorst: 1990s *Solving Linear Systems on Vector and Shared Memory Computers* [20], which was superseded by 1998s *Numerical Linear Algebra for High-Performance Computers* [21].

Dan's primary software contribution was the development of ARPACK [36]. With an automatic, stable restart procedure and a numerically efficient scheme to maintain numerical orthogonality of the Arnoldi basis vectors, the implicitly restarted Arnoldi method was now ripe for implementation in software as a robust solver for large-scale eigenvalue problems.

During the academic year 1991–92, Phuong Vu (at that time with Cray Research) was granted permission to work, through a half-time appointment to the NSF Center for Research on Parallel Computation (CRPC) at Rice University, on the initial development of ARPACK. Doctoral students Rich Lehoucq and Chao Yang joined the development effort during the next several years. Postdoc Kristi Maschhoff provided the first distributed-memory parallel implementation, P_ARPACK. ARPACK remains the first choice method for general-purpose large-scale nonsymmetric and symmetric eigenvalue computations; indeed, now the full ARPACK software is embedded in MATLAB® via the `eigs` command. Dan and co-authors went on to consider variations of this algorithm in the papers [14,35,54]; further convergence theory is proposed in [9,51]. This work on large-scale eigenvalue computations naturally dovetailed into Dan's later work on Krylov subspace techniques for model reduction of large-scale dynamical systems.

5. Model reduction

Dan's interest in model order reduction (MOR for short, also referred to as dimension, model, or order reduction) was piqued in the mid-1990s. The goal of MOR is to replace a given model for the dynamics of a large-scale system of ordinary differential equations (ODE) – often resulting from a spatial semi-discretization of a time-dependent partial differential equation – by one of lower complexity. If a system theoretic description of the process model is used, then one is merely interested in a good model for the mapping of inputs to outputs, rather than an accurate model for the dynamical behavior of the states. For linear-time invariant (LTI) systems, transformed to frequency domain via a Laplace (or Fourier) transform, this amounts to approximating the system's transfer function. As the transfer function of an LTI system is a rational matrix-valued function of the frequency parameter, this problem can be cast as a rational approximation problem; that is, one aims at replacing the high-degree transfer function of order n of the original model by a rational matrix-valued function of reduced order (degree) $r \ll n$. Using realization theory, this reduced-order transfer function then also leads to a new state-space model, i.e., an LTI system residing in an r-dimensional state-space. The MOR problem can be tackled by Padé approximation, i.e., the best approximation of the transfer function by a rational function of given order. Best approximation is understood in the way that the approximant's power series agrees with the power series of the original transfer in as many coefficients as possible for the given degree. As the coefficients in this power series are often called *moments*, MOR techniques based on this approach are often called *moment-matching methods*.

In the early 1990s, researchers began to recognize that Krylov subspace methods, in particular the nonsymmetric Lanczos process, can be used to compute Padé and Padé-like approximants of transfer functions in a reliable way [24,25,27]. A disadvantage of this approach, which became popular in particular in the electronics industry, is that the reduced-order models obtained by this *Padé-via-Lanczos* (PVL) process are often unstable, even if the original model is stable. Depending on the stimulus, this may introduce undesirable effects in the dynamical behavior of the reduced-order model. Thus in [29], Dan's implicit restarting technique so successfully employed in large-scale eigenvalue computations was proposed as a method to remove unstable poles of the system. Another property shared by many LTI systems arising in circuit theory is passivity. Again, the usual PVL approaches do not preserve this property in the reduced-order model. In [3], Dan's Rice colleague Thanos Antoulas derived sufficient conditions for an interpolant of the transfer function to preserve passivity: if the reduced-order model interpolates the full model in its spectral zeros, then passivity is preserved. This spurred Dan to develop a robust numerical method for computing a rational approximation to the original transfer function, using the implicitly restarted Arnoldi method to generate a reduced model that interpolates some of the spectral zeros [52].

Since his first MOR paper [29], Dan has contributed in a variety of ways to MOR for LTI systems. A very well received community service was the early MOR survey [5]; he also co-edited one of the early books

on MOR [11] as well as a special issue of LAA on this subject [10]. One contribution of the survey [5] was to show that, thanks to recent efforts to employ advanced techniques from numerical linear algebra, the method of balanced truncation could provide a viable alternative to Krylov subspace-based MOR methods for large-scale systems. Numerical experiments in [5] on standard benchmarks show that *approximate balanced truncation* (as suggested, e.g., in [12,37,41]) yields basically the same accuracy as traditional balanced truncation using the direct solution of the underlying Lyapunov equations, which is often incorrectly considered "exact" balanced truncation in the literature. As "direct" solvers [1] exhibit cubic complexity, in order to come up with an efficient approximate balanced truncation method, it is therefore of paramount importance to be able to solve Lyapunov equations in (almost) linear complexity by exploiting the sparsity of the coefficient matrix and low-rank structure of the right-hand side. Such a method is suggested by Dan and co-workers in [31], where they consider a modification of the low-rank Smith method discussed in [40]. Almost all methods for large-scale Lyapunov equations, including the one suggested in [31], heavily rely on the observation that the solution's eigenvalues (or singular values, as these solution matrices are symmetric positive semi-definite) frequently decay to zero rapidly (if ordered by magnitude). Given Dan's quest for mathematical rigor, he could not accept this observation without understanding the principle behind it. In [6], he and his co-workers were able to provide new bounds on the eigenvalue decay of Lyapunov solutions, and in particular obtained the first results for the case of non-symmetric (but diagonalizable) coefficient matrices. Also, an important contribution of this paper is that the effect of the right-hand side on the eigenvalue decay is taken into account.

In recent years, Dan has focused his attention on model reduction for nonlinear systems. A popular method in this area is proper orthogonal decomposition (POD). When applied to nonlinear ODE systems, POD suffers from a significant drawback: while it often produces a significant reduction of the state-space dimension, the nonlinearity still must be evaluated in the high-dimensional space – leading to no substantial performance gain. In recent work with Saifon Chaturantabut [15], Dan shows how the well known empirical interpolation method used in reduced basis-type methods for approximating nonlinear parameter-dependent terms by parameter-affine functions [8] can be employed to overcome this deficiency of POD. The resulting method – the *Discrete Empirical Interpolation Method (DEIM)* – has already led to a variety of applications in different areas by Dan and others [16,33], and points to a promising vein of future work.

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