#### **Structured Low Rank Approximation Lecture II: General Approach**

## Moody T. Chu

North Carolina State University

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# **Syllabus**

- Objectives:
	- $\Diamond$  To provide some preliminaries.
	- $\diamond$  To treat some mathematics.
	- $\Diamond$  To point out some applications.
	- $\diamond$  To describe some algorithms.
- Topics:
	- $\diamond$  Lecture I: Introduction
	- Lecture II: General Approach
	- Lecture III: Distance Geometry and Protein Structure
	- Lecture IV: Singular Value Assignment with Low Rank Matrices
	- Lecture V: Nonnegative Matrix Factorization
- Assignments:
	- Quite <sup>a</sup> few open questions to be answered.
	- Try out various existing optimization codes on large scale low rank approximation problems.

# **Lecture II:**

# **General Approach**

Joint work with Robert Funderlic and Robert Plemmons

# **Outline**

- Problem Description
- Algebraic Structure:
	- Algebraic Varieties
	- $\diamond$ Rank Deficient $3 \times 3$  Toeplitz Matrices
- Constructing Lower Rank Structured Matrices:
	- Lift and Project Method
	- $\diamond$  Parameterization by SVD
- Implicit Optimization
	- Engineers' Misconception
	- $\diamond$  Simplex Search Method
- Explicit Optimization
	- **fmincon** in MATLAB
	- **LANCELOT** on NEOS

# **Structure Preserving Rank Reduction Problem**

• Given

- $\Diamond$  A target matrix  $A \in \mathbb{R}^{n \times n}$ ,
- $\Diamond$  An integer k,  $1 \leq k < \text{rank}(A)$ ,
- $\Diamond$  A class of matrices  $\Omega$  with a specified structure,
- $\Diamond$  a fixed matrix norm  $\|\cdot\|;$

#### Find

 $\Diamond A$  matrix  $\hat{B} \in \Omega$  of rank k, such that

$$
||A - \hat{B}|| = \min_{B \in \Omega, \text{rank}(B) = k} ||A - B||. \tag{1}
$$

# **Difficulties**

- No easy way to characterize, either algebraically or analytically, <sup>a</sup> given class of structured lower rank matrices.
- Lack of explicit description of the feasible set  $\implies$  Difficult to apply classical optimization techniques.
- Little discussion on whether lower rank matrices with specified structure actually exist.

## Feasibility and Approximations

• The Toeplitz matrix

$$
H := \begin{bmatrix} h_n & h_{n+1} & \dots & h_{2n-1} \\ \vdots & & & \vdots \\ h_2 & h_3 & \dots & h_{n+1} \\ h_1 & h_2 & \dots & h_n \end{bmatrix}
$$

with

$$
h_j := \sum_{i=1}^k \beta_i z_i^j, \quad j = 1, 2, \dots, 2n - 1,
$$

where  $\{\beta_i\}$  and  $\{z_i\}$  are two sequences of arbitrary nonzero numbers satisfying  $z_i \neq z_j$  whenever  $i \neq j$  and  $k \leq n$ , is a Toeplitz matrix of rank k.

- The genera<sup>l</sup> Toeplitz structure preserving rank reduction problem as described in (1) remains open.
	- Existence of lower rank matrices of specified structure does not guarantee closest such matrices.
	- $\Diamond$  No  $x > 0$  for which  $1/x$  is minimum.

#### Other Structures?

- For other types of structures, the existence question usually is <sup>a</sup> hard algebraic problem.
- Given real general matrices  $B_0, B_1, \ldots, B_n \in \mathbb{R}^{m \times n}, m \geq n$ , and an integer  $k < n$ ,
	- $\Diamond$  Open Question: Can values of  $\mathbf{c} := (c_1, \ldots, c_n)^\top \in \mathbb{R}^n$  be found such that

$$
B(\mathbf{c}) := B_0 + c_1 B_1 + \ldots + c_n B_n
$$

is of rank k precisely?

