SQP Algorithms for Solving Toeplitz Matrix Approximation Problem

Suliman Al-Homidan
Department of Mathematical Sciences, King Fahd University of Petroleum and Minerals, Dhahran 31261, PO Box 119, Saudi Arabia E-mail: homidan@kfupm.edu.sa

Abstract

Given an $n \times n$ matrix F, we find the nearest symmetric positive semi-definite Toeplitz matrix T to F. The problem is formulated as a nonlinear minimization problem with positive semi-definite Toeplitz matrix as constraints. Then a computational framework is given. An algorithm with rapid convergence is obtained by l_1Sequential Quadratic Programming (SQP) method.

Key words : non-smooth optimization, positive semi-definite matrix, Toeplitz matrix, SQP method, l_1SQP Method.
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1 Introduction

The problem we are interested in is the best approximation of a given matrix by a positive semi–definite symmetric Toeplitz matrix. Toeplitz matrices appear naturally in a variety of problems in engineering. Since positive semi–definite Toeplitz matrices can be viewed as shift invariant autocorrelation matrices, considerable attention has been paid to them, especially in the areas of stochastic filtering and digital signal processing applications [7] and [12]. Several problems in digital signal processing and control theory require the computation of a positive definite Toeplitz matrix that closely approximates a given matrix. For example, because of rounding or truncation errors incurred while evaluating F, F does not satisfy one or all conditions. Another example in the power spectral estimation of a wide–sense stationary process from a finite number of data, the matrix F formed from the estimated autocorrelation coefficients, is often not a positive definite Toeplitz matrix [11]. In control theory, the Gramian assignment problem for discrete–time single input system requires the computation of a positive definite Toeplitz matrix, which also satisfies certain inequality constraints [9].

We consider the following problem: Given a data matrix $F \in \mathbb{R}^{n \times n}$, find the nearest symmetric positive semi-definite Toeplitz matrix T to F and rank $T = m$. Use of the Frobenius norm as a measure gives rise to

$$\begin{array}{ll} \text{minimize} & \phi = \|F - T\| \\ \text{subject to} & T \in K, \end{array} \tag{1.1}$$

where K is the set of all $n \times n$ symmetric positive semi-definite Toeplitz matrices

$$K = \{T : T \in \mathbb{R}^{n\times n}, T^T = T,\ T \geq 0 \ \text{ and } \ T \ \in \ \mathcal{T}\} \tag{1.2}$$

where $\mathcal{T}$ is the set of all Toeplitz matrices.

The problem is formulated as a nonlinear minimization problem with positive semi-definite Toeplitz matrix as constraints. Then a constraints formulation is given. An algorithm with rapid convergence is obtained by the l_1Sequential Quadratic Programming method. In Section 4 we give some numerical examples.

A symmetric Toeplitz matrix T is denoted by

$$T = \begin{bmatrix} t_1 & t_2 & \dots & t_n \\ t_2 & t_1 & \dots & t_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ t_n & t_{n-1} & \dots & t_1 \\ \end{bmatrix} = \text{Toeplitz}(t_1, t_2, \dots, t_n). \tag{1.3}$$

Matrices innerproduct is defined by

$$A : B = \sum a_{ij} b_{ij} + tr(A^T B)$$

2 Constraints Formulation

It is difficult to deal with the matrix cone constraints in (1.2) since it is not easy to specify if the elements are feasible. Using partial LDL^T factorization of T, this difficulty can be overcome. Since m, the rank of T, is known, therefore for F sufficiently close to T, the partial factors $T = LDL^T$ can be calculated such that

$$L \ = \ \begin{bmatrix} L_{11} & \\ L_{21} & I \end{bmatrix}, D \ = \ \begin{bmatrix} D_1 & \\ & D_2 \end{bmatrix}, T \ = \ \begin{bmatrix} T_{11} & T_{21}^T \\ T_{21} & T_{22} \end{bmatrix}, \tag{2.1}$$

where L_{11}, D_1 and T_{11} are $m \times m$ matrices; I, D_2 and T_{22} are $n - m \times n - m$ matrices; L_{21} and T_{21} are $n - m \times m$ matrices; D_1 is diagonal and $D_1 > 0$ and D_2 has no particular structure other than symmetry. At the solution, $D_2 = 0$ and T is symmetric positive semi-definite Toeplitz matrix. In general,

$$D_2(T) \ = \ T_{22} \ - \ T_{21} T_{11}^{-1} T_{21}^T. \tag{2.2}$$

Now if the structure of the matrix T is in a Toeplitz form, i.e.

