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BOOK OF ABSTRACTS

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An Explicit Formula for the Singular Values of the Sylvester–Kac Matrix

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The object of our interest is the $(n+1) \times (n+1)$ tridiagonal matrix

$$P = \begin{bmatrix} 0 & n & & & \cdots & 0 \\ 1 & 0 & n-1 & & & \vdots \\ & 2 & 0 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ \vdots & & & \ddots & \ddots & 1 \\ 0 & \cdots & & & n & 0 \end{bmatrix},$$

that appears in a variety of problems in statistical mechanics and quantum physics. The spectral decomposition of this matrix has been studied by a number of authors. The question arises: does there exist an explicit formula for the singular values? A few years ago Professor Sigurd Falk (TU Braunschweig) noticed via numerical examples that if $n = 2m$ then at least $m+1$ of the squared singular values of P are integers. In this paper we prove the following Theorem.

Theorem. *Let $n = 2m$ for a nonnegative integer m, then the numbers*

$$\sqrt{(2m+1)^2 - (2i+1)^2} \qquad (i = 0, 1, 2, \ldots, m)$$

are singular values of P.

The proof of the theorem is arranged in four sections. In Section 2 we begin by permuting the rows and columns of P so that we obtain a 2×2 block matrix with zero blocks on the main diagonal and nonzero blocks on the antidiagonal. We then recognize that the "well-behaved" singular values of P are associated with one of the nonzero blocks. In Section 3 we replace the singular value problem with the equivalent symmetric eigenvalue problem of the tridiagonal matrix $R = 4[r_{ij}]$ where

$$r_{kk} = (m-k)^2 - k^2 \qquad (k = 0, 1, 2, \ldots, m),$$

$$r_{k+1,k} = r_{k,k+1} = k \cdot (m-k+1) \qquad (k = 1, 2, \ldots, m).$$

In Section 4 we use the method of generating functions to represent the elements of the unknown eigenvectors as coefficients of polynomials. These polynomials satisfy a second-order differential equation in which the eigenvalue appears as a free parameter. In Section 5 we seek the general solution of the differential equation in the form of a Frobenius series, and show that polynomial solutions exist only for certain discrete values of the free parameter.

Polynomial Extension of Rational Realization of Minimum Rank Matrices in a Sign Pattern Class

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A *sign pattern matrix* is a matrix whose entries are from the set $\{+,-,0\}$. The minimum rank of a sign pattern matrix A is the minimum of the ranks of the real matrices whose entries have signs equal to the corresponding entries of A. It is conjectured that the minimum rank of every sign pattern matrix can be realized by a rational matrix. The equivalence of this conjecture to several seemingly unrelated statements are established. For some special cases, such as when A is entrywise nonzero, or the minimum rank of A is at most 2, or the minimum rank of A is at least $n-1$ (where A is $m \times n$), the conjecture is shown to hold. Connections between this conjecture and the existence of positive rational solutions of certain systems of homogeneous quadratic polynomial equations with each coefficient equal to either -1 or 1 are investigated.

This is joint work with Marina Arav, Selcuk Koyuncu, Zhongshan Li, and Bhaskara Rao.

Partitions into Nonobtuse Simplices

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Acute and nonobtuse simplicial partitions are very useful in numerical analysis, since they yield irreducible and diagonally dominant stiffness matrices, when solving the Poisson problem by the standard linear conforming finite elements in a bounded polytopic domain. In this case the discrete maximum principle takes place and linear simplicial elements have optimal interpolation properties. We show that there does not exist a face-to-face partition of the Euclidean space into acute simplices when its dimension is greater than 4.

