Rational Krylov subspaces for Hermitian matrices properties and applications

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Where it all started...

Householder Symposium XII on Numerical Algebra, Lake Arrowhead, CA, June 1993

My (very) personal recollection of the meeting's highlights:

- A beautiful venue (nice bungalows, tennis court, good food, ...)
- Alston Householder attended! (shortly before he passed away)
- An impressive number of other *important* people

Report on SIAM News by Stephen Vavasis

Householder Symposium,

continued from page 1

structured algorithms for the solution of both continuous-time and discrete-time algebraic Riccati equations. These algorithms are based on a simple but elegant proof of the existence of particular square roots of matrices with Hamiltonian or symplectic structure. Xu derived an error analysis and showed how to use iterative refinement for ill-conditioned Riccati equations. He also tested the new algorithms thoroughly to verify theoretical error bounds. Xu is currently a member of the mathematics department at Fudan University.

Beresford Parlett, speaking for the Householder award committee, said that the selection criteria for the Householder award were mathematical innovation, thoroughness of computational experiments, and applicability of the results.

Parlett said that, in addition to the two winners, the committee had selected one nominee, Ali Sayed, for special mention. Sayed received his PhD in electrical engineering from Stanford in August 1992 under the direction of Thomas Kailath. His dissertation describes how a variant of Gaussian elimination can be applied to a variety of problems in linear algebra and control theory, including Toeplitz systems and Padé tables, to yield efficient algorithms. The key concept in the dissertation is a generalization of "low displacement rank." Sayed's work unifies many previous and seemingly complicated algorithms in the literature. Sayed is headed for the electrical engineering department at the University of California, Santa Barbara.

Many Applications to PDEs, Signal and Image Processing

The bulk of the meeting was devoted to 30 plenary lectures, spread over five days. The lectures covered various topics of current interest, including parallel linear algebra, sparse systems, boundary value problems, updating and downdating factorizations, perturbation bounds, and structured systems. Many of the talks described applications of linear algebra, including applications to partial differential equations and signal and image processing. In addition to the plenary lectures, there were concurrent sessions in the evenings on parallel computation, multigrid and domain decomposition methods, eigenvalue algorithms, and other topics.

The meeting opened with plenary talks by Paul Van Dooren (Illinois), Hong-yuan Zha (Penn State), and Sabine Van Huffel (Leuven) on matrix factorizations arising in signal processing and statistics. Van Dooren spoke on numerically stable simultaneous factorization of a product of matrices arising in control. Algorithms for canonical correlations in statistics were the subject of Zha's presentation. Van Huffel compared structured total least squares with constrained total least squares and discussed their application to biomedical problems.

A sequence of talks by James Demmel (Berkeley), Roy Mathias (William & Mary), and Nicholas Higham (Manchester) focused on the relation between parallelism and numerical stability in linear algebra. Demmel described an eigenvalue toolkit that uses new algorithms based on the matrix sign function. Although the method is ideal for parallelism, its stability properties are weaker than those of traditional sequential methods. Mathias showed the computing of signatures by parallel prefix methods to be less stable than traditional accumulation. In his talk on parallel triangular solvers, Higham showed that several proposed algorithms are not as stable as sequential back-substitution.

Two speakers considered sparse matrix methods. John Gilbert (Xerox) described the implementation of and experimentation with geometric mesh partitioning, which is important for parallel iterative methods and sparse Gaussian elimination in finite element problems. Stanley Eisenstat (Yale) described new approaches to sparse unsymmetric factorization that attempt to incorporate successful ideas from symmetric algorithms.

Several talks focused on iterative algorithms for solving nonsymmetric and indefinite linear systems. Gerald Sleijpen (Utrecht) showed how to prevent stagnation in the BiCGSTAB iterative algorithm in an extension denoted BiCGSTAB(l). Anne Greenbaum (NYU) described a new analysis of the GMRES algorithm that can better distinguish matrices for which the method will converge quickly. Michael Saunders (Stanford) compared two iterative methods, LSQR and Craig's method, showing equivalence in some cases.

