Toeplitz Matrix Approximation

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Abstract

This paper deals with numerical Toeplitz matrix approximation. Our approach is based on (i) a projection algorithm which converges globally but slowly; and (ii) the quasi-Newton method which is faster. Hybrid methods that attempt to combine the best features of both methods are then considered.

Key words : Alternating projections, least distance functions, non-smooth optimization, positive semi-definite matrix, Toeplitz matrix, quasi-Newton method.

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 [12] and [21]. 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 [18]. 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 [16]. 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 that minimizes

$$\text{minimize} \quad \phi = \|F \ - \ T\|_F \tag{1.1}$$

where $\|.\|_F$ denotes the Frobenius norm.

A similar problem was studied by Suffridge et. al. [17]. They solve the problem using the self-inversive polynomial $P(x)$. The roots of the derivative of $\frac{P(z)}{z^{n-1}}$ enable them to approximate the data matrix. They also solve (1.1) using the ideas of a modified alternating projection algorithm that was successfully used in solving similar approximation problems for distance matrices [3]. In [9], alternating convex projection techniques are used to solve the problem. Oh et. al. [15] use alternating projection onto fuzzy convex sets when three or more convex sets do not intersect. Toeplitz matrix approximations are also discussed in [5] and [13].

In the past ten years, there has been much interest in the interior point methods applied to problems with semidefinite matrix constraints (e.g. the survey papers [20], [19] and [22] and the references therein). Semidefinite programming optimizes a linear function subject to positive semidefinite matrix. It is a convex programming problem since the objective and the constraints are convex. In this paper, we deal with a little different problem since the objective is quadratic; also an additional rank constraint is added which makes the problem unconvex and harder to solve. Here, we use a different approach than the interior point methods.

In Section 2, (1.1) is solved using the von Neumann algorithm. In Section 3, the problem is formulated as a smooth unconstrained minimization problem, then solved using the BFGS method. In Section 4, two new hybrid methods are described to solve (1.1): firstly, there is Algorithm 1, which starts with the projection method to determine the rank $m^{(k)}$ and continues with the BFGS method; and secondly, Algorithm 2 is described which solves the problem by the BFGS method and uses the projection method to update the rank.

A symmetric Toeplitz matrix A is denoted by

$$T = \begin{bmatrix} t_1 & t_2 & \dots & t_n \\ t_2 & t_1 & \dots & t_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ t_n & t_{n-1} & \dots & t_1 \end{bmatrix} = \text{Toeplitz}(t_1, t_2, \dots, t_n). \tag{1.2}$$

2 The Projection Algorithm

In this section, we describe a projection algorithm for solving (1.1). This algorithm is derived from an alternating projection algorithm due to Dykstra [6] for finding the least distance from a fixed point to an intersection of convex sets. This algorithm is given independently by Han [10]. An important feature of this algorithm is the generation of formulae for certain projection maps that are needed.

The Dykstra-Han algorithm solves the problem

$$\begin{aligned} &\text{minimize} && \|\mathbf{f} - \mathbf{x}\|_2 \\ &\text{subject to} && \mathbf{x} \in \bigcap_{i=1}^{m} K_i, \end{aligned}$$

where K_i are convex sets in $\mathbb{R}^n$ and $\mathbf{f}$ is given. The algorithm initializes $\mathbf{f}^0 = \mathbf{f}$ and generates a sequence $\{\mathbf{f}^{(k)}\}$ using the iteration formula

$$\mathbf{f}^{(k+1)} = \mathbf{f}^{(k)} + P_m(\ldots P_1(\mathbf{f}^{(k)})\ldots) - P_1(\mathbf{f}^{(k)}). \tag{2.1}$$

Here, $P_i(\mathbf{f})$ denotes the l_2 projection of $\mathbf{f}$ on to K_i; that is, the (unique) nearest vector to $\mathbf{f}$ in K_i. It is shown by Boyle and Dykstra [4] that $P_i(\ldots P_1(\mathbf{f}^{(k)})\ldots) \to \mathbf{x}^*$ for any $i \geq 1$. However, the sequence $\{\mathbf{f}^{(k)}\}$ does not, in general, converge to $\mathbf{x}^*$ (see [2]).