$$T = \text{Toeplitz}(x_1, x_2, \dots, x_n), \tag{2.3}$$

then (2.2) enables the constraint $T \in K$ to be written in the form

$$D_2(T(\mathbf{x})) = 0 \tag{2.4}$$

Hence, (1.1) can now be expressed as

$$\begin{aligned} &\text{minimize} \quad \phi \\ &\text{subject to} \quad D_2(T) \;=\; 0 = Z^T T Z, \end{aligned} \tag{2.5}$$

where

$$Z \;=\; \begin{bmatrix} -T_{11}^{-1}T_{21}^T \\ I \end{bmatrix}$$

is the basis matrix for the null space of T when $D_2 = 0$. The Lagrange multipliers for the constraint (2.4) is Λ relative to the basis Z and the Lagrangian for porblem (2.5) is

$$\mathcal{L}(\mathbf{x}^{(k)}, \Lambda^{(k)}) \;=\; \phi - \Lambda : Z^T T Z. \tag{2.6}$$

This approach has been studied in a similar way by [5].

3 The SQP Algorithms

In this section various iterative schemas are investigated in order to develop an algorithms for solving problem (2.5). We use techniques related to SQP which provide global convergence at a second order rate. The structure of the Toeplitz matrix T has been given in (2.3), then

$$\begin{aligned} \phi \quad &= \sum_{i,j=1}^{n} (f_{ij} - a_{ij})^2 \\ &= \sum_{i,j=1}^{n} (f_{ij} - x_{|i-j+1|})^2, \end{aligned} \tag{3.1}$$

and $\bigtriangledown\phi \;=\; (\partial\phi/\partial x_1, \ldots, \partial\phi/\partial x_n)^T$ where ∇ denotes the gradient operator $(\partial/\partial x_1, \;\ldots,\; \partial/\partial x_n)^T$. Therefore

$$\frac{\partial\phi}{\partial x_1} = 2\sum_{i=1}^{n}(x_1 - f_{ii})$$

and

$$\frac{\partial\phi}{\partial x_{s+1}} = 2\{\sum_{i=1}^{n-s}(x_{s+1} - f_{i+s,i}) \;+\; (x_{s+1} - f_{i,i+s})\}$$

where $s = 1, \cdots, n-1$. Differentiating again gives

$$\frac{\partial^2\phi}{\partial x_r \partial x_s} = 0 \qquad \mathit{if} \quad r \neq s,$$

$$\frac{\partial^2 \phi}{\partial x_1^2} = 2(n)$$

and

$$\frac{\partial^2 \phi}{\partial x_{s+1}^2} = 4(n-s) \tag{3.2}$$

where $s = 1, \cdots, n-1$.

The advantage of formula (2.4) is that expressions for both first and second derivatives of the constraints with respect to the elements of T can be obtained. The simple form of (2.2) is utilized by writing the constraints $D_2(T) = 0$ in the following form:

$$d_{ij}(\mathbf{x}) \;=\; x_{|i-j+1|} - \sum_{k,l=1}^{m} x_{i-k+1}[T_{11}^{-1}]_{kl}\; x_{j-l+1} = 0$$

where $i, j = m+1, \cdots, n$ and $[T_{11}^{-1}]_{kl}$ denotes the element of T_{11}^{-1} in kl–position.

