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Structured low rank approximation

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Abstract

This paper concerns the construction of a structured low rank matrix that is nearest to a given matrix. The notion of structured low rank approximation arises in various applications, ranging from signal enhancement to protein folding to computer algebra, where the empirical data collected in a matrix do not maintain either the specified structure or the desirable rank as is expected in the original system. The task to retrieve useful information while maintaining the underlying physical feasibility often necessitates the search for a good structured lower rank approximation of the data matrix. This paper addresses some of the theoretical and numerical issues involved in the problem. Two procedures for constructing the nearest structured low rank matrix are proposed. The procedures are flexible enough that they can be applied to any lower rank, any linear structure, and any matrix norm in the measurement of nearness. The techniques can also be easily implemented by utilizing available optimization packages. The special case of symmetric Toeplitz structure using the Frobenius matrix norm is used to exemplify the ideas throughout the discussion. The concept, rather than the implementation details, is the main emphasis of the paper.

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1. Introduction

Finding a low rank approximation of a general data matrix is a critical task in many disciplines. The list of applications includes images compression, noise reduction, seismic inversion, latent semantic indexing (LSI), principal component analysis, regularization for ill-posed problems, and so on. A practical means to tackle this low rank approximation, if the 2-norm or the Frobenius norm is used in the measurement of closeness, is the truncated singular value decomposition (TSVD) method [5,6,17,22]. When the desired rank is relatively low and the data matrix is large and sparse, a complete SVD becomes too expensive. Some less expensive alternatives for numerical computation, e.g., the Lanczos bidiagonalization process [30,37] and the Monte-Carlo algorithm [34], are available. Some geometric properties of low rank symmetric matrices are discussed in [25]. None of these methods, however, can address the underlying matrix structure that is also part of the constraint. This introductory note is meant to provide some initial investigations into this structured low rank approximation problem. We shall treat some mathematical properties, point out some interesting applications, and outline some numerical procedures.

A general structured low rank approximation problem can be described as follows.

Problem 1.1. Given a matrix $A \in \mathbb{R}^{m\times n}$, an integer k, $1 \leqslant k < \operatorname{rank}(A)$, a class of matrices Ω, and a fixed matrix norm $\|\cdot\|$, find a matrix $\hat{B} \in \Omega$ of rank k such that

$$\|A - \hat{B}\| = \min_{B\in\Omega,\ \operatorname{rank}(B)=k} \|A - B\|. \tag{1.1}$$

We point out immediately that any feasible approximation B must satisfy both the structural constraint specified by Ω and the rank constraint specified by k. As such, the problem is sometimes referred to as a *structure preserving rank reduction problem*. The structural constraint is immaterial if Ω is simply the entire space $\mathbb{R}^{m\times n}$. On the other hand, the low rank approximation by specially structured matrices becomes a much harder problem. We should also point out that the measurement used in problem (1.1) need not be the usual 2-norm or the Frobenius norm. If other norms are used, solving (1.1) presents another degree of difficulty for TSVD-based methods. We shall see that our approach is capable of handling this general case.

It is worth noting that the low rank approximation can be considered using different settings. Suppose a given matrix A is known a priori to have k singular values larger than ϵ. An idea in [42], for instance, is to find all rank-k approximates $\hat{A}$ such that $\|A - \hat{A}\|_2 < \epsilon$. See also [20] for a similar approximation. The objective in [42] is not to compute an approximate $\hat{A}$ of rank k that minimizes $\|A - \hat{A}\|_2$, but

rather to compute the one in which the approximation error is limited. In contrast, there are no restrictions on the singular values of A in our formulation. Furthermore, our methods compute a best approximate matrix $\hat{A}$ belonging to a specified affine subspace Ω.

A serious challenge associated with problem (1.1) is that generally there is no easy way to characterize, either algebraically or analytically, a given class of structured lower rank matrices. This lack of explicit description of the feasible set makes it difficult to apply classical optimization techniques. In this note we first provide some theoretical insight into the structure preserving low rank approximation problem. We then propose two numerical procedures to tackle this structure preserving rank reduction problem. Our discussion by no means is complete. Further investigation is needed both theoretically and numerically. There appears to be little information available in the literature. We thus consider this article as merely a beginning step toward fully understanding the problem. Nonetheless, we stress that the framework we are about to outline is quite flexible in that the procedures can be applied to problems of any rank, any linear structure, and any matrix norm.

This paper is organized as follows: We first outline some applications in Section 2. In Section 3 we offer some theoretical bases for solving (1.1). Particularly, the existence question of structured low rank matrices is considered. We query the solvability of (1.1) even after knowing that the feasible set is not empty. In Section 4 we discuss a practical way to track down a structured low rank matrix. We utilize a lift-and-project method that alternates iterations between low rank matrices and structured matrices to introduce a point-to-point map $\mathscr{P}_k$ so that from any given initial matrix T its image $\mathscr{P}_k(T)$ is expected to satisfy both the structural and the rank conditions. In Section 5 we propose two procedures that reformulate the problem in such a way that standard optimization software can be applied directly to seek for numerical solutions. The first approach uses the SVD as a way to characterize low rank matrices. The desired matrix structure is then formulated as a set of equalities among the singular values and singular vectors. The resulting formulation becomes an equality constrained optimization problem. The second approach involves using the point-to-point map $\mathscr{P}_k(T)$ as a handle to capture structured low rank matrices. The resulting formulation becomes an unconstrained optimization problem. Along with the discussions of these methods, we demonstrate our ideas by experimenting with some existing software packages. The structure preserving rank reduction problem presents many challenges in both analytic and computational aspects. It is hoped that the discussion in this article will help to generate some further interest and research in this direction.