 $\Diamond$  Or,  $B(c)$  has a prescribed set of singular values  $\{\sigma_1, \ldots, \sigma_n\}.$ 

## Another Hidden Catch

- The set of all  $n \times n$  matrices with rank  $\leq k$  is a closed set.
- The approximation problem

$$
\min_{B \in \Omega, \text{rank}(B) \le k} \|A - B\|
$$

is always solvable, so long as the feasible set is non-empty.

- $\Diamond$  The rank condition is to be less than or equal to k, but not necessarily exactly equal to k.
- It is possible that a given target matrix A does not have a nearest rank k structured matrix approximation, but does have a nearest structured matrix approximation of rank  $k - 1$  or lower.

# Our Approach

- Introduce two procedures to tackle the structure preserving rank reduction problem numerically.
- The procedures can be applied to problems of any norm, any *linear* structure, and any matrix norm.
- Use the symmetric Toeplitz structure with Frobenius matrix norm to illustrate the ideas.

#### Some other approaches

- (van der Veen'96) Given  $A \in \mathbb{R}^{m \times n}$  which is known to have k singular values less than  $\epsilon$ , find all rank-k matrices  $B \in \mathbb{R}^{m \times n}$  such that
	- $||A B||_2 < \epsilon$ .
	- $\Diamond$  Not seeking the best approximation, only the one in the  $\epsilon$ -neighborhood of A.
	- $\diamond$  No structure involved.
	- Open Question: Can it be done this way for structured matrices?
- (Manton, Mahony, and Hua'03) Consider the weighted low rank approximation

$$
\min_{B \in \mathbb{R}^{m \times n}, \text{rank}(B) \le k} \|A - B\|_{Q}^2,
$$

where

$$
||X||_Q^2 = \text{vec}(X)^\top Q \text{vec}(X)
$$

and  $Q \in \mathbb{R}^{mn \times mn}$  is a SPD matrix.

 $\diamond$  Reformulate the minimization as

$$
\min_{N \in \mathbb{R}^{n \times (n-k)}, N^{\top}N = I} \underbrace{\left(\min_{B \in \mathbb{R}^{m \times n}, BN = 0} \|A - B\|_{Q}^{2}\right)}_{\text{A quadratic prememming problems}}.
$$
\n(2)

A quadratic programming problem

 $\Diamond$  (Schuermans, Lemmerling, Van Huffel'03) Using a modified operator vec<sub>2</sub> to dictate the underlying linear structure.

• (Frieze, Kannan, and Vempala'98) Monte-Carlo algorithm for finding a matrix  $B^*$  of rank at most k so that

$$
||A - B^*||_F \le \min_{B \in \mathbb{R}^{m \times n}, \text{rank}(B) \le k} ||A - B||_F + \epsilon ||A||_F
$$

holds with probability  $1 - \delta$ .

- $\Diamond$  The algorithm takes time polynomial in k,  $1/\epsilon$  and log( $1/\delta$ ) only, and is independent of m, n.
- $\Diamond$  Open question: Can a structure be built in? With what probability?

• Identify a *symmetric* Toeplitz matrix by its first row,

$$
T = T([t_1, \ldots, t_n]) = \begin{bmatrix} t_1 & t_2 & \cdots & t_n \\ t_2 & t_1 & \cdots & t_{n-1} \\ \vdots & & & & \\ t_n & \cdots & & & \\ t_n & t_{n-1} & \cdots & t_2 & t_1 \end{bmatrix}.
$$

 $\Diamond$  T = The affine subspace of all  $n \times n$  symmetric Toeplitz matrices.

• Spectral decomposition of symmetric rank k matrices:

$$
M = \sum_{i=1}^{k} \alpha_i \mathbf{y}^{(i)} \mathbf{y}^{(i)^\top}.
$$
 (3)

• Write  $T = T([t_1, \ldots, t_n])$  in terms of  $(3) \implies$ 

$$
\sum_{i=1}^{k} \alpha_i \mathbf{y}_j^{(i)} \mathbf{y}_{j+s}^{(i)} = t_{s+1}, \ s = 0, 1, \dots, n-1, \ 1 \le j \le n-s
$$
\n<sup>(4)</sup>

 $\Diamond$  Low rank matrices form an *algebraic variety*, i.e, solutions of polynomial systems.