Alston Householder, with Martin Gutknecht (*left*) and Walter Gander (*right*), at the Householder meeting in Lake Arrowhead, June 1993. The photo was taken by a member of the Gander family.

Boundary value problems were the subject of three talks. Stephen Vavasis (Cornell) proposed new elimination methods for solving boundary value problems that are guaranteed to be numerically stable in the presence of wild variation in the coefficient field. Andrew Wathen (Bristol) proposed new preconditioned iterative methods for Stokes' flow with optimal bounds on the condition number. Coincidentally, both of these speakers analyzed properties of the symmetric indefinite linear system

$$\begin{bmatrix} H & A \\ A^T & 0 \end{bmatrix}$$

to obtain their results. Hans Munthe-Kaas (Bergen) showed how to unify various fast Poisson solvers in terms of Abelian groups.

A number of talks focused on updating, downdating, and rank-detection algorithms. These algorithms are very important in signal processing, where it is necessary to maintain such information as numerical rank for a time-varying signal. In a time-varying signal, "old" information must somehow be eliminated from the factorization and rank approximations as time passes. C.-T. Pan (Northern Illinois) spoke on recent progress in rank-revealing QR factorization, which is used as an efficient substitute for the full singular value decomposition.

Haesun Park (Minnesota) spoke on a hybrid, more stable method for downdating the URV decomposition, also used for monitoring numerical rank. Ming Gu (Yale) proposed new algorithms for downdating the singular value decomposition itself. Franklin Luk (RPI) derived a new factorization of matrix pairs that is amenable to updating.

Chris Paige (McGill), who delivered the plenary address at the banquet, described the history of the C–S decomposition and angles between subspaces. Tracing the history of this area back to the work of Jordan, Paige focused on recent contributions by C. Davis, W. Kahan and G.W. Stewart.

Perturbation theory was the subject of several talks. Michael Overton (NYU) discussed a new way to analyze stability in Hamiltonian systems; the stability issue can be expressed as an eigenvalue perturbation problem. Jiguang Sun (Umea) gave new backward-perturbation estimates for a wide variety of least-squares and eigenvalue problems that are the best possible estimates in many cases. Ilse Ipsen (Yale) described a new method for analyzing a variety of eigenvalue perturbation problems; her method is based on writing additive perturbations as matrix multiplications. L.N. Trefethen (Cornell) presented experimental comparisons of the effects of perturbations of the coefficients of a polynomial on its zeros and of perturbations of a companion matrix, and discussed the connection between numerical errors in Gaussian quadrature computation and the Lanczos iteration. Roland Freund (AT&T) discussed the stabilization of "fast" ($O(n^2)$ flops) algorithms for Toeplitz systems that use look-ahead procedures. Martin Gutknecht (ETH-Zurich) described new "superfast" ($O(n (\log n)^2)$ flops) algorithms for the same problems.

Leslie Foster (San Jose State) gave examples arising in differential and integral equations for which Gaussian elimination with partial pivoting (GEPP) is numerically unstable. It is known from work done by Wilkinson that, theoretically, GEPP can be unstable because of the "growth factor," but many researchers have believed that this instability does not occur in practical problems. Because of examples like Foster's and other recent work, implementors of GEPP, including the LAPACK designers, are planning to build additional safeguards into software to detect unstable behavior.

Important Role for Laptops

In addition to the plenary talks, there were a total of 18 informal sessions spread over three evenings. One very popular session was organized by Cleve Moler (MathWorks) to demonstrate upcoming developments in MATLAB, which is an interactive software package for numerical computation produced by The MathWorks, Inc. Moler demonstrated some of the features of the latest version of MATLAB and gave a preview of a toolbox under development that integrates Maple, a symbolic mathematics package from the University of Waterloo, with MATLAB.