2. Applications

In this paper we shall limit our attention to the case where the structured matrices form an affine subspace Ω. This class of constraints arises naturally in applications

due to the interrelation of matrix elements in some prescribed fashion. The so called *linear structure* in [5], for instance, is an affine constraint. Some examples of linear structure include symmetric Toeplitz, block Toeplitz, Hankel, upper Hessenberg, Sylvester, or banded matrices with fixed bandwidth. On the other hand, the low rank condition is often predestined and is inherent to the system behind the physical setup. In addition to being of theoretical interest in its own right, the structure preserving rank reduction problem (1.1) deserves consideration also for practical reasons. We shall briefly mention some applications in this sections.

Low rank approximation is a common tool used for noise removal in signal processing or image enhancement. Many research results, particularly in the signal processing application, can be found. We mention [3–5,12,28,36,38,43,44] as a few starting points for further study. Because research activities in this area have been vigorous and literature is abundantly available, we shall not discuss any specific application to save space. Generally speaking, the underlying covariance matrix often has Toeplitz or block Toeplitz structure. The rank to be removed corresponds to the noise level where the signal to noise ratio is low.

Likewise, low rank approximation can be used for model reduction problems in speech encoding and filter design [14,35,41]. The underlying structure often is Hankel [15,29,33,39]. The rank to be restored corresponds to the number of sinusoidal components contained in the original signal. An example is given in Section 3.1.

Structured low rank approximation also finds applications in computer algebra. One fundamental question in algebra is to compute the greatest common divisor (GCD) of polynomials. To compute the exact GCD for a system of polynomials, it suffices to know how to compute the GCD for two given two polynomials. Given two polynomials $p(x) = a_n \prod_{i=1}^{n}(x - \alpha_i)$ and $q(x) = b_m \prod_{j=1}^{m}(x - \beta_j)$, it is known that the resultant of $p(x)$ and $q(x)$ with respect to x, is zero if and only if $p(x)$ and $q(x)$ have common divisors. The resultant is the determinant of the Sylvester matrix $S(p(x), q(x))$ where

$$S(p(x), q(x)) = \begin{bmatrix} a_n & a_{n-1} & \dots & a_0 & 0 & \dots & 0 \\ 0 & a_n & \dots & & a_0 & & \\ \vdots & & \ddots & & & & \\ 0 & 0 & 0 & a_n & a_{n-1} & \dots & a_0 \\ b_m & b_{m-1} & \dots & & b_0 & \dots & 0 \\ \vdots & & \ddots & & & \ddots & \\ 0 & 0 & 0 & b_m & & \dots & b_0 \end{bmatrix}. \tag{2.1}$$

The rank deficiency of $S(p(x), q(x))$ therefore is precisely the degree of the GCD [11,27]. Suppose now the coefficients of the given polynomials are inexact. An interesting question is to compute a pair of polynomials with a nontrivial common divisor close to the given polynomials. In this way, the problem of approximating the GCD for polynomials can be formulated as a low rank approximation problem with Sylvester structure. Similar formulation can be set up for multivariate polynomials.

Low rank approximation can also be applied to molecular structure modelling for the protein folding problem in $\mathbb{R}^3$. It is known that the three-dimensional shape of a protein largely determines how the protein functions or acts. It is an incredibly important problem of determining a three-dimensional structure of a protein. Assuming that the sequence of amino acid molecules are located at points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in $\mathbb{R}^3$, their relative positions then gives rise to the Euclidean distance matrix $E = [e_{ij}] \in \mathbb{R}^{n\times n}$ where $e_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2$ for $i, j = 1, \ldots, n$. If we knew all the interatomic distances in the protein, the three-dimensional structure would relatively easy to be generated. It can be proved that D is of rank no more than five [18]. The trouble is that with current technologies, such as X-ray crystallography, we cannot "see" well the entries in the matrix D. Thus we have an observed matrix that is not quite a distance matrix. A symmetric and nonnegative matrix of rank 5 is a necessary condition for the approximation [19].

Finally, we remark that in LSI application, the low rank approximation should be the principal factors capturing the random nature of the indexing matrix [9]. Also, there are some discussions on using structure preserving rank reduction computation as a regularization tool in the solution of certain ill-posed inverse problems [22,23].

3. Theoretical considerations

In this section we address some primary notions related to the approximation by structured low rank matrices. Two basic questions are raised in this section with only partial answers: the first question concerns the feasible set. Can structured matrices have arbitrary lower rank? The second question concerns the solvability. Can a given matrix always be approximated by a matrix with a specific structure and a specific lower rank?

3.1. Substance of feasible set

Before any numerical method is attempted, a fundamental question associated with problem (1.1) is whether low rank matrices with specified structure actually exist. Toward that end, we first observe the following result.

Theorem 3.1. *Given a matrix $A \in \mathbb{R}^{m\times n}$, an integer k, $1 \leqslant k < \operatorname{rank}(A)$, a closed subset Ω of matrices in $\mathbb{R}^{m\times n}$, and a fixed matrix norm $\|\cdot\|$, the matrix approximation problem*

$$\min_{B\in\Omega,\ rank(B)\leqslant k} \|A - B\| \tag{3.1}$$

is always solvable, as long as the feasible set is nonempty.

