The Minimum-Rank Gram Matrix Completion via Modified Fixed Point Continuation Method

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Abstract
The problem of computing a representation for a real polynomial as a sum of minimum number of squares of polynomials can be casted as finding a symmetric positive semidefinite real matrix (Gram matrix) of minimum rank subject to linear equality constraints. In this paper, we propose algorithms for solving the minimum-rank Gram matrix completion problem, and show the convergence of these algorithms. Our methods are based on the modified fixed point continuation (FPC) method. We also use the Barzilai-Borwein (BB) technique and a specific linear combination of two previous iterates to accelerate the convergence of modified FPC algorithms. We demonstrate the effectiveness of our algorithms for computing approximate and exact rational sum of squares (SOS) decompositions of polynomials with rational coefficients.

1. Introduction
Let \( x = [x_1, \ldots, x_s] \) and \( f \in \mathbb{R}[x] \), then \( f \) is a sum of squares (SOS) in \( \mathbb{R}[x] \) if and only if it can be written in the form
\[
    f(x) = m_d(x)^T \cdot W \cdot m_d(x),
\]
in which \( m_d(x) \) is a column vector of monomials of degree less than or equal to \( d \) and \( W \) is a real positive semidefinite matrix \([39, \text{Theorem 1}] \) (see also \([10] \)). \( W \) is also called a Gram matrix for \( f \).

Problem 1. Let \( f \in \mathbb{Q}[x_1, \ldots, x_s] \) be a polynomial of the degree \( 2d \), compute a representation for it as a sum of minimum number of squares of polynomials in \( \mathbb{Q}[x_1, \ldots, x_s] \).

The set of all matrices \( W \) for which (1) holds is an affine subspace of the set of symmetric matrices. If the intersection of this affine subspace with the cone of positive semidefinite (PSD) matrices is nonempty, then \( f \) can be written as a sum of squares. Since the components of \( m_d(x) \) are not algebraically independent, \( W \) is in general not unique. Problem 1 can be restated as finding a Gram matrix with minimum rank satisfying a given set of constraints:

\[
\begin{align*}
    \min & \quad \text{rank}(W) \\
    \text{s.t.} & \quad f(x) = m_d(x)^T \cdot W \cdot m_d(x) \\
    & \quad W \succeq 0, W^T = W
\end{align*}
\]

For \( s = 1 \), Pourchet’s main theorem \([35]\) implies that every positive definite univariate polynomial in \( \mathbb{Q}[x] \) is a sum of five squares in \( \mathbb{Q}[x] \). Therefore, the minimum rank of the Gram matrix
satisfying (2) is bounded by 5 for \( s = 1 \). For \( s > 1 \), Pfister’s general theorem \([37]\) shows that every positive definite polynomial in \( \mathbb{R}[x_1, \ldots, x_s] \) is a sum of \( 2^s \) squares of rational functions in \( \mathbb{R}(x_1, \ldots, x_s) \). It is well known that there exist positive semidefinite polynomials which cannot be written as sums of polynomial squares. However, as shown in \([21]\), various exceptional SOS problems in the literature by Motzkin, Delzell, Reznick, Leep and Starr, the IMO’71 problem by A. Lax and P. Lax, and the polynomial Vor2 in \([11]\) can be written as sums of less than 10 squares of polynomials after multiplying by suitable polynomials. The advantage of computing a numerical Gram matrix with small rank is that we can refine the approximately computed Gram matrix to high accuracy by structure preserved Gauss-Newton iteration more efficiently in order to recover the exact SOS representation of \( f \) \([20, 21, 35, 36]\).

In general, the rank minimization is an intractable problem and is in fact provably NP-hard due to the combinational nature of the non-convex rank function \([9]\). In \([12, 13, 41]\), they showed that \( \text{rank}(W) \) can be replaced by the nuclear norm of \( W \), which is the best convex approximation of the rank function over the unit ball of matrices. Expanding the right-hand side of the equality condition of (2), matching coefficients of the monomials, we obtain a set of linear equations for the entries of \( W \) which can be written as

\[
\begin{aligned}
&\min \|W\|_* \\
\text{s.t.} &\quad \mathcal{A}(W) = b \\
&\quad W \succeq 0, \ W^T = W
\end{aligned}
\]

(3)

where the nuclear norm \( \|W\|_* \) is defined as the sum of its singular values. The constraint \( \mathcal{A}(W) = b \) can also be relaxed, resulting in either the problem

\[
\begin{aligned}
&\min \|W\|_* \\
\text{s.t.} &\quad \|\mathcal{A}(W) - b\|_2 \leq \epsilon \\
&\quad W \succeq 0, \ W^T = W
\end{aligned}
\]

(4)

or its Lagrangian version

\[
\begin{aligned}
&\min_{W \in S_n^+} \mu \|W\|_* + \frac{1}{2} \|\mathcal{A}(W) - b\|_2^2,
\end{aligned}
\]

(5)

where \( S_n^+ \) is the set of symmetric positive semidefinite matrices and \( \mu > 0 \) is a parameter.

In \([1, 16, 24, 25, 26]\), they studied how to determine whether partially specified positive semidefinite matrices can be completed to fully specified matrices satisfying certain prescribed properties. A number of recent work has also shown that the low-rank solution can be recovered exactly via minimizing the nuclear norm under certain conditions \([7, 8, 41, 42]\). Several algorithms based on the interior point method have been proposed in \([4, 5, 28, 41, 43, 45]\) for solving the semidefinite programming problem derived from the rank minimization problem (3). Since most of these methods use second-order information, the memory requirement for computing descent directions quickly becomes too large as the problem size increases. Recently, several fast algorithms using only first-order information have been developed in \([6, 14, 19, 30, 31, 47]\). These first-order methods, based on function values and gradient evaluation, cannot yield as high accuracy as interior point methods, but much larger problems can be solved since no second-order information needs to be computed and stored.