Underscoring the informal nature of the meeting, one session (on geometry, eigenvalues, and optimization, organized by Alan Edelman of Berkeley and Michael Overton of NYU) was held at the conference center's outdoor picnic area. For the first time at a Householder meeting, laptop computers played an important scientific role as many participants demonstrated software to one another and conducted experiments during the breaks. One use of the laptops, which were provided by UCLA and Cleve Moler, was to analyze an impromptu graph made at the meeting showing co-authorship relationships among participants. The graph was started by Nick Trefethen, but most of the participants joined in. Gene Golub turned out to have by far the greatest number of co-authors.

In addition to the technical presentations, there were many recreational activities available at the scenic conference site. Boat tours for the participants showed off the beauty of Lake Arrowhead and the surrounding palatial summer homes owned by movie stars. Of the 16 people who hiked up Mount San Gorgonio with Petter Bjørstad (Bergen), six went to the summit at 11,499 feet. Finally, two milestones were celebrated at the meeting. Gene Golub was feted for his recent election to the National Academy of Sciences, and Alan Edelman turned 30 during the meeting. Congratulations to Gene and Alan!

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The Gatlinburg leaders

One of the subsequent generations

Michele's model

Since then, he has been rocking a more furtive appearance

Going to the math

CIME Summer School, 2015

Unveiling hidden structure. Two recent instances:

- Decay "without" banded structure
- Short-term recurrences "without" symmetric structure

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Decay of matrix function entries

The classical bound (Demko, Moss & Smith):

A **spd** and banded with bandwidth β, then

$$|(A^{-1})_{ij}| \le \gamma q^{\frac{|i-j|}{\beta}}, \qquad q := \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} < 1 \ (\kappa = cond(A))$$

If f analytic in region containing $\mathrm{spec}(A)$: $|f(A)_{ij}| \le Cq^{\frac{|i-j|}{\beta}}$

with C, q depending on $\mathrm{spec}(A)$ and f (*Benzi & Golub, 1999*)

♣ Large number of contributions and large evidence of applicability

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Decay of matrix function entries - non-Hermitian case

[Pozza - Simoncini 2019] Let A be banded with bandwidths (β, γ) with field of values contained in a convex continuum E. Moreover, let ϕ be the conformal map sending the exterior of E onto the exterior of the unitary disk, and let ψ be its inverse. For any $\tau > 1$ so that f is analytic on the level set G_τ defined as the complement of the set $\{\psi(z) \; : \; |z| > \tau\}$, we get[a]

$$\left|(f(A))_{k,\ell}\right| \leq 2\frac{\tau}{\tau - 1} \max_{|z|=\tau} |f(\psi(z))| \left(\frac{1}{\tau}\right)^{\xi}$$

[a] $\xi := \begin{cases} \lceil(\ell - k)/\beta\rceil, & \text{if } k < \ell \\ \lceil(k - \ell)/\gamma\rceil, & \text{if } k \geq \ell \end{cases}$

Earlier refs for non-normal matrices:
Benzi - Razouk 2007, Mastronardi - Ng - Tyrtyshnikov 2010
Iserles 2000, Benzi - Boito 2014, Wang - Ye 2017, etc.

A more subtle setting. First the easy case.

Given a matrix $A \in \mathbb{R}^{N \times N}$ with spectrum $\lambda(A)$ and a vector $\boldsymbol{v} \neq 0$:

Polynomial Krylov recurrence

the mth step of the Arnoldi algorithm produces the $N \times m$ matrix $U_m = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m]$ whose orthonormal columns are a basis of the (polynomial) Krylov subspace $\mathcal{K}_m(A, \boldsymbol{v})$, and

$$AU_m = U_m T_m + t_{m+1,m} \boldsymbol{u}_{m+1} \boldsymbol{e}_m^T,$$

with T_m $m \times m$ upper Hessenberg matrix.