We quickly point out that problem (3.1) is different from problem (1.1). In (3.1) the rank condition is less than or equal to k while in (1.1) the rank condition is

required to be exactly equal to k. In (3.1) the feasible matrices form a closed set while in (1.1) the feasible set might be open. Pathologically it is possible that a given target matrix A does not have a nearest structured rank-k matrix approximation, but does have a nearest structured matrix approximation that is of rank $k-1$ or lower. That is, it is pathologically possible that problem (3.1) has a solution while (1.1) does not. See Section 3.2 for more comments.

For special classes of matrices, it is sometime possible to prove that low rank matrices with specified structures do exist. We mention two specific examples below.

Theorem 3.2. *Symmetric Toeplitz matrices can have arbitrary lower rank.*

Theorem 3.3. *There are $n \times n$ Hankel matrices with any given lower rank.*

The construction in Theorem 3.3 in fact is a known correspondence between low rank Hankel matrices and noiseless time-domain signals comprising k components of exponentially decaying sinusoids [3,6,31,33]. When noise is added to H, the rank k is lost. In this instance, one of the prevailing reasons for considering (1.1) where A stands for the noisy data matrix is to gain insight into the original signal by removing the noise, maintaining the Hankel structure, and reducing the rank. A specific and detailed application of the structure preserving rank reduction problem to medical science can be found in the lecture note by de Beer [3].

For engineering applications, the existence question might not be as important as deriving a reliable method for achieving a closest possible approximation matrix. The question itself, however, is an important step before such an achievement can be obtained. For other types of linear structures, the existence question generally is a challenging algebraic problem that is of interest in its own right. We are not aware of any definitive studies on this subject.

3.2. Solvability of nearest approximation

Even if we could establish the fact that the feasible set of (1.1) is not empty, it remains to find a nearest approximation to the given (noisy) target matrix from within the feasible set. We must be cautious, however, that the existence of lower rank matrices of specified structure does not guarantee that one of such matrices will be *closest* to a given target matrix.

It appears that very little is known about the solvability of problem (1.1). Similar comments were echoed in the discussion [33]. A proof that problem (1.1) is solvable (recall Theorem 3.1) for a specific structure Ω would be a significant accomplishment. We speculate that one of the difficulties in proving the solvability is due to its *finite dimensionality*. For the infinite-dimensional case, the solvability issue is completely settled by the following result [1,2]. It does not seem possible that the proof can be extended to finite-dimensional matrices.

Theorem 3.4. *Suppose the underlying matrices are of infinite dimension. Then the closest approximation to a Hankel matrix by a low rank Hankel matrix always exists and is unique.*

The difference between finding a structured low rank matrix and finding the closest structured low rank approximation to a given target matrix need to be carefully discerned. Indeed, in the latter part of this paper we shall point out that a popular method, the Cadzow algorithm [3,6], somehow has overlooked this distinction. As a result, the Cadzow algorithm only finds a structured low rank matrix that is *nearby* a given target matrix, but certainly is not the closest even in the local sense. We shall provide a numerical example that shows that the Cadzow algorithm does not give rise to the nearest structured low rank approximation.

4. Tracking structured low rank matrices

If low rank matrices with a specified structure cannot be characterized analytically, we must devise other means to accomplish this construction. In this section we introduce a mechanism that is capable of tracking down low rank matrices of any linear structure iteratively, if such a matrix exists. The idea is equivalent to a special application of Cadzow's composite property mapping algorithm [5] that, in turn, is a variation of von Neumann's alternating projection scheme [8,16,24,40].

4.1. Alternating projection method

Imagine that the set of all rank-k matrices forms a surface $\mathscr{R}(k)$ and the set Ω comprising matrices with the specified structure forms another surface. Then the desired set of structured rank-k matrices can be regarded as the intersection of these two geometric entities. A linearly convergent method, called *lift-and-project*, can be formulated to find points at this intersection. The basic idea is to alternate projections between these two sets so that the rank constraint and the structural constraint are satisfied alternatively while the distance in between is being reduced. The algorithm is outlined below. The geometry of lift and project is depicted in Fig. 1.

Algorithm 4.1 (*Lift-and-project algorithm*). Let Ω denote the set of matrices with the specified structure. Starting with an arbitrary $A^{(0)} = A \in \Omega$, iterate the following two steps for $\nu = 0, 1, \ldots$ until convergence:

1. **LIFT**. Compute the rank-k matrix $B^{(\nu)}$ in $R(k)$ that is nearest to $A^{(\nu)}$.
2. **PROJECT**. Compute the projection $A^{(\nu+1)}$ of $B^{(\nu)}$ onto the subspace Ω.