Motivated by these exciting work, in this paper, we present two algorithms for solving the minimum-rank Gram matrix completion problem (3). Our algorithms are based on the modified
fixed point continuation method. By modifying the shrinkage operator in FPC and using the Barzilai-Borwein technique to compute explicit dynamically updated step sizes, we get an algorithm, called modified fixed point continuation method with the Barzilai-Borwein technique (MFP-C-BB). We prove the convergence of our algorithm under certain condition. Some accelerated gradient algorithms were proposed in [3, 19, 32, 33, 34, 47, 49]. These algorithms rely on computing the next iterate based not only on the previous one, but also on two or more previously computed iterates. These accelerated gradient methods have an attractive convergence rate of $O(1/k^2)$, where $k$ is the iteration counter. We incorporate this accelerating technique in the MFPC-BB algorithm to get an accelerated fixed point continuation algorithm with the Barzilai-Borwein technique (AFPC-BB), which shares the improved rate $O(1/k^2)$ of the optimal gradient method.

We also notice that algorithms in the literature mostly focus on recovering a randomly generated large-scale matrix from incomplete samples of its entries. Although it has been pointed out briefly in [47] that these algorithms can be adapted easily to solve the regularized semidefinite linear least squares problem (5), it is interesting for us to investigate how to use these newly developed techniques to compute approximate and exact rational sum of squares (SOS) decompositions of polynomials with rational coefficients.

**Notations:** Let $S_n \subset \mathbb{R}^{n \times n}$ denote the space of symmetric $n \times n$ matrices. The inner product between two elements $X, Y \in S_n$ is denoted by $\langle X, Y \rangle = \text{Tr}(X^T Y)$. The Frobenius norm of a matrix $X$ is denoted by $\|X\|_F$, the nuclear norm by $\|X\|_*$, and the operator norm (or spectral norm) by $\|X\|_2$.

The rest of the paper is organized as follows. In Section 2, we derive the modified fixed point iterative algorithm for the minimum-rank Gram matrix completion problem. In Section 3, we establish the convergence result for the iterations given in Section 2 and prove that it converges to the optimal solution of the regularized linear least squares problem (5). In Section 4, we introduce two techniques to accelerate the convergence of our algorithm and present MFPC-BB and AFPC-BB algorithms for solving problem (5). We demonstrate the performance and effectiveness of our algorithms through numerical examples for computing approximate and exact rational sum of squares decompositions of polynomials with rational coefficients in Section 5.

### 2. Modified fixed point iterative algorithm

Let $f : \mathbb{R}^{n_1 \times n_2} \to \mathbb{R}$ be a convex function, the subdifferential of $f$ at $X^* \in \mathbb{R}^{n_1 \times n_2}$ denoted by $\partial f$ is the compact convex set defined by

$$\partial f(X^*) := \{Z \in \mathbb{R}^{n_1 \times n_2} : f(Y) \geq f(X^*) + \langle Z, Y - X^* \rangle, \forall Y \in \mathbb{R}^{n_1 \times n_2}\}.$$

Following discussions in [27, Theorem 3.1] and [51], we derive the expression of the subdifferential of the nuclear norm at a symmetric matrix.

**Theorem 1.** Let $W \in S^n$, then

$$\partial \|W\|_* = \{Q^{(1)}Q^{(1)T} - Q^{(2)}Q^{(2)T} + Z : Q^{(i)T}Z = 0, i = 1, 2, \text{ and } \|Z\|_2 \leq 1\},$$

where $Q^{(1)}$ and $Q^{(2)}$ are orthogonal eigenvectors associated with the positive and negative eigenvalues of $W$ respectively.

**Proof.** Suppose that the eigenvalues of a symmetric matrix $W$ can be ordered as $\lambda_1 \geq \cdots \geq \lambda_t > 0 > \lambda_{t+1} \geq \cdots \geq \lambda_s$, $\lambda_{s+1} = \cdots = \lambda_n = 0$. Let $W = QAQ^T$ be a Schur decomposition of $W$, where
Consider \( Z \) between \( W \) if and only if \( W = Z \) and \( f(V) \geq f(W) + \langle U, V - W \rangle \), \( \forall V \in S_+^n \). This shows that \( W^* \) is an optimal solution of the problem (7).

Conversely, suppose \( W^* \) is the optimal solution of the problem (7), and (8) does not hold, i.e., there exists \( U \in \partial f(W^*) \), such that

\[ \exists \ V \in S_+^n, \quad s.t. \ \langle U, V - W^* \rangle < 0. \] (9)

Consider \( Z(t) = tW^* + (1 - t)V \), where \( t \in [0, 1] \) is a parameter. Since \( Z(t) \) is on the line segment between \( W^* \) and \( V \), and \( S_+^n \) is a convex set, \( Z(t) \in S_+^n, \forall t \in [0, 1] \). By [44, Theorem 23.4], the

\[ \sum_{i=1}^n \frac{1}{\lambda_i} \]

is an orthogonal matrix and \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \). These matrices can be partitioned as

\[
Q = \begin{pmatrix} Q^{(1)} & Q^{(2)} & Q^{(3)} \end{pmatrix}, \quad \Lambda = \begin{pmatrix} \Lambda^{(1)} & 0 & 0 \\ 0 & \Lambda^{(2)} & 0 \\ 0 & 0 & \Lambda^{(3)} \end{pmatrix},
\]

(6)

with \( Q^{(1)}, Q^{(2)}, Q^{(3)} \) having \( t, s - t, n - s \) columns and being associated with \( \Lambda^{(1)} = \text{diag}(\lambda_1, \ldots, \lambda_t) \), \( \Lambda^{(2)} = \text{diag}(\lambda_{t+1}, \ldots, \lambda_s) \), and \( \Lambda^{(3)} = \text{diag}(\lambda_{s+1}, \ldots, \lambda_n) \), respectively.