Note: $T_m = U_m^* A U_m$ (but also contains the orth coefficients)

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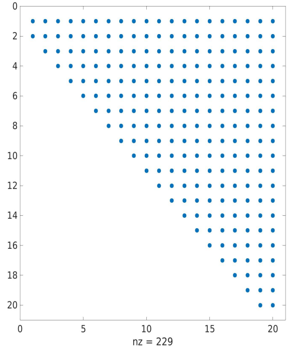
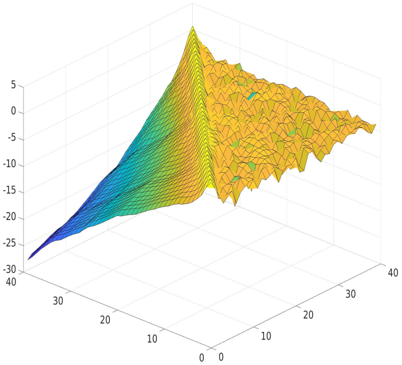
Decay properties of the reduced matrix

The entries of $f(T_m)$ behave as predicted by the theory





Rational Krylov recurrence

$$\mathcal{RK}_m(A, \boldsymbol{v}, \boldsymbol{\sigma}_{m-1}) := \mathrm{span}\{\boldsymbol{v}, (A - \sigma_1 I)^{-1}\, \boldsymbol{v}, \ldots, \prod_{j=1}^{m-1} (A - \sigma_j I)^{-1}\, \boldsymbol{v}\}$$

the mth step of the rational Arnoldi algorithm produces the $N \times m$ matrix $V_m = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m]$ whose orthonormal columns are a basis of the rational Krylov subspace $\mathcal{RK}_m(A, \boldsymbol{v})$, and

$$A\, V_m H_m = V_m K_m - h_{m+1,m}(A - \sigma_m I)\boldsymbol{v}_{m+1} \boldsymbol{e}_m^T$$

with $H_m := (h_{i,j})_{i,j=1,\ldots,m}$ upper Hessenberg, and $K_m = I + H_m\, \mathrm{diag}(\boldsymbol{\sigma}_m)$;

(Ruhe 1994, Güttel 2013, etc.)

Rational Krylov recurrence. Reduced matrix.

$$J_m := V_m^* A V_m = K_m H_m^{-1} - h_{m+1,m} V_m^* (A - \sigma_m I)\, \boldsymbol{v}_{m+1} \boldsymbol{e}_m^T H_m^{-1},$$

The matrix J_m is not generally a Hessenberg matrix, except for some special choices of the shifts
(Druskin -Knizhnerman 1998, Jagel - Reichel 2009, etc.)

This holds irrespective of the symmetry of A!

Structure of J_m is more complex
(see also Fasino 2005, Van Buggenhout, Van Barel, Vandebril, 2018)

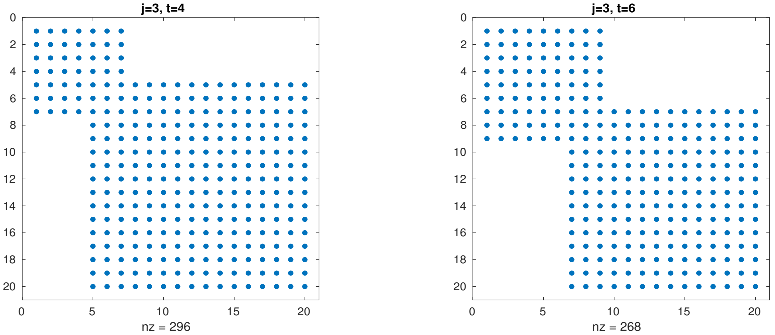
Sparsity pattern of the reduced matrix J_m

Consider the rational function (Pozza - Simoncini, 2021)

$$s_j^{(t)}(x) := \frac{q_j(x)}{(x-\sigma_t)\cdots(x-\sigma_{t+j-1})},$$

with $t \geq 1$ and $q_j(x)$ a polynomial of degree at most j. If the indexes k, ℓ are such that $k \geq t+2$ and $\ell \leq t$, then