To carry out these steps in action, we remark that the lift usually can be done by the TSVD. That is, from $A^{(\nu)} \in \Omega$, first compute its SVD

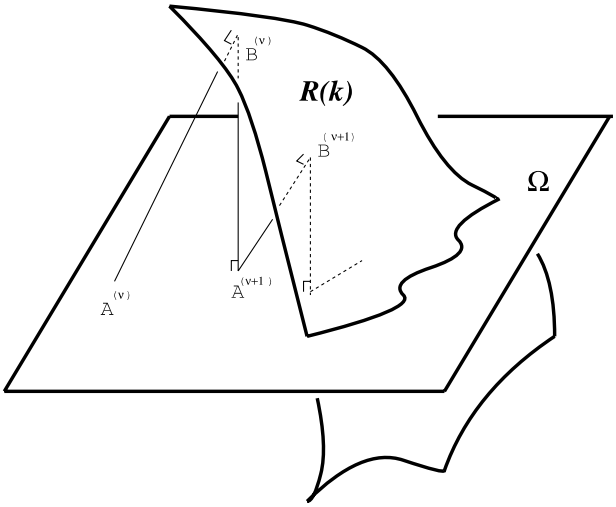

Fig. 1. Algorithm 4.1 with intersection of lower rank matrices and Toeplitz matrices.

$$A^{(\nu)} = U^{(\nu)}\Sigma^{(\nu)}V^{(\nu)^{\mathrm{T}}}.$$

Let $s_1^{(\nu)}, s_2^{(\nu)}, \ldots$ denote the singular values along the diagonal of $\Sigma^{(\nu)}$. Replace the matrix $\Sigma^{(\nu)}$ by $\mathrm{diag}\{s_1^{(\nu)}, \ldots, s_k^{(\nu)}, 0, \ldots, 0\}$ and define

$$B^{(\nu)} := U^{(\nu)}\Sigma^{(\nu)}V^{(\nu)^{\mathrm{T}}}.$$

In turn, the projection usually involves solving a few simple (linear) equations whose setup depends upon the structure in Ω.

In the process of lifting and projecting, the sequence $\{A^{(\nu)}\}$ of matrices will not necessarily have the desirable rank k. However, it is clear that

$$\|A^{(\nu+1)} - B^{(\nu+1)}\|_{\mathrm{F}} \leqslant \|A^{(\nu+1)} - B^{(\nu)}\|_{\mathrm{F}} \leqslant \|A^{(\nu)} - B^{(\nu)}\|_{\mathrm{F}}. \tag{4.1}$$

Thus, Algorithm 4.1 is a descent method. In the above, we should clarify that this descent property (4.1) is measured only with respect to the Frobenius norm which is not necessarily the same norm used in problem (1.1). Regardless of whichever norm $\|\cdot\|$ is used in (1.1), the descent property (4.1) of Algorithm 4.1 guarantees that if all $A^{(\nu)}$ are distinct then the iteration converges to a structured matrix of rank k. In principle, it is possible that the iteration could be trapped in an impasse where $A^{(\nu)}$ and $B^{(\nu)}$ will not improve any more. That will be the case when, for example, $\mathscr{R}(k) \cap \Omega = \emptyset$.

As an illustration, the projection for the case $\Omega = \mathscr{T}_n$ of symmetric Toeplitz matrices is particularly simple. The diagonals of $A^{(\nu+1)}$ are simply the averages of diagonals of $B^{(\nu)}$, respectively. For structures other than Toeplitz, only minor modification in the projection part is needed (see, for example [19,26]).

4.2. A point-to-point map

The usefulness of the above lift and project approach is that it provides a means to calculate a point $P_k(T) \in \Omega \cap \mathscr{R}(k)$ for each given $T \in \Omega$. The map

$$P_k : \Omega \longrightarrow \Omega \cap \mathscr{R}(k) \tag{4.2}$$

is defined to be the limit point $P_k(T)$ if the above lift-and-project iteration procedure starting with T converges.

Despite of the descent property (4.1), one must not be mistaken to think that $P_k(T)$ is the *closest* rank-k matrix in Ω to T. Given a target matrix A, the resulting $P_k(A)$ is *not* the solution to the structure preserving rank reduction approximation problem (1.1). Unfortunately, we have seen in many references citing that $P_k(A)$ is the solution.

It is worth noting that, even in the case $n = 2$, the iteration procedure in Algorithm 4.1 with $k = 1$ applied to toeplitz$(t_1, 0)$ or toeplitz$(0, t_2)$ converges to the zero matrix, instead of a rank one matrix. This observation suggests that the map P_1 can be at most piecewise continuous. This observation also reiterates what we have discussed in Theorem 3.1, that the nearest point is not necessarily of the desired rank k matrix.

5. Numerical methods

In this section we begin to touch upon numerical methods for solving the structure preserving rank reduction problem (1.1). With the understanding that there is a mammoth volume of research on this topic in engineering literature alone and that new methods are continually being developed, our goal has to be limited. Our purpose is not to evaluate or compare existing methods. Rather, we are proposing a general computational framework that can accommodate any kind of structure, any kind of norm, and any low rank and. It is also helpful that our formulation can easily adapt existing optimization package to solve the problem. It is the concept, not the implementation details, that we want to emphasize in this section.

We shall recast the problem in two different optimization formulations. The difference between these two formulations is the way we parameterize the structured low rank matrices. Along with the discussion, we shall use some very primitive experimental results to demonstrate our approach. A similar setting, employing penalty techniques, has recently been studied in [33].