Let \( \lambda = (\lambda_1, \ldots, \lambda_n)^T \) and recall that

\[
\|\lambda\|_1 = \{ y \in \mathbb{R}^n : y_i = 1, i = 1, \ldots, t; \ y_j = -1, j = t + 1, \ldots, s; \ |y_k| < 1, k = s + 1, \ldots, n \}.
\]

Let \( Y \in \partial \|W\|_* \), by [27, Theorem 3.1], we have

\[ Y = Q \text{diag}(d) Q^T, \]

where \( d \in \partial \|\lambda\|_1 \). Therefore

\[ Y = Q^{(1)}Q^{(1)T} - Q^{(2)}Q^{(2)T} + Q^{(3)}DQ^{(3)T}, \]

where \( D \) is an \((n - s) \times (n - s)\) diagonal matrix with diagonal elements less than 1 in modulus.

Let \( Z = Q^{(3)}DQ^{(3)T} \), we have \( Q^{(j)T}Z = 0, i = 1, 2. \) Let \( \sigma_1(\cdot) \) denote the largest singular value of a given matrix, then we have

\[ \|Z\|_2 = Q^{(3)}DQ^{(3)T} \leq \sigma_1(D) < 1, \]

which completes the proof.

The optimality condition in [30, Theorem 2] can be generalized to the optimality condition for the constrained convex optimization problem (5).

**Theorem 2.** Let \( f : S^n \to \mathbb{R} \) be a proper convex function, i.e. \( f < +\infty \) for at least one point and \( f > -\infty \) for every point in its domain. Then \( W^* \) is an optimal solution to the problem

\[ \min_{W \in S_+^n} f(W) \]

(7)

if and only if \( W^* \in S_+^n \), and there exists a matrix \( U \in \partial f(W^*) \) such that

\[ \langle U, V - W^* \rangle \geq 0, \ for \ all \ V \in S_+^n. \]

(8)

Proof. Suppose \( U \in \partial f(W^*) \) and satisfies the inequality condition (8), hence

\[ f(V) \geq f(W^*) + \langle U, V - W^* \rangle, \quad \forall V \in S_+^n, \]

we have \( f(V) \geq f(W^*) \), for all \( V \in S_+^n \). This shows that \( W^* \) is an optimal solution of the problem (7).

Conversely, suppose \( W^* \) is the optimal solution of the problem (7), and (8) does not hold, i.e., there exists \( U \in \partial f(W^*) \), such that

\[ \exists \ V \in S_+^n, \quad s.t. \ \langle U, V - W^* \rangle < 0. \] (9)
one-sided directional derivative of \( f \) at \( Z(1) \) with respect to the vector \( W^*-V \) satisfies the following equation

\[
f'(Z(t); W^*-V)_{|t=1} = f'(W^*; W^*-V) = \sup\{\langle W, W^*-V \rangle : W \in \partial f(W^*)\}.
\]

According to (9), we have

\[
f'(Z(t); W^*-V)_{|t=1} \geq \langle U, W^*-V \rangle > 0.
\]

Therefore, for a small value \( \epsilon > 0 \), we have \( f(Z(1-\epsilon)) < f(W^*) \), which is contradict to the fact that \( W^* \) is optimal to the problem (7). □

Based on above theorems, we can introduce a thresholding operator and extend the fixed point iterative scheme for solving (5).

**Definition 1.** Suppose \( W = QAQ^T \) is a Schur decomposition of a matrix \( W \in \mathbb{S}^n \), where \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \) and \( Q \) is a real orthogonal matrix. For any \( \nu \geq 0 \), the matrix thresholding operator \( \mathcal{T}_\nu(\cdot) \) is defined as

\[
\mathcal{T}_\nu(W) := Q \mathcal{T}_\nu(\Lambda) Q^T, \quad \mathcal{T}_\nu(\Lambda) = \text{diag}(\{\lambda_i - \nu\}_+),
\]

where \( t_+ = \max(0, t) \).

We should point out that the idea of using the eigenvalue decomposition of \( Y^k \) has also appeared in [17, Remark 3]. However, to our best knowledge, there exists no convergence analysis about the eigenvalue thresholding operator in the literature.

Let \( \mu \) and \( \tau \) be positive real numbers and \( X^0 \) be an initial starting matrix. For \( k = 0, 1, 2, \ldots \), we compute

\[
\begin{cases}
Y^k &= X^k - \tau A^*(A(X^k) - b), \\
X^{k+1} &= \mathcal{T}_\tau(Y^k),
\end{cases}
\]

until a stopping criterion is reached.

**Theorem 3.** Suppose a matrix \( W^* \in \mathbb{S}^n_+ \) satisfies

1. \( \|A(W^*) - b\|_2 < \mu/n \) for a small positive number \( \mu \).
2. \( W^* = \mathcal{T}_{\tau\mu}(h(W^*)) \), where \( h(\cdot) = I(\cdot) - \tau A^*(A(\cdot) - b) \) and \( I(\cdot) \) is an identity operator.