It is convenient to define two convex sets for the purpose of reconstructing (1.1). The set of all $n \times n$ symmetric positive semi-definite matrices

$$K_{\mathbb{R}} \;=\; \{A : A \in \mathbb{R}^{n\times n},\;\; A^T \;=\; A \text{ and } \mathbf{z}^T A\mathbf{z} \;\geq\; 0 \qquad \forall\, \mathbf{z} \in \mathbb{R}^n\} \tag{2.2}$$

is a convex cone of dimension $n(n+1)/2$. Also, define

$$K_{\mathrm{T}} \;=\; \{T : T \in \mathbb{R}^{n\times n},\; T \text{ is Toeplitz}\}, \tag{2.3}$$

which is a subspace of dimension n.

In applying the Dykstra-Han algorithm to the Toeplitz matrix approximation, it is appropriate to use the Frobenius matrix norm, and to express (1.1) as

$$\begin{array}{ll} \text{minimize} & \|F - T\|_F \\ \text{subject to} & T \in K_{\mathbb{R}} \cap K_T, \end{array} \tag{2.4}$$

where $K_{\mathbb{R}}$ and K_T are given by (2.2) and (2.3), respectively.

To apply algorithm (2.1), we need formulae for the projection maps $P_{\mathbb{R}}(.)$ and $P_T(.)$, corresponding, respectively, to $P_1(.)$ and $P_2(.)$ in (2.1). These are the maps from $K = \{A :\; A \in \mathbb{R}^{n\times n}\}$ on to $K_{\mathbb{R}}$ and K_T. The projection map $P_{\mathbb{R}}(F)$ formula on to $K_{\mathbb{R}}$ is given by [11]

$$P_{\mathbb{R}}\,(F) \;= U\Lambda^+ U^T, \tag{2.5}$$

where

$$\Lambda^+ \;=\; \begin{bmatrix} \Lambda_m & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \tag{2.6}$$

and $\Lambda_m \;=\; \text{diag}\,[\lambda_1,\; \lambda_2,\; \ldots,\; \lambda_m]$ is the diagonal matrix formed from the positive eigenvalues of F.

The projection map $P_T(F)$ formula on to K_T is given by

$$P_T(F) \;= \text{Toeplitz}(t_1, t_2, \ldots, t_n), \tag{2.7}$$

where

$$t_{k+1} = \frac{1}{2(n-k)} \sum_{i=1}^{n-k} (f_{i\;\, i+k} + f_{i+k\;\, i}). \qquad k = 1, 2, \ldots, n.$$

We can now use the projection maps $P_{\mathbb{R}}(F)$ and $P_T(F)$ given by (2.5) and (2.7) to implement the Dykstra-Han algorithm (2.1). Given a distance matrix $F \in \mathbb{R}^{n\times n}$, the algorithm is initialized by $F^{(0)} = F$ and the iteration formula is

$$F^{(k+1)} = F^{(k)} + (P_T(P_{\mathbb{R}}(F^{(k)}))) - P_{\mathbb{R}}(F^{(k)}). \tag{2.8}$$

It follows from [4] that both The sequences $\{P_{\mathbb{R}}(F^{(k)})\}$ and $\{P_T(P_{\mathbb{R}}(F^{(k)}))\}$ generated by (2.8) globally converge to the solution A^* of (2.4) and hence (1.1). This algorithm was also given by [9] and [17] in a similar manner.

3 Solution by Unconstrained Minimization

In the previous section, the alternating projection algorithm computes a unique solution for (2.4) since the sets $K_{\mathbb{R}}$ and K_T are convex. When quasi-Newton methods are applied to solve the problem, this requires the knowledge of the rank of the matrix (T); hence (2.4) loses convexity and this increases the difficulty. In this section, we consider a different approach to (2.4). The main idea is to replace (2.4) by a smooth unconstrained optimization problem in order to use superlinearly convergent quasi-Newton methods. Problem (2.4) is solved by BFGS method, also the relevant formulae for derivatives are given. Partial connection between the problem and signal processing is given in the following factorization.