5.1. Explicit optimization

One convenient way to parameterize low rank matrices is via the SVD. That is, any rank k square matrix M can be identified by the triplet (U, Σ, V) if $M = U\Sigma V^{\mathrm{T}}$, where U and V are orthogonal matrices and $\Sigma = \mathrm{diag}\{s_1, \ldots, s_k, 0, \ldots, 0\}$ with $s_1 \geqslant \cdots \geqslant s_k > 0$. We use the singular values $s_1, \ldots, s_k$ as well as entries in U and

V as parameters to specify a low rank matrix. Any structural constraints can then be qualified via a set of algebraic equalities among these variables. A rewriting of (1.1) in this way is called an *explicit formulation*, inferring that every constraint is explicitly represented in the description of the problem. If symmetry is part of the structural constraint, then nonzero eigenvalues and the corresponding eigenvectors in the spectral decomposition could be used as the parameterization variables instead. This would effectively reduce the number of unknowns.

Using the symmetric Toeplitz structure to exemplify this idea, in the explicit formulation we intend to minimize the objective function

$$g(\alpha_1, \ldots, \alpha_k, \mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(k)}) := \|A - M(\alpha_1, \ldots, \alpha_k, \mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(k)})\| \quad (5.1)$$

subject to the constraints that, if

$$M(\alpha_1, \ldots, \alpha_k, \mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(k)}) := \sum_{i=1}^{k} \alpha_i \mathbf{y}^{(i)} \mathbf{y}^{(i)^{\mathrm{T}}} = [m_{ij}], \quad (5.2)$$

then

$$m_{j,j+s-1} = m_{1,s}, \quad s = 1, \ldots, n-1, \quad j = 2, \ldots, n-s+1, \quad (5.3)$$

$$\alpha_i \neq 0 \text{ and } \mathbf{y}^{(i)^{\mathrm{T}}} \mathbf{y}^{(j)} = \delta_{ij}, \quad i, j = 1, \ldots, k. \quad (5.4)$$

The algebraic interrelationship among variables $\alpha_1, \ldots, \alpha_k, \mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(k)}$ are used to ensure that M is symmetric Toeplitz, of rank k, and that vectors $\mathbf{y}^i$, $i = 1, \ldots, k$, are mutually orthonormal.

The idea in forming an equality constrained optimization problem such as above can be extended to general cases. For nonsymmetric or rectangular matrices, singular values and singular vectors are used as variables. To reflect various types of structures, we only need to modify the constraint statements (5.3) for the structure and (5.4) for the orthogonality accordingly. Note again that the norm used in (5.1) to measure the closedness of approximation can be arbitrary.

The notion of explicit formulation outlined above is fairly robust. Almost all kinds of structure preserving low rank approximation problems can be rewritten in this way. The drawback, however, is that it induces considerable redundancy in the description of the problem. As an example, it is well known that symmetric Toeplitz matrices have special spectral properties, i.e., $\lceil n/2 \rceil$ of the eigenvectors are symmetric and $\lfloor n/2 \rfloor$ are skew-symmetric [7]. This additional structure of eigenvectors $\mathbf{y}^{(j)}$ has not been taken into account in (5.3). Even if we do want to include this structure in the constraint statements, we face another dilemma because we are not sure which eigenvalue should be associated with, say, an even eigenvector. The formulation does not exploit any additional internal relationship among the current equality constraints. This could cause, inadvertently, additional computational complexity and difficulties as we report below.

In our first experiment, we take advantage of the matrix manipulation capacity in MATLAB and existing routines in its Optimization Toolbox for our application.

Clearly, many other software packages (e.g., [13,32]) can be used as well. The algorithm FMINCON in MATLAB uses a sequential quadratic programming technique to focus on the solution of the Kuhn–Tucker equations that, in turn, are solved by a quasi-Newton updating procedure. As an experiment, we consider the symmetric Toeplitz matrix $A = \text{toeplitz}([1, 2, 3, 4, 5, 6])$ as the given target matrix whose rank is to be reduced. Let the termination tolerance required on the solution as well as on the objective function be set at 10^{-6}. Start with $T^{(0)} = P_k(A)$ as the initial value, we simply ask FMINCON to solve problem (1.1) for $k = 5, 4, 3, 2, 1$, respectively. By default, the code estimates any required derivative information by finite difference approximations. Denote, for each k, the calculated optimal solution by T_k^*, if the algorithm converges. We find that T_5^* (whose values are listed later in Table 2) does give smaller objective value than $P_5(A)$. However, for $k < 5$, the iterations by FMINCON simply will not improve the objective values throughout the computation. The exit condition of FMINCON reports that the optimization is terminated successfully, but we find that $\|T_k^* - P_k(A)\| \approx 10^{-6}$, indicating that the optimal solution claimed is considered to be the same as the initial point. One might mistakenly think then (and many did in the literature and applications) that $T_k^* = P_k(A)$ for $k = 4, 3, 2, 1$. However, we shall see below by using other software or algorithms under the same circumstances that this is not the case.

Suppose we turn to the package LANCELOT as the next optimization solver. This code, available on the NEOS Server [10,13,21], is a standard Fortran 77 package for solving large-scale nonlinearly constrained optimization problems. As it turns out, LANCELOT is able to find optimal solutions of problem (5.1) for all values of k without any difficulties. Furthermore, the solutions obtained by using LANCELOT agree, up to the required accuracy 10^{-6}, with those obtained by using our second method (see Table 2). The overhead cost of using LANCELOT for our test problem is reported in Table 1. The "# of variables" used by LANCELOT is $(n + 1)k$ for a problem of size n and desired rank k. The "# of f/c calls" refers to the number of function/gradient evaluations as well the constraint/Jacobian evaluations. The total time in seconds given in Table 1 seems to suggest that the choice of the rank affects the computational cost nonlinearly.