Loss and Recapture of Correlation between Two Arnoldi Bases of the Krylov Subspace

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Let us compute recursively two Arnoldi bases of the Krylov subspace

$$K_n(A, r^0) = \text{span}\{r^0, Ar^0, \ldots, A^{n-1}r^0\},\ A \in \mathbb{R}^{N\times N},$$

using two methods, namely the Iterated Modified Gram-Schmidt and Householder orthogonalization, where both methods preserve the orthonormality up to the machine precision ϵ_M. In the nth step, $n \leq N$, let $V_n = [v_1, v_2, \ldots, v_n]$ and $W_n = [w_1, w_2, \ldots, w_n]$ denote the Arnoldi basis computed by the first and second method, respectively. In rare cases, for some matrices A, an interesting effect of the loss and recapture of correlation between V_n and W_n has been observed, i.e., the n by n correlation matrix $C = V_n^T W_n$ becomes non-diagonal in some index regions where its diagonal values are less than one. However, after some iteration steps the full correlation is recaptured, whereby the loss and recapture of orthonormality can repeat several times during computation.

We discuss the necessary and sufficient conditions for the loss of correlation to occur. The decisive role is played by the existence of very close pairs of singular values of matrix A. Taking one such pair $(\sigma_i,\ \sigma_{i+1})$, the corresponding left and right singular vectors, x_i, x_{i+1} and y_i, y_{i+1}, respectively, are ill-conditioned. Consequently, at the beginning of the $(n+1)$st iteration step, the angle $\angle(\text{fl}(Av_n), \text{fl}(Aw_n))$ may have any value in the interval $[0,\ \pi/2]$, i.e., the vectors $\text{fl}(Av_n)$ and $\text{fl}(Aw_n)$ may become de-correlated. We show that under mild assumptions their de-correlation is restricted into the subspaces corresponding to ill-conditioned right singular vectors, whereas both vectors are fully correlated in subspaces corresponding to well-conditioned right singular vectors. This remains true also after the orthogonalization of new vectors against all previously computed members of corresponding bases.

The recapture of correlation is connected with the absorption of 'bad' singular subspaces (i.e., of those corresponding to ill-conditioned right and left singular vectors) into $\text{span}\{V_n\}$ and $\text{span}\{W_n\}$. Since both methods preserve the orthonormality to $O(\epsilon_M)$, once absorbed the new members of both bases can not have significant components in 'bad' singular spaces (up to the round-off error). Since the de-correlation is restricted to 'bad' spaces, this means the recapture of correlation for subsequent members of both bases. Of course, the absorption must not be full; then the instability region may emerge again depending on the relative role played by close pairs of singular values.

We provide an interesting numerical example using the 240 by 240 matrix `STEAM1`. Because of the very special geometrical relationship between the singular vectors and eigenvectors of this matrix, we can say much more about the subsequent absorption of singular subspaces into $\text{span}\{V_n\}$ and $\text{span}\{W_n\}$ than in general case.

Linear Algebra for Monitoring of Industrial Processes in Heavy Industry

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The numerical linear algebra is used as a basis for the information retrieval in the retrieval strategy called Latent Semantic Indexing (LSI), see for instance [1, 2, 3]. Originally, LSI was used as an efficient tool for semantic analysis of large amount of text documents. The main reason is that more conventional retrieval strategies (such as vector space and extended Boolean) are not very efficient for real data, because they retrieve information solely on the basis of keywords. LSI can be viewed as a variant of a vector space model, where the database is represented by the document matrix, and a user's query of the database is represented by a vector. LSI also contains a low-rank approximation of the original document matrix via the Singular Value Decomposition (SVD) or the other numerical methods. The SVD is used as an automatic tool for identification and removing redundant information and noise from data. In our contribution, we present our experience with using the LSI method for monitoring of industrial processes [4] in heavy industry environment. The aim is to monitor the coking process quality in real time. We have no information about application of LSI for image retrieval in heavy industry. Important implementation details of SVD will be discussed as well.