Then \( W^* \) is the unique optimal solution of the problem (5).

**Proof.** Let \( \nu = \tau\mu \) and \( Y^* = h(W^*) = W^* + E \in \mathbb{S}^n \), where \( E = -\tau A^*(A(W^*) - b) \). We claim that \( \mathcal{T}_\nu(Y^*) \) is the unique optimal solution to the following problem

\[
\min_{W \in \mathbb{S}^n_+} \nu\|W\|_* + \frac{1}{2}\|W - Y^*\|_F^2.
\]

In fact, since the objective function \( \nu\|W\|_* + \frac{1}{2}\|W - Y^*\|_F^2 \) is strictly convex, there exists a unique minimizer, and we only need to prove that it is equal to \( \mathcal{T}_\nu(Y^*) \). Without loss of generality, we assume that the eigenvalues of \( Y^* \) can be ordered as

\[
\lambda_1(Y^*) \geq \cdots \geq \lambda_t(Y^*) \geq \nu > \lambda_{t+1}(Y^*) \geq \cdots > 0 > \cdots \geq \lambda_s(Y^*) = \cdots = \lambda_n(Y^*) = 0.
\]
We compute a Schur decomposition of $Y^*$ as

$$Y^* = Q^{(1)}\Lambda^{(1)}Q^{(1)T} + Q^{(2)}\Lambda^{(2)}Q^{(2)T},$$

where $\Lambda^{(1)} = \text{diag}(\lambda_1, \ldots, \lambda_s)$, $\Lambda^{(2)} = \text{diag}(\lambda_{s+1}, \ldots, \lambda_t)$, $Q^{(1)}$ and $Q^{(2)}$ are block matrices corresponding to $\Lambda^{(1)}$ and $\Lambda^{(2)}$ respectively. Let $\tilde{X} = T_\nu(Y^*)$, we have

$$\tilde{X} = Q^{(1)}(\Lambda^{(1)} - \nu I)Q^{(1)T},$$

therefore,

$$Y^* - \tilde{X} = \nu(Q^{(1)}Q^{(1)T} + Z), \quad Z = \nu^{-1}Q^{(2)}\Lambda^{(2)}Q^{(2)T}.$$  

By definition, $Q^{(1)T}Z = 0$.

- If $\lambda_{t+1}(Y^*) \geq |\lambda_s(Y^*)|$, then $\|Z\|_2 = \lambda_{t+1}(Y^*)/\nu < 1$.
- Otherwise, let $y = (y_1, \ldots, y_p)^T = A(W^*) - b \in \mathbb{R}^p$, then

$$\|E\|_F^2 = \tau^2\|A^*y\|_F^2 \leq \tau^2n^2(y_1^2 + \cdots + y_p^2) < \tau^2\mu^2.$$  

Notice that $E \in \mathbb{S}^n$ and $W^* \in \mathbb{S}^n_+$, by [15] Theorem 8.1.5], we have

$$\|Z\|_2 = \frac{|\lambda_s(Y^*)|}{\nu} = \max\{|\lambda_1(E)|, |\lambda_n(E)|\} \leq \frac{\|E\|_F}{\nu} < 1.$$  

Hence, according to Theorem[1], we have $Y^* - \tilde{X} \in \nu^\partial\|\tilde{X}\|_*$, which means that $0 \in \nu^\partial\|\tilde{X}\|_* + \tilde{X} - Y^*$.

By Theorem[2] we immediately conclude that $T_\nu(Y^*)$ is an optimal solution of the problem (11).

Since the objective function of the problem (5) is strictly convex, its optimal solution is also unique. If $W^* = T_{\tau\mu}(Y^*)$, by Theorem[2] there exists a matrix $U \in \nu^\partial\|W^\|_* + W^* - Y^*$ such that

$$\langle U, V - W^* \rangle \geq 0, \quad \forall \ V \in \mathbb{S}^n_+.$$  

Let $\tilde{U} = U/\tau$, by substituting $\nu = \tau\mu$ and $Y^* = W^* - \tau A^*(A(W^*) - b)$ into the above subdifferential function, we have $\tilde{U} \in \mu^\partial\|W^\|_* + A^*(A(W^*) - b)$ satisfying

$$\langle \tilde{U}, V - W^* \rangle \geq 0, \quad \forall \ V \in \mathbb{S}^n_+.$$  

By applying Theorem[2] once again, it is true that $W^*$ is the optimal solution of the problem (5). □

3. Convergence analysis

In this section, we analyze the convergence properties of the modified fixed point iterative scheme (10). We begin by recording two lemmas which establish the non-expansivity of the thresholding operator $T_\nu(h(\cdot))$.