The experience that FMINCON in MATLAB fails and LANCELOT in NEOS succeeds in solving the very same problem (5.1) is a clear signal that any numerical solutions obtained by one algorithm need to be compared carefully with results from

Table 1
Cost overhead in using LANCELOT for $n = 6$

	Rank k				
	5	4	3	2	1
# of variables	35	28	21	14	7
# of f/c calls	108	56	47	43	19
Total time	12.99	4.850	3.120	1.280	0.4300

Table 2
Test results for a case of $n = 6$ symmetric Toeplitz structure using FMINUNC

	Rank k				
	5	4	3	2	1
# of iterations	59	49	39	29	18
# of SVD calls	1013	2914	2200	1860	589
Optimal solution	$\begin{bmatrix}1.1046\\1.8880\\3.1045\\3.9106\\5.0635\\5.9697\end{bmatrix}$	$\begin{bmatrix}1.2408\\1.8030\\3.0352\\4.1132\\4.8553\\6.0759\end{bmatrix}$	$\begin{bmatrix}1.4128\\1.7980\\2.8171\\4.1089\\5.2156\\5.7450\end{bmatrix}$	$\begin{bmatrix}1.9591\\2.1059\\2.5683\\3.4157\\4.7749\\6.8497\end{bmatrix}$	$\begin{bmatrix}2.9444\\2.9444\\2.9444\\2.9444\\2.9444\\2.9444\end{bmatrix}$
$\|A - T_k^*\|$	0.5868	0.9581	1.4440	3.2890	8.5959
Singular values	$\begin{bmatrix}17.9851\\7.4557\\2.2866\\0.9989\\0.6164\\3.4638\text{e}-15\end{bmatrix}$	$\begin{bmatrix}17.9980\\7.4321\\2.2836\\0.8376\\2.2454\text{e}-14\\2.0130\text{e}-14\end{bmatrix}$	$\begin{bmatrix}18.0125\\7.4135\\2.1222\\1.9865\text{e}-14\\9.0753\text{e}-15\\6.5255\text{e}-15\end{bmatrix}$	$\begin{bmatrix}18.2486\\6.4939\\2.0884\text{e}-14\\7.5607\text{e}-15\\3.8479\text{e}-15\\2.5896\text{e}-15\end{bmatrix}$	$\begin{bmatrix}17.6667\\2.0828\text{e}-14\\9.8954\text{e}-15\\6.0286\text{e}-15\\2.6494\text{e}-15\\2.1171\text{e}-15\end{bmatrix}$

other algorithms. We should stress that it is not clear whether the proposed formulation would run into the same difficulties even with LANCELOT as those we have experienced with FMINCON, when the problem size becomes larger. We also should point out that there are many other algorithms available from NEOS [13,21] that we have not tried yet for our problem.

5.2. Implicit optimization

By regarding the function $P_k(T)$ in (4.2) as a way to characterize low rank matrices, the rank reduction problem (1.1) can now be formulated as minimizing the objection function

$$f(T) = \|A - P_k(T)\| \tag{5.5}$$

with $T \in \Omega$. Though $P_k(T)$ may not be defined for all T, the above formulation at least provides us with a handle to manipulate the objective function for most matrices T.

It is important to note that $P_k(T)$ is *not* necessarily the closest rank k approximation to T. Nowhere in Algorithm 4.1 is it suggested that $P_k(A)$ is a solution to (1.1). Unfortunately, in the literature and in many applications, $P_k(A)$ has been mistaken to be the nearest approximation to A. For instance, a quote by Cadzow [5,6] claims that Algorithm 4.1 alone (namely, $P_k(A)$) would serve "as a cleansing process whereby any corrupting noise, measurement distortion or theoretical mismatch present in the given data set (namely, A) is removed". Similar misconception seems to prevail in many other applications using Cadzow's algorithm [3,15,29] and in the discussion in [33]. We emphasize that more need to be done in order to find the *closest* structured low rank approximation to the given A since $P_k(A)$ is known to be merely one candidate in the feasible set. The fact that more has to be done to obtain the *closest* structured low rank matrix has somehow been overlooked. An interesting discussion in [14] suggests that this situation does have some impact on real applications.

With the formulation (5.5) in hand, the structure preserving rank reduction problems become more tractable. The constraint that $T \in \Omega$ can easily be handled. For example, if $\Omega = \mathscr{T}_n$, then only n independent variables $t_1, \ldots, t_n$ are needed to specify $T = \text{toeplitz}([t_1, \ldots, t_n])$. Therefore, the function $P_k(T)$ can actually be written as $P(t_1, \ldots, t_n)$ and can be evaluated point by point by the *black box* function described earlier. We call (5.5) an *implicit formulation* of the structure preserving rank reduction problem, inferring to the fact that the constraints, particularly the rank condition, are hidden inside the point-to-point map $P_k(T)$. We stress that this implicit formulation is in fact an *unconstrained* optimization problem because the structural constraint $T \in \Omega$ can be replaced by independent variables. This is in contrast to the explicit formulation discussed in the preceding section.