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Numerical Stability of Iterative Methods

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Iterative methods for linear systems are often the time-critical component in the solution of large-scale problems in computational science and engineering. In recent years a large amount of work has been devoted to Krylov subspace methods which are among the most widely used iterative schemes. Significantly less attention, however, has been paid to their numerical stability. Rounding errors occurring in finite-precision implementations of iterative methods can have two main effects on their numerical behavior. They can delay the rate of convergence given by the (theoretical) properties of a solved system and there is a limitation to the accuracy of computed approximate solution which does not decrease below a certain level (called usually maximum attainable or limiting accuracy). A comprehensive survey of error analysis for stationary iterative methods was given by Higham in his book, who addressed the problem how small can be the forward or backward error for various classical schemes. Several results for Krylov subspaces methods on both the accuracy of computed solution and the rate of convergence have been presented in last decades. Based on the pioneering papers of Paige on the (symmetric) Lanczos process, Greenbaum, Strakoš and others worked on a rounding error analysis of the CG method. These articles gave rise to the main result on the delay of convergence (due to rounding errors) which is essentially given by the rank-deficiency of the computed basis vectors. The maximal attainable accuracy of various iterative schemes with short recurrences has been analyzed by Greenbaum, van der Vorst, Strakoš, Gutknecht and others. In this contribution we will review the main results on the numerical behavior of the GMRES method, the most widely known and used representative of nonsymmetric Krylov subspace methods. This method consists of constructing the basis of associated Krylov subspace and then solving the transformed Hessenberg least squares problem at each iteration step. In the talk we analyze different computational variants of the Arnoldi process used in the orthogonalization part of GMRES, including its Householder (HH), classical (CGS) and modified (MGS) Gram-Schmidt implementation. We will examine how important is the orthogonality of computed Arnoldi vectors and to what extent its has an influence on the accuracy of different implementations of GMRES. In particular, we show that there is an important relation to the relative backward error, which gives us the link between the loss of orthogonality in the MGS Arnoldi and the convergence of GMRES. Using this result we will prove that the most usual MGS-GMRES implementation is backward stable. This theoretically justifies the observed fact that the linear independence of Arnoldi vectors in MGS-GMRES is effectively maintained until the convergence to the level of limiting accuracy. Based on a recently obtained bound for the loss of orthogonality in the CGS process, an analogous statement can be formulated also for CGS-GMRES. Presented results lead to important conclusions about the practical use of the GMRES and other iterative methods.

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On Semiregular Digraphs of the Congruence $x^k \equiv y \pmod{n}$

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We assign to each pair of positive integers n and $k \geq 2$ a digraph $G(n, k)$ whose set of vertices is $H = \{0, 1, \ldots, n-1\}$ and for which there is a directed edge from $a \in H$ to $b \in H$ if $a^k \equiv b \pmod{n}$. The digraph $G(n, k)$ is semiregular if there exists a positive integer d such that each vertex of the digraph has indegree d or 0. Generalizing our earlier results for the case in which $k = 2$, we characterize all semiregular digraphs $G(n, k)$ when $k \geq 2$ is arbitrary.

ABS Methods for Linear Diophantine Problems

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ABS methods have been introduced at the beginning of the 80's originally to solve linear algebraic continuous systems, and have been later extended to linear least squares, nonlinear equations and optimization problems. They provide a unification in a parametric form, based upon the use of the Egervary matrix rank-one decreasing process, of most methods for solving linear algebraic continuous systems and linearly constrained continuous optimization (via feasible direction processes, the LP case being a special case). More than 400 papers on ABS methods have been written up to now, including two monographs. Recently ABS methods have been extended to linear Diophantine problems (linear equations, linear inequalities and LP problems), by extending the approach that Egervary developed only for the homogeneous case. We discuss our results in this case, including a method that does not need computing the greatest common divisor, and a technique to reduce the growth of the integers generated by the algorithm.

Gerschgorin Discs and the Numerical Range

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We intend to discuss these classical concepts in connection with the behaviour of the powers of operators. A number of open questions will be mentioned.