**Lemma 1.** The thresholding operator $T_\nu$ is non-expansive, i.e., for any $X_1, X_2 \in \mathbb{S}^n$,

$$\|T_\nu(X_1) - T_\nu(X_2)\|_F \leq \|X_1 - X_2\|_F. \quad (12)$$  

Moreover,

$$\|X_1 - X_2\|_F = \|T_\nu(X_1) - T_\nu(X_2)\|_F \iff X_1 - X_2 = T_\nu(X_1) - T_\nu(X_2).$$
Proof. Let $X_1 = Q^{(1)} \Lambda^{(1)} Q^{(1)T}$ and $X_2 = Q^{(2)} \Lambda^{(2)} Q^{(2)T}$ be Schur decompositions of $X_1$ and $X_2$, respectively, where

$$
\Lambda^{(1)} = \begin{pmatrix} \text{diag}(\lambda_1) & 0 \\ 0 & 0 \end{pmatrix}, \quad \Lambda^{(2)} = \begin{pmatrix} \text{diag}(\lambda_2) & 0 \\ 0 & 0 \end{pmatrix},
$$

$\lambda_1 = (\alpha_1, \ldots, \alpha_s)^T$ and $\lambda_2 = (\beta_1, \ldots, \beta_t)^T$ are vectors of eigenvalues of $X_1$ and $X_2$ respectively, and $Q^{(1)}, Q^{(2)}$ are orthogonal matrices. Suppose that $\alpha_1 \geq \cdots \geq \alpha_k \geq \nu > \alpha_{k+1} \geq \cdots \geq \alpha_s$ and $\beta_1 \geq \cdots \geq \beta_l \geq \nu > \beta_{l+1} \geq \cdots \geq \beta_t$, then we have

$$
\tilde{X}_1 := T_\nu(X_1) = Q^{(1)} \tilde{\Lambda}^{(1)} Q^{(1)T}, \quad \tilde{X}_2 := T_\nu(X_2) = Q^{(2)} \tilde{\Lambda}^{(2)} Q^{(2)T},
$$

where

$$
\tilde{\lambda}_1 = (\alpha_1 - \nu, \ldots, \alpha_k - \nu) \quad \text{and} \quad \tilde{\lambda}_2 = (\beta_1 - \nu, \ldots, \beta_l - \nu).
$$

Therefore, we have

$$
\|X_1 - X_2\|_F^2 - \|\tilde{X}_1 - \tilde{X}_2\|_F^2
= \text{Tr}((X_1 - X_2)^T(X_1 - X_2)) - \text{Tr}((\tilde{X}_1 - \tilde{X}_2)^T(\tilde{X}_1 - \tilde{X}_2))
= \text{Tr}(X_1^TX_1 - \tilde{X}_1^T\tilde{X}_1 + X_2^TX_2 - \tilde{X}_2^T\tilde{X}_2) - 2\text{Tr}(X_1^TX_2 - \tilde{X}_1^T\tilde{X}_2)
= \sum_{i=1}^s \alpha_i^2 - \sum_{i=1}^k (\alpha_i - \nu)^2 + \sum_{i=1}^t \beta_i^2 - \sum_{i=1}^l (\beta_i - \nu)^2 - 2\text{Tr}(X_1^TX_2 - \tilde{X}_1^T\tilde{X}_2).
$$

It is known that for symmetric matrices $X, Y$,

$$
\text{Tr}(XY) \leq \lambda(X)^T \lambda(Y),
$$

with equality if and only if there exists an orthogonal matrix $Q$ such that

$$
X = Q \text{diag}(\lambda(X)) Q^T, \quad Y = Q \text{diag}(\lambda(Y)) Q^T,
$$

where $\lambda(X), \lambda(Y)$ are the vectors of eigenvalues of $X$ and $Y$ respectively (see [27, Theorem 2.2]). Hence, without loss of generality, assuming $k \leq l \leq s \leq t$, we have

$$
\text{Tr}(X_1^TX_2 - \tilde{X}_1^T\tilde{X}_2) \leq \lambda(X_1 - \tilde{X}_1)^T \lambda(X_2 - \tilde{X}_2) + \lambda(X_1 - \tilde{X}_1)^T \lambda(\tilde{X}_2) + \lambda(\tilde{X}_1)^T \lambda(X_2 - \tilde{X}_2)
\leq \sum_{i=1}^l \alpha_i \nu + \sum_{i=l+1}^s \alpha_i \beta_i + \sum_{i=1}^k (\beta_i - \nu) \nu + \sum_{i=k+1}^l \alpha_i (\beta_i - \nu)
$$

Therefore,

$$
\|X_1 - X_2\|_F^2 - \|\tilde{X}_1 - \tilde{X}_2\|_F^2 \geq \sum_{i=1}^s \alpha_i^2 - \sum_{i=1}^k (\alpha_i - \nu)^2 + \sum_{i=1}^t \beta_i^2 - \sum_{i=1}^l (\beta_i - \nu)^2
- 2(\sum_{i=1}^l \alpha_i \nu + \sum_{i=l+1}^s \alpha_i \beta_i + \sum_{i=1}^k (\beta_i - \nu) \nu + \sum_{i=k+1}^l \alpha_i (\beta_i - \nu))
\geq (\sum_{i=l+1}^s \alpha_i^2 + \sum_{i=l+1}^t \beta_i^2 - 2 \sum_{i=l+1}^s \alpha_i \beta_i) + \sum_{i=k+1}^l (2\beta_i \nu - \nu^2 + \alpha_i^2 - 2\alpha_i \beta_i).$$
Since \( t \geq s \) and \( \alpha_i^2 + \beta_i^2 - 2\alpha_i\beta_i \geq 0 \), we obtain
\[
\sum_{i=1}^s \alpha_i^2 + \sum_{i=t+1}^s \beta_i^2 - 2 \sum_{i=t+1}^s \alpha_i\beta_i \geq 0.
\]
Moreover, since the function \( g(x) = 2\beta_i x - x^2 + \alpha_i^2 - 2\alpha_i\beta_i \) is monotonically increasing in \([ -\infty, \beta_i ]\), and \( \alpha_i \leq \nu \leq \beta_i \), \( i = k + 1, \ldots, l \),

\[
2\nu\beta_i - \nu^2 + \alpha_i^2 - 2\alpha_i\beta_i > 0, \quad i = k + 1, \ldots, l.
\]

Hence, we have
\[
\|X_1 - X_2\|_F^2 - \|\tilde{X}_1 - \tilde{X}_2\|_F^2 \geq 0,
\]
i.e., (12) holds.