Knowing how to compute $P_k(T)$ point by point is sufficient for the application of a wide spectrum of unconstrained optimization methods to problem (5.5). An

ad hoc optimization technique that does not use the gradient information, for example, is the Nelder–Mead simplex search method. The simplex search method (e.g., FMINSEARCH in Matlab) requires only function evaluations, a feature that our point-to-point map $P_k(T)$ can satisfactorily provide. For more sophisticated methods, the gradient information can be calculated by using either numerical or automatic differentiation techniques. Using exactly the same example as in the previous section for the explicit formulation, we apply the the MATLAB routine FMINUNC, a BFGS quasi-Newton method using a mixed quadratic and cubic line search procedure, to the implicit formulation. The results are summarized in Table 2. The "# of iterations" refers to the number of function evaluations of the map P called by the search in FMINUNC. Each call of P requires the computation of SVD several times. The "# of SVD calls" is the number of lifts done in Algorithm 4.1 for the entire calculation. The large number of SVD calls even for this small size toy problem seems to indicate the degree of difficulty for this structure preserving rank reduction problem.

Three important observations are due from this experiment. First, we are able to calculate *all* low rank matrices while maintaining the symmetric Toeplitz structure. This is somewhat surprising. We know from Theorem 3.2 that symmetric Toeplitz matrices can have arbitrary lower rank, but there is no general theory that guarantees the "nearest" symmetric Toeplitz approximation of any lower rank to a given matrix. Is this observation true in general? Does it extend to other structures? This existence question of a solution to problem (1.1) deserves further investigation. Secondly, we note in Table 2 that the distance between A and T_k^* is quite significant, strongly indicating that the noisy data could be substantially "filtered" using our numerical procedures. Thirdly, the optimal Toeplitz T_5^* given in Table 2 has a calculated singular value 3.4638×10^{-15}, suggesting that T_5^* is computationally of rank 5. We remark that T_5^* can only be perceived as a local minimizer, as is generally expected for nonlinear optimization problems. Nevertheless, we note that $\|T_5^* - A\| \approx 0.586797 < 0.589229 \approx \|P_5(A) - A\|$. Although this difference only represents a slight improvement on the objective value, it is a piece of clear evidence that the Cadzow's initial iteration alone does not give rise to an optimal approximation to the noisy data.

6. Conclusions

The structure preserving rank reduction problem concerns the construction of the nearest approximation to a given matrix by a matrix with a specific rank and a specific linear structure. This approximation is needed in many important applications. In this paper we have investigated some theoretical and numerical issues associated with structure preserving rank reduction problems. Many questions remain to be answered. We have proposed two general frameworks to reformulate the problem. We have illustrated how the resulting optimization problems can then be tackled numerically by utilizing existing software packages. Our approach can readily be

generalized to rank reduction problems of any given linear structure and of any given matrix norm.

References

[1] V.J. Adamjan, D.Z. Arov, M.G. Krein, Analytic properties of Schmidt pairs for a Hankel operator and the generalized Schur-Takagi problem, Mat. USSR Sbornik 15 (31–73) (1971).

[2] A. Antoulas, Approximation of linear operators in the 2-norm, Linear Algebra Appl. 278 (1998) 309–316.

[3] R. de Beer, Quantitative in vivo NMR (nuclear magnetic resonance on living objects), http://dutnsic.tn.tudelft.nl:8080/c59_to_html/c59.html, University of Technology Delft, Netherlands, 1995.

[4] J.P. Burg, D.G. Luenberger, D.L. Wenger, Estimation of structured covariance matrices, Proc. IEEE 70 (1982) 963–974.

[5] J.A. Cadzow, Signal enhancement: a composite property mapping algorithm, IEEE Trans. Acoust. Speech Signal Process. ASSP-36 (1988) 39–62.

[6] J.A. Cadzow, D.M. Wilkes, Signal enhancement and the SVD, in: Proceedings of the Second International Workshop on SVD and Signal Processing, University of Rhode Island, Kingston, RI, 1990, pp. 144–151.

[7] A. Cantoni, P. Butler, Eigenvalues and eigenvectors of symmetric centrosymmetric matrices, Linear Algebra Appl. 13 (1976) 275–288.

[8] W. Cheney, A. Goldstein, Proximity maps for convex sets, Proc. Am. Math. Soc. 10 (1959) 448–450.

[9] M. Chu, R. Funderlic, The centroid decomposition: relationships between discrete variational decompositions and SVD, SIAM Matrix Anal. Appl. 23 (2002) 1025–1044.

[10] A.R. Conn, N.I.M. Could, Ph.L. Toint, LANCELOT: a Fortran package for large-scale nonlinear optimization (Release A), in: Springer Series in Computational Mathematics, vol. 17, Springer-Verlag, New York, 1992.

[11] R.M. Corless, P.M. Gianni, B.M. Trager, S.M. Watt, The singular value decomposition for polynomial system, in: Proceedings of the International Symposium on Symbolic and Algebraic Computation, Montreal, Canada, July, 1995, pp. 195–207.

[12] G. Cybenko, Moment problems and low rank Toeplitz approximations, Circuits Systems Signal Process. 1 (1983) 3–4.

[13] J. Czyzyk, M. Mesnier, J. Moré, The network-enabled optimization system (NEOS) server, Preprint MCS-P615-1096, Argonne National Laboratory, 1996. See also http://www.mcs.anl.gov/neos/Server.