Classical results about Toeplitz matrices that go back to [7] may be re-stated according to which a nonsingular positive semi-definite Toeplitz matrix can be represented as the product of a Vandermonde matrix and its transpose and a diagonal matrix in between

$$T = VDV^T, \tag{3.1}$$

where D is an $m\times m$ diagonal matrix with positive diagonal entries and V is an $n\times m$ Vandermonde matrix

$$V = [x_j^i], \quad i = 0,\ldots,n-1, \quad j = 1,\ldots,m \tag{3.2}$$

(see [1, 14]).

We assume that the rank of T is known to be m. If the rank m is known, it is possible to express (1.1) as a smooth unconstrained optimization problem in the following way: Since the unknown in (1.1) is the matrix T, therefore the unknowns are chosen to be the elements of the matrices V; $x_1,\ldots,x_m$ and D; $d_{11},\ldots,d_{mm}$ introduced in (3.1). This gives us an equivalent unconstrained optimization problem to (1.1) in $2m$ unknowns expressed as

$$\text{minimize} \qquad \phi(V,D) \;=\; \|F - VDV^T\|_F^2. \tag{3.3}$$

Then the objective function $\phi(V,D)$ is readily calculated by first forming T from V and D as indicated by (3.1) and (3.2), after which ϕ is given by $\phi(V,D) = \|F -$

$T\|_F^2 \;=\; \|F - VDV^T\|_F^2$. The elements of the matrix T take the form

$$t_{ij} \;=\; \sum_{k=1}^{m} d_{kk} x_k^{i+j-2}. \tag{3.4}$$

Hence

$$\phi(V,D) = \sum_{i,j=1}^{n} (t_{ij} \;-\; f_{ij})^2 = \sum_{i,j=1}^{n} (\{\sum_{k=1}^{m} d_{kk} x_k^{i+j-2}\} \;-\; f_{ij})^2. \tag{3.5}$$

Our chosen method to minimize $\phi(X)$ is the BFGS quasi-Newton method (see for example [8]). This requires expressions for the first partial derivatives of ϕ, which are given from (3.5) by

$$\frac{\partial \phi}{\partial d_{ss}} \;=\; \sum_{i,j=1}^{n} 2(\{\sum_{k=1}^{m} d_{kk} x_k^{i+j-2}\} \;-\; f_{ij}) x_s^{i+j-2} \tag{3.6}$$

$$\frac{\partial \phi}{\partial x_s} \;=\; \sum_{\substack{i,j=1 \\ i=j\neq 1}}^{n} 2(\{\sum_{k=1}^{m} d_{kk} x_k^{i+j-2}\} \;-\; f_{ij})(i+j-2) d_{ss} x_s^{i+j-3} \tag{3.7}$$

The BFGS method also requires the Hessian approximation to be initialized. Where necessary, we do this using a unit matrix.

Some care has to be taken when choosing the initial value of the matrices V and D, in particular the rank m. If not, the minimization method may not be able to increase m. An extreme case occurs when the initial matrix $V = 0$ and $D = 0$ is chosen, and $F \neq 0$. It can be seen from (3.6) and (3.7) that the components of the gradient vector are all zero, so that $V = 0$ and $D = 0$ is a stationary point, but not a minimizer. A gradient method will usually terminate in this situation, and so fail to find the solution.

An advantage of the unconstrained method is that it allows the spatial dimensions to be chosen by the user. This is useful when the rank is already known. For example if the entries in F are derived from a matrix that has rank $m = 2$ or $m = 3$.

In general however the rank of the matrix is not known, for example the matrix that assumed has rank $m = 3$ might be irreducibly embedded in matrix with rank $m = 1$ or $m = 2$. We therefore must consider an algorithm in which we are prepared to revise our estimate of m. A simple strategy is to repeat the entire unconstrained method for different values of m. If m^* denotes the correct value of m which solves (1.1), then it is observed that the BFGS method converges rapidly if $m \leq m^*$, and exhibits superlinear convergence. On the other hand if $m > m^*$ then slow convergence is observed. One reason is that there are more variables in the problem. Also redundancy in the parameter space may have an effect. Thus it makes sense to start with a small value of m, and increase it by one until the solution is recognised. One way to recognise termination is when $T^{(k)}$ agrees sufficiently well with $T^{(k+1)}$, where $T^{(k)}$ denotes the positive semi-definite Toeplitz matrix obtained by minimizing ϕ in the kth iteration.