$$\left(s_j^{(t)}(J_m)\right)_{k,\ell} = 0, \quad j = 1, \ldots, k-t-1.$$

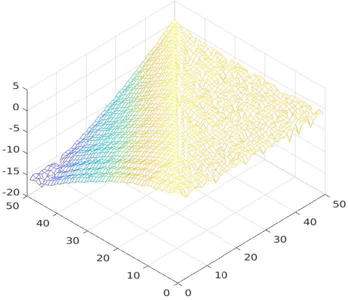


Decay properties of the reduced matrix J_m

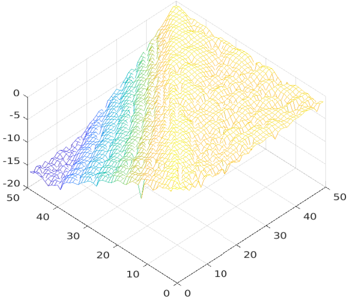
Hidden structure of J_m leads to decay properties

- The entries of J_m decay exponentially (depending on field of values of A)
- The entries of $f(J_m)$ also decay exponentially (depending on field of values of A)

$$|f(J_m)_{k,\ell}| \leq 3\frac{\tau}{\tau - 1} \max_{|z|=\tau} |f(\psi(z))| \prod_{t=\ell}^{k-2} \frac{\tau + |\phi(\sigma_t)|}{|\phi(\sigma_t)|\tau + 1}$$



J_{50}



$\exp(J_{50})$ Pozza - Simoncini, 2021

Rational Krylov iteration for A symmetric

The standard implementation of rational Krylov does not take advantage of symmetry

Deckers - Bultheel (2007,2012) developed a three-term recurrence relation to generate a sequence of orthogonal rational functions to be used with $\mathcal{RK}$

Güttel (PhD thesis, 2010) proposed the corresponding (vector) recurrence:

$$\beta_j \left(I - \xi_j^{-1} A\right) \boldsymbol{q}_{j+1} = A\boldsymbol{q}_j - \alpha_j \left(I - \xi_{j-1}^{-1} A\right) \boldsymbol{q}_j - \beta_{j-1} \left(I - \xi_{j-2}^{-1} A\right) \boldsymbol{q}_{j-1}$$

Usual formulation and Arnoldi-type relation recovered by rearrangements of the terms

⇒ Block version readily available...

Q: Can this recurrence be useful? (*It is somewhat more expensive, except for implicit orth.*)

A: Yes, whenever we can do without $Q_m = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m]$

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Applications

Instances where Q_m-less approach can be relevant:

- $e_1^T f(J_m) e_1 \approx v^T f(A)\, v$
- $\Rightarrow \quad \mathrm{tr}(f(A)) \approx \frac{1}{\ell}\sum_{k=1}^{\ell} \tau_k$, where $\quad \tau_k \approx z_k^* f(A) z_k$ (Monte-Carlo approx)
- $\mathcal{H}_2$-norm approximation for dynamical system output control
- $\Rightarrow \quad$ Approximation to control function

All examples explicitly use J_m but not Q_m

Q_m-less implementation

Computational issue. How to determine the (full) matrix

$$J_m = Q_m^* A Q_m$$

without having Q_m handy?

At the j-th iteration the last column (or row) of $J_j = Q_j^T A Q_j$ is given by

$$J_j e_j = \widehat{y}_j - \frac{\beta_j^2}{\xi_j^2} \frac{\xi_j - \eta}{\omega_j} t_j,$$

where $\widehat{y}$ satisfies

$$\widehat{y}_1 = \alpha_1, \quad \widehat{y}_j = \begin{bmatrix} -\widehat{y}_{j-1} \frac{\beta_{j-1}}{\xi_{j-2}\omega_j} \\ \beta_{j-1} e_{j-1}^T y_j + \frac{\alpha_j}{\omega_j} \end{bmatrix} + \frac{\beta_{j-1}}{\omega_j} e_{j-1}, \quad \text{for } j > 1$$

Here $\{y_j\}$, $\{t_j\}$ and $\{\omega_j\}$ are also updated by two-term recursive formulas
(Palitta - Pozza - Simoncini, 2022)

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Conclusions

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The Gatlinburg leaders - a replica

Conformal mappings associated with $W(A)$