[14] B. DeMoor, Total least squares for affinely structured matrices and the noisy realization problem, IEEE Trans. Signal Process. 42 (1994) 3104–3113.

[15] M. Dendrinos, S. Bakamidis, G. Carayannis, Speech enhancement from noise: a regenerative approach, Speech Commun. 10 (45–57) (1991).

[16] F. Deutsch, von Neumann's alternating method: the rate of convergence, in: C. Chui, L. Schumaker, J. Ward (Eds.), Approximation Theory IV, Academic Press, New York, 1983, pp. 427–434.

[17] G.H. Golub, C.F. Van Loan, Matrix Computations, third ed., Johns Hopkins University Press, Baltimore, MD, 1996.

[18] J.C. Gower, Eculidean distance geometry, Math. Scientist 7 (1982) 1–14.

[19] W. Glunt, T.L. Hayden, S. Hong, J. Wells, An alternating projection algorithm for computing the nearest Euclidean distance matrix, SIAM J. Matrix Anal. Appl. 11 (1990) 589–600.

[20] S.A. Goreinov, E.E. Tyrtyshnikov, N.L. Zamarashkin, A theory of pseudoskeleton approximations, Linear Algebra Appl. 261 (1997) 1–21.

[21] W. Gropp, J. Moré, Optimization environments and the NEOS server, Preprint MCS-P654-0397, Argonne National Laboratory, 1997.

[22] P.C. Hansen, The truncated SVD as a method for regularization, BIT 27 (534–553) (1987).
[23] P.C. Hansen, Truncated SVD solution to discrete ill-posed problems with ill-determined numerical rank, SIAM J. Sci. Stat. Comput. 11 (503–518) (1991).
[24] S.P. Han, A successive projection method, Math. Programming 40 (1988) 1–14.
[25] U. Helmke, J. Moore, Optimization and Dynamical Systems, Springer-Verlag, London, 1994.
[26] N.J. Higham, Computing the nearest correlation matrix, preprint, NA Report 369, University of Manchester, 2000.
[27] N.K. Karmarkar, Y.N. Lakshman, On approximate GCDs of unvariate polynomials, J. Symbolic Comput. 26 (1998) 653–666.
[28] H.B. Li, P. Stoica, J. Li, Computationally efficient maximum likelihood estimation of structured covariance matrices, IEEE Trans. Signal Process. 47 (1999) 1314–1323.
[29] B.T. Lilly, K.K. Paliwal, Robust speech recognition using singular value decomposition based speech enhancement, IEEE TENCON—Speech Image Tech. Comput. Telecommun. (1997) 257–260.
[30] G.L. Millhauser, A.A. Carter, D.J. Schneider, J.H. Freed, R.E. Oswald, Rapid singular value decomposition for time-domain analysis of magnetic resonance signals by use of the Lanczos algorithm, J. Magn. Reson. 82 (1989) 150–155.
[31] H.D. Mittelmann, J.A. Cadzow, Continuity of closest rank-p approximations to matrices, IEEE Trans. Acoust. Speech Signal Process. ASSP-35 (1987) 1211–1212.
[32] J.J. Moré, S.J. Wright, Optimization sofware guide, Frontiers Appl. Math. 14 (1993) 11–22.
[33] H. Park, Z. Lei, J.B. Rosen, Low rank approximation of a Hankel matrix by structured total least norm, BIT 39 (1999) 757–779.
[34] A. Prieze, R. Kannaa, Fast Monte-Carlo algorithm for finding low rank approximations, http://www.cs.yale.edu/∼kannan/.
[35] L.L. Scharf, D.W. Tufts, Rank reduction for modeling stationary signals, IEEE Trans. Acoust. Speech Signal Process. 35 (1987) 350–355.
[36] T.J. Schulz, Penalized maximum-likelihood estimation of covariance matrices with linear structure, IEEE Trans. Signal Process. 45 (1997) 3027–3038.
[37] H.S. Simon, H. Zha, Low rank matrix approximation using the Lanczos bidiagonalization process, Technical Report CSE-97-008, Computer Science and Engineering Dept., Penn. State Univ., 1997.
[38] A.K. Shaw, R. Kumaresan, Some structured matrix approximation problems, in: IEEE International Conference on Acoustics, Speech and Signal Processing, New York, NY, April, 1988, pp. 2324–2327.
[39] A.K. Shaw, S. Pokala, R. Kumaresan, Toeplitz and Hankel approximation using structured approach, in: IEEE International Conference on Acoustics, Speech and Signal Processing, Seattle, WA, May, 1998.
[40] T.J. Suffridge, T.L. Hayden, Approximatin by a Hermitian positive semidefinite Toeplitz matrix, SIAM J. Matrix Anal. Appl. 14 (1993) 721–734.
[41] D.W. Tufts, A.A. Shah, Estimation of a signal wave-form from noisy data using low rank approximation to a data matrix, IEEE Trans. Signal Process. 41 (1993) 1716–1721.
[42] A. van der Veen, A Schur method for low-rank matrix approximation, SIAM J. Matrix Anal. Appl. 17 (1996) 139–160.
[43] D.E. Williams, D.H. Johnson, Robust estimation on structured covariance matrices, IEEE Trans. Signal Process. 41 (1993) 2891–2906.
[44] A.E. Yagle, A convergent composite mapping Fourier domain iterative algorithm for 3-D discrete tomography, Linear Algebra Appl. 339 (2001) 91–109.