#### Some Examples

• The case  $k = 1$  is trivial.

 $\diamond$  Rank-one Toeplitz matrices form two simple one-parameter families,

$$
T = \alpha_1 T([1, ..., 1]), \text{ or}
$$
  
\n
$$
T = \alpha_1 T([1, -1, 1, ..., (-1)^{n-1}])
$$

with arbitrary  $\alpha_1 \neq 0$ .

• For  $4 \times 4$  symmetric Toeplitz matrices of rank 2, there are 10 unknowns in 6 equations (by dropping the references to  $t_1,\ldots,t_4$ ).

$$
\left\{\begin{array}{ccl} \alpha_1 &:=& \frac{\alpha_2\left(y_1^{(2)}-y_2^{(2)}{}^2\right)}{-y_1^{(1)}{}^2+y_2^{(1)}{}^2},\\ y_3^{(1)} &:=& \frac{y_2^{(1)}y_1^{(2)}y_1^{(1)}+2\,y_2^{(2)}y_2^{(1)}-y_2^{(2)}y_1^{(1)}{}^2}{y_3^{(1)}y_1^{(2)}+y_1^{(1)}y_2^{(2)}}-\\ y_4^{(1)} &:=& -\frac{y_2^{(1)}{}^3y_1^{(2)}{}^2-4\,y_2^{(1)}y_2^{(2)}{}^2-4\,y_1^{(1)}y_1^{(2)}y_2^{(2)}y_2^{(1)}{}^2-2\,y_2^{(1)}y_1^{(1)}{}^2y_1^{(2)}{}^2+3\,y_2^{(1)}y_2^{(2)}y_1^{(1)}{}^2+2\,y_1^{(2)}y_2^{(2)}y_1^{(1)}{}^3}{y_2^{(1)}{}^2y_1^{(2)}{}^2+2\,y_2^{(1)}y_2^{(2)}y_1^{(1)}y_2^{(2)}+y_1^{(1)}y_2^{(2)}{}^2}\\ y_3^{(2)} &:=& -\frac{y_2^{(1)}\,y_1^{(2)}{}^2-2\,y_2^{(1)}y_2^{(2)}-y_1^{(2)}y_2^{(2)}y_1^{(1)}}{y_2^{(1)}y_1^{(2)}+y_1^{(1)}y_2^{(2)}}+\\ y_4^{(2)} &:=& -\frac{3\,y_2^{(1)}{}^2y_1^{(2)}{}^2y_2^{(2)}-4\,y_2^{(1)}y_2^{(2)}{}^3+2\,y_2^{(1)}y_1^{(1)}y_1^{(2)}{}^3-4\,y_2^{(1)}y_1^{(1)}y_2^{(2)}y_1^{(2)}-2\,y_2^{(2)}y_1^{(1)}{}^2y_1^{(2)}+y_1^{(1)}y_2^{(2)}{}^2}{y_2^{(1)}y_1^{(2)}y_1^{(2)}+y_1^{(1)}y_2^{(2)}y_2^{(2)}+y_1^{(1)}y_2^{(2)}{}^2}
$$

The eigstructure of symmetric and centrosymmetric matrices has <sup>a</sup> special parity property, but that has not been taken into account.

Explicit description of algebraic equations for higher dimensional low rank symmetric Toeplitz matrices becomes unbearably complicated.

## About Uniqueness

- Consider rank deficient  $T([t_1, t_2, t_3])$ 
	- $\varphi \det(T)=(t_1 t_3)(t_1^2 + t_1t_3 2t_2^2) = 0.$
	- A union of two algebraic varieties.



Figure 1: Low rank, symmetric, Toeplitz matrices of dimension 3 identified in  $\mathbb{R}^3$ .