Furthermore, if \( \|X_1 - X_2\|_F = \|T_{\nu}(X_1) - T_{\nu}(X_2)\|_F \), then \( s = t, k = l \) and \( \alpha_i = \beta_i, i = k + 1, \ldots, s \), which further implies that \( \Lambda^{(1)} - \Lambda^{(1)} = \Lambda^{(2)} - \Lambda^{(2)} \) and \( \text{Tr}((X_1 - \tilde{X}_1)^T(X_2 - \tilde{X}_2)) \) achieves its maximum. Hence, there exists an orthogonal matrix \( Q \) such that
\[
X_1 - \tilde{X}_1 = Q(\Lambda^{(1)} - \Lambda^{(1)})Q^T = Q(\Lambda^{(2)} - \Lambda^{(2)})Q^T = X_2 - \tilde{X}_2,
\]
which implies that
\[
X_1 - X_2 = T_{\nu}(X_1) - T_{\nu}(X_2). \tag{13}
\]
Suppose (13) holds, then \( \|X_1 - X_2\|_F = \|T_{\nu}(X_1) - T_{\nu}(X_2)\|_F \), which completes the proof.

The following lemma and its proof are analogous to results in \[17, 30\].

**Lemma 2.** Suppose that the step size \( \tau \) satisfies \( \tau \in (0, 2/\|A\|_2^2) \). Then the operator \( h(\cdot) = I(\cdot) - \tau A^*(A(\cdot) - b) \) is non-expansive, i.e., for any \( X_1, X_2 \in S^n \),

\[
\|h(X_1) - h(X_2)\|_F \leq \|X_1 - X_2\|_F.
\]

Moreover, we have
\[
\|h(X_1) - h(X_2)\|_F = \|X_1 - X_2\|_F \iff h(X_1) - h(X_2) = X_1 - X_2,
\]
where \( I(\cdot) \) is an identity operator.

We now claim that the modified fixed point iterations (10) converge to the optimal solution of the problem (5).

**Theorem 4.** Let \( \tau \in (0, 2/\|A\|_2^2) \) and \( W^* \in S^n_+ \) satisfy

1. \( \|A(W^*) - b\|_2 < \mu/n \) for a small positive number \( \mu \).
2. \( W^* = T_{\tau\mu}(h(W^*)), \) where \( h(\cdot) = I(\cdot) - \tau A^*(A(\cdot) - b) \).

Then the sequence \( \{X^k\} \) obtained via modified fixed point iterations (10) converges to \( W^* \).
Proof. Let \( \nu = \tau \mu \). Since both \( \mathcal{T}_\nu(\cdot) \) and \( h(\cdot) \) are non-expansive, \( \mathcal{T}_\nu(h(\cdot)) \) is also non-expansive. Therefore, \( \{X^k\} \) lies in a compact set and must have a limit point. Suppose \( \bar{X} = \lim_{j \to \infty} X^k \) satisfying \( \|A(\bar{X}) - b\|_2 < \mu/n \). By \( W^* = \mathcal{T}_\nu(h(W^*)) \), we have

\[
\|X^{k+1} - W^*\|_F = \|\mathcal{T}_\nu(h(X^k)) - \mathcal{T}_\nu(h(W^*))\|_F \leq \|h(X^k) - h(W^*)\|_F \leq \|X^k - W^*\|_F,
\]

which means that the sequence \( \{\|X^k - W^*\|_F\} \) is monotonically non-increasing. Therefore

\[
\lim_{k \to \infty} \|X^k - W^*\|_F = \|\bar{X} - W^*\|_F,
\]

where \( \bar{X} \) can be any limit point of \( \{X^k\} \). By the continuity of \( \mathcal{T}_\nu(h(\cdot)) \), we have

\[
\mathcal{T}_\nu(h(\bar{X})) = \lim_{j \to \infty} \mathcal{T}_\nu(h(X^k)) = \lim_{j \to \infty} X^{k+1},
\]

i.e., \( \mathcal{T}_\nu(h(\bar{X})) \) is also a limit point of \( \{X^k\} \). Therefore, we have

\[
\|\mathcal{T}_\nu(h(\bar{X})) - \mathcal{T}_\nu(h(W^*))\|_F = \|\mathcal{T}_\nu(h(\bar{X})) - W^*\|_F = \|\bar{X} - W^*\|_F.
\]

Using Lemma 1 and Lemma 2 we obtain

\[
\mathcal{T}_\nu(h(\bar{X})) - \mathcal{T}_\nu(h(W^*)) = h(\bar{X}) - h(W^*) = \bar{X} - W^*,
\]

which implies \( \mathcal{T}_\nu(h(\bar{X})) = \bar{X} \). By Theorem 3, \( \bar{X} \) is the optimal solution to the problem (5), i.e., \( \bar{X} = W^* \). Hence, we have

\[
\lim_{k \to \infty} \|X^k - W^*\|_F = 0,
\]

i.e., \( \{X^k\} \) converges to its unique limit point \( W^* \). \( \square \)

4. Implementation

This section provides implementation details of the modified FPC algorithm for solving the minimum-rank Gram matrix completion problem.

4.1. Evaluation of the eigenvalue thresholding operator

The main computational cost of the modified FPC algorithm is computing the Schur decompositions. Following the strategies in [6,47], we use PROPACK [23] in Matlab to compute a partial Schur decomposition of a symmetric matrix.