Thus (2.5) can be expressed as

$$\begin{aligned} &\text{minimize} \;\; \phi = \sum_{i,j=1}^{n} (f_{ij} - x_{|i-j+1|})^2. \\ &\text{subject to } d_{ij}(\mathbf{x}) \;=\; 0 \end{aligned} \tag{3.3}$$

In this problem, since the equivalent constraints $d_{ij}(\mathbf{x}) = 0$ and $d_{ji}(\mathbf{x}) = 0$ are both present, they would be stated only for $i \geq j$.

In order to write down the SQP method applied to (3.3), it is necessay to derive first and second derivatives of d_{ij} which enable a second order rate of convergence to be achieved.

Let I_s be an $m \times m$ matrix given by

$$I_s = \text{Toeplitz}(0, \ldots, 0, 1, 0, \ldots, 0),$$

where the "1" appears in the s-position. Hence the matrix I_s is a matrix that contains "1"s in two off diagonal and zeros elsewhere. Now differentiating $T_{11}T_{11}^{-1} = I$ gives

$$\begin{aligned} \frac{\partial T_{11}}{\partial x_s} T_{11}^{-1} + T_{11}\frac{\partial T_{11}^{-1}}{\partial x_s} &= 0 \qquad s = 1, \ldots, n \\ \Rightarrow \qquad T_{11}\frac{\partial T_{11}^{-1}}{\partial x_s} &= -\frac{\partial T_{11}}{\partial x_s} T_{11}^{-1} \end{aligned}$$

then

$$\frac{\partial T_{11}^{-1}}{\partial x_s} \;=\; -\; T_{11}^{-1}\,\frac{\partial T_{11}}{\partial x_s} T_{11}^{-1},$$

but since

$$\frac{\partial T_{11}}{\partial x_s} \;=\; I_s$$

then

$$\frac{\partial T_{11}^{-1}}{\partial x_s} \;=\; -\; T_{11}^{-1}\; I_s\; T_{11}^{-1}. \tag{3.4}$$

Hence from (2.2)

$$\frac{\partial D_2}{\partial x_s} \;=\; \frac{\partial}{\partial x_s}(T_{22} \;-\; T_{21}T_{11}^{-1}T_{21}^T) \tag{3.5}$$

$$\begin{aligned} &= \; II_s - \; III_sT_{11}^{-1}T_{21}^T + \; T_{21}T_{11}^{-1}I_sT_{11}^{-1}T_{21}^T \\ &\qquad\qquad -\; T_{21}T_{11}^{-1}III_s^T \end{aligned} \tag{3.6}$$

where

$$\frac{\partial T_{22}}{\partial x_s} = II_s$$

and

$$\frac{\partial T_{21}}{\partial x_s} = III_s$$

are matrices similar to I_s with II_s being an $n-m \times n-m$ matrix which contains ones in two off diagonal and zeros elsewhere, and III_s is an $n-m \times m$ matrix which contains ones in one off diagonal and zeros elsewhere.

Let

$$V^T = -T_{21}T_{11}^{-1} \quad \mathit{and} \quad W = III_sV$$

then (3.6) becomes

$$\frac{\partial D_2}{\partial x_s} \;=\; II_s + V^T I_s V + W^T + W$$

Furthermore, differentiating (3.4), we get

$$\frac{\partial^2 D_2}{\partial x_s \partial x_r} = Y + Y^T$$

where

$$Y = -Z_r^T T_{11}^{-1} Z_s \quad \mathit{and} \quad Z_t = I_tV - III_t^T$$

Therefore

$$\frac{\partial^2 d_{ij}}{\partial x_s \partial x_r} \;=\; y_{ij} + y_{ji}$$

where $i, j = m+1, \cdots, n$.