• The number of *local* solutions to the structured lower rank approximation problem is not unique.

## Dimensionality

• (Adamjan, Arov and Krein'71) Suppose the underlying matrices are of infinite dimension. Then the closest approximation to <sup>a</sup> Hankel matrix by <sup>a</sup> low rank Hankel matrix always exists and is unique.

## **Constructing Lower Rank Toeplitz Matrices**

• Idea:

- $\Diamond$  Rank k matrices in  $R^{n \times n}$  form a surface  $\mathcal{R}(k)$ .
- $\Diamond$  Rank k Toeplitz matrices =  $\mathcal{R}(k) \bigcap \mathcal{T}$ .
- Two approaches:
	- $\diamond$  Parameterization by SVD:
		- $\triangleright$  Identify  $M \in \mathcal{R}(k)$  by the triplet  $(U, \Sigma, V)$  of its singular value decomposition  $M = U \Sigma V^{\top}$ .
			- · U and V are orthogonal matrices, and
			- $\cdot \Sigma = \text{diag}\{s_1, \ldots, s_k, 0, \ldots, 0\}$  with  $s_1 \geq \ldots \geq s_k > 0$ .
		- $\triangleright$  Enforce the structure.
	- $\Diamond$  Alternate projections between  $\mathcal{R}(k)$  and  $\mathcal T$  to find intersections. (Cheney & Goldstein'59, Catzow'88)

## **Lift and Project Algorithm**

- Given  $A^{(0)} = A$ , repeat projections until convergence:
	- $\Diamond$  **LIFT**. Compute  $B^{(\nu)} \in \mathcal{R}(k)$  nearest to  $A^{(\nu)}$ :
		- $\triangleright$  From  $A^{(\nu)} \in \mathcal{T},$  first compute its SVD

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

 $\rhd$  Replace  $\Sigma^{(\nu)}$  by  $diag\{s_1^{(\nu)}, \ldots, s_k^{(\nu)}, 0, \ldots, 0\}$  and define

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

**◇ PROJECT**. Compute  $A^{(\nu+1)}$  ∈ T nearest to  $B^{(\nu)}$ :

 $\triangleright$  From  $B^{(\nu)}$ , choose  $A^{(\nu+1)}$  to be the matrix formed by replacing the diagonals of  $B^{(\nu)}$  by the averages of their entries.

- The general approach remains applicable to any other linear structure, and symmetry can be enforced.
	- $\Diamond$  The only thing that needs to be modified is the projection in the projection (second) step.

Geometric Sketch



Figure 2: Lift-and-project algorithm with intersection of low rank matrices and Toeplitz matrices

#### Black-box Function

• Descent property:

$$
||A^{(\nu+1)} - B^{(\nu+1)}||_F \le ||A^{(\nu+1)} - B^{(\nu)}||_F \le ||A^{(\nu)} - B^{(\nu)}||_F.
$$

Descent with respect to the Frobenius norm which is not necessarily the norm used in the structure preserving rank reduction problem.

• If all  $A^{(\nu)}$  are distinct then the iteration converges to a Toeplitz matrix of rank k.

 $\Diamond$  In principle, the iteration could be trapped in an impasse where  $A^{(\nu)}$  and  $B^{(\nu)}$  would not improve any more, but not experienced in practice.

• The lift and project iteration provides a means to define a *black-box function* 

$$
P: \mathcal{T} \longrightarrow \mathcal{T} \bigcap \mathcal{R}(k).
$$

 $\Diamond$  The  $P(T)$  is presumably piecewise continuous since all projections are continuous.

## The graph of  $P(T)$

• Consider  $P: R^2 \longrightarrow R^2$ :

- $\Diamond$  Use the xy-plane to represent the domain of P for 2  $\times$  2 symmetric Toeplitz matrices  $T(t_1, t_2)$ .
- $\Diamond$  Use the *z*-axis to represent the image  $p_{11}(T)$  and  $p_{12}(T)$ ), respectively.