4 Hybrid Methods

A combination of both algorithms is introduced. Projection methods are globally convergent and hence potentially reliable, but often converge slowly, which can be very inefficient. Quasi-Newton methods are reliable and have a superlinear order rate of convergence, but require the correct rank m^* to be known. We therefore consider hybrid methods in which the projection algorithm is used sparingly as a way of establishing the correct rank, whilst the BFGS method is used to provide rapid convergence.

In order to ensure that each component method is used to best effect, it is important to transfer information from one method to the other. In particular, the result from one method is used to provide the initial data for the other, and vice versa. This mechanism has a fixed point property so that if one method finds a solution, then the other method is initialized with an iterate that also corresponds to the solution. It is clear how to use the output data from BFGS in the projection method but, unfortunately, the reverse is not easy.

We will evaluate two different algorithms which differ in respect of how $m^{(0)}$ is initialized. Algorithm 1 is expressed as follows: Given any data matrix $F \in \mathbb{R}^{n\times n}$, let s be some pre-selected positive integer number and ϵ some small number. Then the following algorithm solves (1.1)

Algorithm 1 $(T^{(0)} := F, s, \epsilon)$:

repeat projection method
until $m^{(l)} = m^{(l-j)} \quad j = 1, 2, \ldots, s.$
repeat
  Apply one iteration of projection method;
  $m^{(0)} := m^{(l)}$;
  repeat BFGS method;
  until $\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\| \leq \epsilon$ and $\|\mathbf{d}^{(k-1)} - \mathbf{d}^{(k)}\| \leq \epsilon$;
  $T^{(k)} = VDV^T$; ($\mathbf{x}^{(k)}$ and $\mathbf{d}^{(k)}$ from BFGS method)
until $\|T^{(k-1)} - T^{(k)}\| \leq \epsilon$;
return $(T^* := T^{(k)}, \mathbf{x}^* := \mathbf{x}^{(k)}, \mathbf{d}^* := \mathbf{d}^{(k)}, m^* := m^{(k)})$.

where $\mathrm{diag}(\mathbf{d}) = D$. The choice of s is a compromise between two effects. If s is small then the rank may not be accurately estimated, but the number of (expensive) iterations taken in the projection method is small. On the other hand, if s is large then a more accurate rank is obtained but the projection method needs more iterations.

In Algorithm 2, $m^{(0)}$ is supplied by the user. This approach avoids the initial sequence of projection iterations, but works well if the user is able to make a good estimate of the rank, which is often the case. Thus, we can express Algorithm 2 as follows: Given any data matrix $F \in \mathbb{R}^{n\times n}$, let ϵ be some small number; also choose $m^{(0)}$ as a small integer number. Then the following algorithm solves (1.1)

Algorithm 2 $(T^{(0)} := F, m^{(0)}, \epsilon)$:
repeat
repeat BFGS method;
until $\|\mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}\| \leq \epsilon$ and $\|\mathbf{d}^{(k-1)} - \mathbf{d}^{(k)}\| \leq \epsilon$;
$F^{(k)} = VDV^T$; ($\mathbf{x}^{(k)}$ and $\mathbf{d}^{(k)}$ from BFGS method)
Apply one iteration of projection method;
$m^{(0)} := m^{(l)}$;
until $\|T^{(k-1)} - T^{(k)}\| \leq \epsilon$;
return $(T^* := T^{(k)}, \mathbf{x}^* := \mathbf{x}^{(k)}, \mathbf{d}^* := \mathbf{d}^{(k)}, m^* := m^{(k)})$.

Conclusions In this paper, we have studied the Toeplitz matrix approximation problem involving the positive semidefinite matrix constraint, using both projection and BFGS methods. The problem needs more study in terms of the hybrid methods involving some numerical experiment comparisons.

Acknowledgements The author is very grateful to King Fahd University of Petroleum and Minerals for providing excellent research facilities.

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