Now let

$$\begin{aligned} W &= \nabla^2 \mathcal{L}(\mathbf{x}, \Lambda) \\ &= \nabla^2 \phi - \sum_{i,j=m+1}^{n} \lambda_{ij} \nabla^2 d_{ij} \end{aligned} \tag{3.7}$$

where $\nabla^2 \phi$ is given by (3.2) and

$$\sum_{i,j=m+1}^{n} \lambda_{ij} \nabla^2 d_{ij} = \begin{bmatrix} \sum_{i,j} \lambda_{ij} \frac{\partial^2 d_{ij}}{\partial x_1 \partial x_1} & \cdots & \sum_{i,j} \lambda_{ij} \frac{\partial^2 d_{ij}}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \sum_{i,j} \lambda_{ij} \frac{\partial^2 d_{ij}}{\partial x_n \partial x_1} & \cdots & \sum_{i,j} \lambda_{ij} \frac{\partial^2 d_{ij}}{\partial x_n \partial x_n} \end{bmatrix}$$

Therefore, the SQP method applied to (3.3) requires the solution of the QP subproblem

$$\begin{aligned} &\text{minimize}_{\boldsymbol{\delta}} \ \phi + \nabla \phi^T \boldsymbol{\delta} + \tfrac{1}{2} \boldsymbol{\delta}^T W \boldsymbol{\delta} \qquad \boldsymbol{\delta} \in \mathbb{R}^m \\ &\text{subject to } d_{ij} + \nabla d_{ij}^T \boldsymbol{\delta} = 0 \qquad i, j = m+1, \ldots, n \end{aligned} \tag{3.8}$$

giving a correction vector $\boldsymbol{\delta}^{(k)}$, so that $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \boldsymbol{\delta}^{(k)}$. Also, the Lagrange multipliers of the equations in (3.8) become the elements $\lambda_{ij}^{(k+1)}$ for the next iteration. Usually, $\nabla^2 \mathcal{L}$ is positive definite, in which case, if $\mathbf{x}^{(k)}$ is sufficiently close to $\mathbf{x}^*$, the basic SQP method converges and the rate is second order (Fletcher [6]). Globally, however (3.8) may not converge. An algorithm with better convergence properties, when $\mathbf{x}^{(k)}$ is remote from $\mathbf{x}^*$, is suggested by Fletcher [4] in which a different subproblem to (3.8) is solved using the expression

$$\begin{aligned} &\text{minimize}_{\boldsymbol{\delta}} \ \phi + \nabla \phi^T \boldsymbol{\delta} + \tfrac{1}{2} \boldsymbol{\delta}^T W \boldsymbol{\delta} + \sigma \sum | \ d_{ij} + \nabla d_{ij}^T \boldsymbol{\delta} | \\ &\text{subject to} \| \boldsymbol{\delta} \| \leq \rho. \end{aligned} \tag{3.9}$$

The solution $\boldsymbol{\delta}^{(k)}$ of this problem is used in the same way as with (3.8).

This description of iterative schemes for solving (3.3) has so far ignored an important constraint that is $D_1 > 0$ in which the varibles $\mathbf{x}^{(k)}$ must permit the matrix $T^{(k)}$ to be factorized as in (2.1). However if m is identified correctly and $\mathbf{x}^{(k)}$ is near the solution this restriction will usually be inactive at the solution. If $\mathbf{x}^{(k)}$ is remote from the solution additional constraints are introduced

$$d_{rr}^{(k)} \ + \ \nabla d_{rr}^{(k)T} \boldsymbol{\delta} > 0. \qquad r = 1, 2, \ldots, m$$

However, strict inequalities are not permissible in an optimization problem and it is also advisable not to allow $d_{rr}(\mathbf{x}^{(k)} + \boldsymbol{\delta})$ to become too close to zero, especially for small r, as this is likely to cause the factorization to fail. Hence the constraints

$$\nabla d_{rr}^{(k)T} \boldsymbol{\delta} \geq -r d_{rr}^{(k)} / m \qquad r = 1, 2, \ldots, m$$

are added to the subproblems (3.8) and (3.9). Finally, it may be that partial factors of the matrix $T^{(k)}$ in the form (2.1) do not exist for some iterates. In this case the parameters $\rho^{(k+1)} = \rho^{(k)}/4$, $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$ and $\Lambda^{(k+1)} = \Lambda^{(k)}$ are chosen for the next iteration in the trust region method.

4 Numerical Examples and Results

For testing the algorithms described above, the following examples are considered:

Example 1.