Figure 3: Graph of  $P(T)$  for 2-dimensional symmetric Toeplitz T.

• Toeplitz matrices of the form  $T(t_1, 0)$  or  $T(0, t_2)$ , corresponding to points on axes, converge to the zero matrix.

## **Implicit Optimization**

• Implicit formulation:

$$
\min_{T=\text{toeplitz}(t_1,\ldots,t_n)} \|T_0 - P(T)\|.\tag{5}
$$

- $\Diamond$  T<sub>0</sub> is the given target matrix.
- $\Diamond P(T)$ , regarded as a black box function evaluation, provides a handle to manipulate the objective function  $f(T) := ||T_0 P(T)||$ .
- $\Diamond$  The norm used in (5) can be any matrix norm.
- Engineers' misconception:
	- $\Diamond P(T)$  is not necessarily the closest rank k Toeplitz matrix to T.
	- $\Diamond$  In practice,  $P(T_0)$  has been used "as a cleansing process whereby any corrupting noise, measurement distortion or theoretical mismatch present in the given data set (namely,  $T_0$ ) is removed."
	- $\Diamond$  More needs to be done in order to find the *closest* lower rank Toeplitz approximation to the given  $T_0$  as  $P(T_0)$  is merely known to be in the feasible set.

## Numerical Experiment

- An ad hoc optimization technique:
	- The simplex search method by Nelder and Mead requires only function evaluations.
	- Routine **fminsearch** in MATLAB, employing the simplex search method, is ready for use in our application.
- An example:
	- $\Diamond$  Suppose  $T_0 = T(1, 2, 3, 4, 5, 6).$
	- $\Diamond$  Start with  $T^{(0)} = T_0$ , and set worst case precision to 10<sup>-6</sup>.
	- $\Diamond$  Able to calculate all lower rank matrices while maintaining the symmetric Toeplitz structure. Always so?
	- $\Diamond$  Nearly machine-zero of smallest calculated singular value(s)  $\Longrightarrow T_k^*$  is computationally of rank k.
	- $\Diamond$  T<sup>\*</sup><sub>k</sub> is only a local solution.
	- $\|\mathcal{F}_{k}^*-T_0\| < \|P(T_0)-T_0\|$  which, though represents only a slight improvement, clearly indicates that  $P(T_0)$  alone does not give rise to an optimal solution.



Table 1: Test results for a case of  $n = 6$  symmetric Toeplitz structure

# **Explicit Optimization**

- Difficult to compute the gradient of  $P(T)$ .
- Other ways to parameterize structured lower rank matrices:
	- $\Diamond$  Use eigenvalues and eigenvectors for symmetric matrices;
	- $\Diamond$  Use singular values and singular vectors for general matrices.
	- $\diamond$  Robust, but might have *overdetermined* the problem.

#### An Illustration

• Define

$$
M(\alpha_1,\ldots,\alpha_k,\mathbf{y}^{(1)},\ldots,\mathbf{y}^{(k)}):=\sum_{i=1}^k \alpha_i \mathbf{y}^{(i)} {\mathbf{y}^{(i)}}^\top.
$$

• Reformulate the symmetric Toeplitz structure preserving rank reduction problem *explicitly* as

$$
\min \qquad \|T_0 - M(\alpha_1, \dots, \alpha_k, \mathbf{y}^{(1)}, \dots, \mathbf{y}^{(k)})\|
$$
\n
$$
\tag{6}
$$

subject to 
$$
m_{j,j+s-1} = m_{1,s}
$$
,  
\n $s = 1,... n - 1$ ,  
\n $j = 2,..., n - s + 1$ , (7)

if  $M = [m_{ij}].$ 

 $\diamond$  Objective function in (6) is described in terms of the non-zero eigenvalues  $\alpha_1, \ldots, \alpha_k$  and the corresponding eigenvectors  $\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(k)}$  of M.

 $\Diamond$  Constraints in (7) are used to ensure that M is symmetric and Toeplitz.