PROPACK can not automatically compute only eigenvalues greater than a given threshold \( \nu \). To use this package, we must predetermine the number \( s_k \) of eigenvalues of \( Y^k \) to compute at the \( k \)-th iteration. Suppose \( X^k = Q^{k-1} \Lambda^{k-1} (Q^{k-1})^T \), we set \( s_k \) equal to the number of diagonal entries of \( \Lambda^{k-1} \) that are no less than \( \varepsilon_k \|\Lambda^{k-1}\|_2 \), where \( \varepsilon_k \) is a small positive number. Notice that \( s_k \) is non-increasing. If \( s_k \) is too small, the non-expansive property (12) of the thresholding operator \( \mathcal{T}_\nu \) may be violated. We increase \( s_k \) by 1 if the non-expansive property is violated 10 times [30].
4.2. Barzilai-Borwein technique

In [30], the authors always set the parameter $\tau = 1$ since their operator $A$ is generated by randomly sampling a subset of $p$ entries from matrices with i.i.d. standard Gaussian entries. For this linear map, the Lipschitz constant for the objective function of (5) is 1. According to Theorem 4, convergence for the Gram matrix completion problem is guaranteed provided that $\tau \in (0, \frac{2}{\|A\|_2^2})$. This choice is, however, too conservative and the convergence is typically slow.

There are many ways to select a step size. For simplicity, we describe a strategy, which is based on the Barzilai-Borwein method [2], for choosing the step size $\tau_k$. Let $g(\cdot) = A^*(A(\cdot) - b)$ and $g^k = A^*(A(X^k) - b)$. We perform the shrinkage iteration (10) along the negative gradient direction $g^k$ of the smooth function $\frac{1}{2}\|A(X^k) - b\|_2^2$, then apply the thresholding operator $T_\nu(\cdot)$ to accommodate the non-smooth term $\|X\|_*$. Hence, it is natural to choose $\tau_k$ based on the function $\frac{1}{2}\|A(X^k) - b\|_2$ alone. Let

$$\Delta X = X^k - X^{k-1}, \quad \Delta g = g^k - g^{k-1}.$$  

The Barzilai-Borwein step provides a two-point approximation to the secant equation underlying quasi-Newton method, specifically,

$$\tau_k = \frac{\langle \Delta X, \Delta g \rangle}{\langle \Delta g, \Delta g \rangle}, \quad \text{or} \quad \tau_k = \frac{\langle \Delta X, \Delta X \rangle}{\langle \Delta X, \Delta g \rangle}.$$

In order to avoiding the parameter $\tau_k$ being either too small or too large, we take

$$\tau_k = \max \{\tau_{\min}, \min \{\tau_k, \tau_{\max}\}\},$$

where $0 < \tau_{\min} < \tau_{\max} < \infty$ are fixed parameters.

The idea of using the BB step to accelerate the convergence of gradient algorithms has also appeared in [52].

4.3. Algorithms

As suggested in [17, 30, 47], we adopt a continuation strategy to solve the regularized linear least squares problem (5). For the problem (5) with a target parameter $\bar{\mu}$ being a moderately small number, we propose solving a sequence of problems (5) defined by a decreasing sequence $\mu_k$. When a new problem, associated with $\mu_{k+1}$, is to be solved, the approximate solution for the current problem with $\mu_k$ is used as the starting point. We use the parameter $\eta$ to determine the rate of reduction of the consecutive $\mu_k$, i.e.,

$$\mu_{k+1} = \max(\eta \mu_k, \bar{\mu}), \quad k = 1, \ldots, L - 1.$$

Our modified fixed point continuation iterative scheme with the Barzilai-Borwein technique for solving (5) is outlined below.

**Algorithm MFPC-BB**

**Input:**  
- Parameters $0 < \tau_{\min} < \tau_0 < \tau_{\max} < \infty$, $\mu_1 > \bar{\mu} > 0$, $\eta > 0$ and a tolerance $\epsilon > 0$  
**Output:**  
- A numeric Gram matrix.

- Set $X^0 = 0$.
- For $\mu = \mu_1, \ldots, \mu_L$, do
1. Choose a step size \( \tau_k \) via the BB technique such that \( \tau_{\text{min}} \leq \tau_k \leq \tau_{\text{max}} \).
2. Compute \( Y^k = X^k - \tau_k A^* (A(X^k) - b) \) and a Schur decomposition of \( Y^k = Q^k \Lambda^k (Q^k)^T \).
3. Compute \( X^{k+1} = Q^k \tau_{\mu_k} (\Lambda^k) (Q^k)^T \).

- If the stop criterion is true, then return \( X_{\text{opt}} \).

- end for.

However, as shown in \[3, 19, 47\], the above algorithm may converge as \( O(1/k) \). Very recently, alternative algorithms that could speed up the performance of the gradient method FPC have been proposed in \[19, 47\]. These algorithms rely on computing the next iterate based not only on the previous one, but also on two or more previously computed iterates. We incorporate this new accelerating technique in our MFPC-BB algorithm to solve the affine constrained low-rank Gram matrix completion problem \[5\]. The accelerated algorithm, called AFPC-BB, keeps the simplicity of MFPC-BB but shares the improved rate \( O(1/k^2) \) of the optimal gradient method.

Algorithm \( \text{AFPC-BB} \)

Input: ▶ Parameters \( 0 < \tau_{\text{min}} < \tau_0 < \tau_{\text{max}} < \infty, \mu_1 > \bar{\mu} > 0, \eta > 0 \) and tolerance \( \epsilon > 0 \)
Output: ▶ A numeric Gram matrix.