Consider problem (3.3) in which

$$F = \begin{bmatrix} 3 & 2 & 3 \\ 2 & 4 & 1 \\ 3 & 1 & 5 \end{bmatrix}, \quad \text{and} \quad m = 2 \tag{4.1}$$

The solution is

$$T^* = \begin{bmatrix} 3.6 & 1.5 & 3.6 \\ 1.5 & 3.6 & 1.5 \\ 3.6 & 1.5 & 3.6 \end{bmatrix} \tag{4.2}$$

T^* is Toeplitz positive semi–definite. Its partial factors are

$$D = \begin{bmatrix} 3.6 & 0 & 0 \\ 0 & 2.975 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \text{and} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ 0.41671 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

Example 2.

Another example for which $n = 4$ is

$$F = \begin{bmatrix} 3 & 2 & 3 & 4 \\ 5 & 7 & 2 & -1 \\ 6 & 2 & 5 & 4 \\ 5 & 3 & 1 & 2 \end{bmatrix}, \quad \text{with} \quad m = 1. \tag{4.3}$$

Let

$$T^* = \begin{bmatrix} x & y & z & u \\ y & x & y & z \\ z & y & x & y \\ u & z & y & x \end{bmatrix}. \tag{4.4}$$

In general, when $n = 4$, the number of constraints is six, of which three are:

$$d_{22} = x^2 - y^2 = 0 \implies x = y, \qquad d_{33} = x^2 - z^2 = 0 \implies x = z$$

and

$$d_{44} = x^2 - u^2 = 0 \implies x = u.$$

Therefore

$$x = y = z = u$$

and this satisfies the rest of the constraints. Hence the problem will be reduced to minimizing

$$\phi = 16x^2 - 106x + c \tag{4.5}$$

where c is a constant. Thus the minimum value of ϕ is for $x = 106/32$. However, if the required rank is two, then we have three new constraints $d_{33} = 0$, $d_{44} = 0$ and $d_{34} = 0$. One of these constraints is

$$d_{33} = x^3 - 2xy^2 - xz^2 + 2zy^2 = 0 \implies x = z.$$

This reduces the next constraint to

$$d_{44} = x^3 - xy^2 - xz^2 - xu^2 + 2yzu = (y-u)^2 = 0 \implies y = u,$$

and this satisfies the constraint d_{34}. Hence the problem will be reduced to minimizing

$$\phi = 8x^2 - 56x + 8y^2 - 50y + c \tag{4.6}$$

where c is a constant. Thus the minimum value of ϕ is for $x = z = 56/16$ and for $y = u = 50/16$.

The algorithm has been tested on randomly generated matrices with values distributed between 10^{-3} and 10^3. A Fortran codes have been written to program solver for (3.9) using filterSQP. $\|F^{(k)} - F^{(k-1)}\| < 10^{-5}$. Table 1 summarizes the results for the filterSQP Algorithm,

For algorithms, the housekeeping associated with each iteration is $O(n^2)$. Also, if care is taken, it is possible to calculate the gradient and Hessian in $O(n^2)$ operations. For the filter-SQP algorithm, the initial value $m^{(0)}$ is tabulated, and m is increased by one until the solution is found. The total number of iterations is tabulated, and within this figure, it is found that fewer iterations are required as m increases. Also the initial value $m^{(0)}$ is rather arbitrary: a smaller value of $m^{(0)}$ would have given an even larger number of iterations.

5 Conclusions

In this paper we have studied the Toeplitz matrix approximation problem involving the positive semi-definite matrix constraint, using the l_1SQP method. Some Numerical examples are also given. However, the problem needs more study in terms of hybrid methods involving both the current method and a projection method, see [10]. Also some numerical experiments need to be carried out.

n	$m^{(0)}$	m^*	Number of iteration by filterSQP	ϕ
4	1	1	10	2644.1
4	1	3	36	2656.5
5	2	4	29	4013.6
6	2	3	28	5741.2
7	3	6	35	6059.3
8	3	6	49	6591.4
8	3	5	39	8270.9
10	3	6	73	9769.8
15	5	10	64	14274
20	7	15	79	19860

Table 1: Numerical Results.

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