- For other types of structures, we only need modify the constraint statement accordingly.
- The norm used in  $(6)$  can be arbitrary but is fixed.

#### Redundant Constraints

- Symmetric centro-symmetric matrices have special spectral properties (Cantoni and Butler'76):
	- $\circ$  [n/2] of the eigenvectors are symmetric; and
	- $\Diamond \lfloor n/2 \rfloor$  are skew-symmetric.
		- $\triangleright \mathbf{v} = [v_i] \in \mathbb{R}^n$  is symmetric (or skew-symmetric) if  $v_i = v_{n-i}$  (or  $v_i = -v_{n-i}$ ).
- Symmetric Toeplitz matrices are symmetric and centro-symmetric.
- The formulation in  $(6)$  does not take this spectral structure of eigenvectors  $y^{(i)}$  into account.
	- $\diamond$  More variables than needed have been introduced.
	- $\Diamond$  May have overlooked any internal relationship among the  $\frac{n(n-1)}{2}$  equality constraints.
	- $\diamond$  May have caused, inadvertently, additional computation complexity.

# **Using fmincon in MATLAB**

#### • Routine **fmincon** in MATLAB:

- Uses <sup>a</sup> sequential quadratic programming method.
- $\Diamond$  Solve the Kuhn-Tucker equations by a quasi-Newton updating procedure.
- $\Diamond$  Can estimate derivative information by finite difference approximations.
- $\diamond$  Readily available in Optimization Toolbox.
- Our experiments:
	- $\diamond$  Use the same data as in the implicit formulation.
	- $\Diamond$  Case  $k = 5$  is computationally the same as before.
	- $\Diamond$  Have trouble in cases  $k = 4$  or  $k = 3$ ,
		- $\triangleright$  Iterations will not improve approximations at all.
		- $\triangleright$  MATLAB reports that the optimization is terminated successfully.



# **Using LANCELOT on NEOS**

- Reasons of failure of MATLAB are not clear.
	- Constraints might no longer be linearly independent.
	- Termination criteria in **fmincon** might not be adequate.
	- Difficult geometry means hard-to-satisfy constraints.
- Using more sophisticated optimization packages, such as **LANCELOT**.
	- A standard Fortran <sup>77</sup> package for solving large-scale nonlinearly constrained optimization problems (Conn, Could, and Toint'92).
	- $\Diamond$  Break down the functions into sums of *element functions* to introduce sparse Hessian matrix.
	- Huge code. See

*http*:*//www.rl.ac.uk/departments/ccd/numerical/lancelot/sif/sifhtml.html.*

- Available on the NEOS Server through <sup>a</sup> socket-based interface.
- $\diamond$  Uses the  $\bf ADIFOR$  automatic differentiation tool.
- **LANCELOT** works, so far.
	- $\diamond$  Find optimal solutions of problem (6) for all values of k.
	- Results from **LANCELOT** agree, up to the required accuracy 10 −6, with those from **fmins**.
	- $\diamond$  Rank affects the computational cost nonlinearly.

rank $k$					
$\#$ of variables	35	28			
$\#$ of f/c calls	108	56		43	19
total time	12.99	4.850	3.120	1.280	.4300

Table 3: Cost overhead in using  $\text{LANCELOT}$  for  $n = 6$ .

- It is not clear whether the **LANCELOT** would run into the same trouble as **fmincon** when applied to larger size problems.
- There are many other algorithms available in NEOS.

# **Conclusions**

- Structure preserving rank reduction problems arise in many important applications, particularly in the broad areas of signal and image processing.
- Constructing the nearest approximation of <sup>a</sup> given matrix by one with any rank and any linear structure is difficult in general.
- We have proposed two ways to formulate the problems as standard optimization computations.
- It is now possible to tackle the problems numerically via utilizing standard optimization packages.
- The ideas were illustrated by considering Toeplitz structure with Frobenius norm.
- Our approach can be readily generalized to consider rank reduction problems for any given linear structure and of any given matrix norm.