- Set \( X^0 = 0 \).

- For \( \mu = \mu_1, \ldots, \mu_L \), do
  1. Choose a step size \( \tau_k \) via the BB technique such that \( \tau_{\text{min}} \leq \tau_k \leq \tau_{\text{max}} \).
  2. Compute \( Z^k = X^k + \frac{t_{k-1}}{t_k} (X^k - X^{k-1}) \).
  3. Compute \( Y^k = Z^k - \tau_k A^* (A(Z^k) - b) \) and a Schur decomposition of \( Y^k = Q^k \Lambda^k (Q^k)^T \).
  4. Compute \( X^{k+1} = Q^k \tau_{\mu_k} (\Lambda^k) (Q^k)^T \).
  5. Compute \( t_{k+1} = \frac{1 + \sqrt{1 + 4t^2_k}}{2} \).

- If the stop criterion is true, then return \( X_{\text{opt}} \).

- end for.

The following theorem shows that by performing the gradient step at the matrix \( Z^k \) instead of at the approximate solution \( X^k \), the convergence rate of the MFPC-BB method can be accelerated to \( O(1/k^2) \).

Theorem 5. \([19, 47]\) Let \( \{X^k\} \) be the sequence generated by the AFPC-BB algorithm. Then for any \( k > 1 \), we have

\[
F(X^k) - F(X^*) \leq \frac{C\|X^* - X^0\|^2}{(k + 1)^2},
\]

where \( C \) is a constant, \( F(X) \) is the objective function and \( X^* \) is the optimal solution of the problem \([2]\).
5. Numerical experiments

In this section, we report the performance of our modified FPC algorithms for writing a real positive semidefinite polynomial as a sum of minimum number of squares of polynomials. In our tests, we generate positive semidefinite matrices $W \in \mathbb{Q}^{n \times n}$ with rank $r$ by randomly sampling an $n \times r$ factor $L$ with rational entries and setting $W = LL^T$. After multiplying the matrix $W$ by a monomial vector $m_d(x)$ and its transpose, we obtain a positive semidefinite polynomial

$$f(x) = m_d(x)^T \cdot W \cdot m_d(x) \in \mathbb{Q}[x].$$

Replacing entries in $W$ by parameters, expanding the right-hand side of the equality and matching coefficients of the monomials, we obtain a set of linear equations which can be written as

$$A(W) = b,$$

where $A$ is the linear map from $\mathbb{S}^n$ to $\mathbb{R}^p$.

Since the SOS representation of a nonnegative polynomial is in general not unique, the solution $X_{\text{opt}}$ returned by MFPC-BB and AFPC-BB algorithms probably doesn’t correspond to the constructed rational Gram matrix $W$. Therefore, in stead of setting relative error equal to $\|X_{\text{opt}} - W\|_F/\|W\|_F$, which is used in [6, 7, 30, 47], we choose to measure the accuracy of the computed solution $X_{\text{opt}}$ by the relative error defined by:

$$\text{error} := \frac{\|A(X_{\text{opt}}) - b\|_2}{\|b\|_2}. \quad (16)$$

The relative error also gives us a stopping criterion for the MFPC, MFPC-BB, AFPC-BB algorithms in our numerical experiments. We declared that the Gram matrix is approximately recovered if the relative error is less than a given tolerance denoted by $\epsilon$.

An $n \times n$ symmetric matrix of rank $r$ depends on $d_r = n(2n - r + 1)/2$ degrees of freedom. Let $FR = d_r/p$ be the ratio between the degrees of freedom in an $n \times n$ symmetric matrix of rank $r$ and the number of linear constrains defined in (15). If $FR$ is large (close to 1), recovering $W$ becomes harder as the number of measurements is close to the degrees of freedom. Conversely, if $FR$ is close to zero, recovering $W$ becomes easier. Note that if $FR > 1$, there might have an infinite number of matrices with rank $r$ satisfying given affine constraints.

Throughout the experiments, we choose an initial matrix $X^0$ to be a zero matrix. For each test, we make an initial estimate of the value $L = \|A\|_2^2$ which is the smallest Lipschitz constant of the gradient of $\frac{1}{2}\|AX - b\|_2^2$. We set the Barzilai-Borwein parameters $\tau_{\text{max}} = 10/L$ and $\tau_{\text{min}} = 10^{-3}/L$. The thresholds 10 and $10^{-3}$ are found after some experimentations.

We have implemented the MFPC-BB and AFPC-BB algorithms in MATLAB, using PROPACK package to evaluate partial eigenvalue decompositions. All runs are conducted on a HP xw8600 workstation with an Inter Xeon(R) 2.67GHz CPU and 3.00 GB of RAM.

5.1. Numerical experiments on random Gram matrix completion problems

In the first series of test, we set $\epsilon = 5 \times 10^{-3}$ and compare the performance of the MFPC, MFPC-BB and AFPC-BB algorithms without continuation technique to solve (5) for randomly generated matrix completion problems with moderate dimensions. In order to see the convergence behaviors of MFPC, MFPC-BB and AFPC-BB clearly, we compute the full Schur decompositions at each iteration.

Table reports the degree of freedom ratio $FR$, the number of iterations, and the error (16) of the three algorithms MFPC, MFPC-BB, AFPC-BB. As can be seen from Table I on the condition
that these three algorithms achieve similar errors, MFPC-BB provides better performance with less number of iterations than MFPC, while AFPC-BB outperforms the other two algorithms greatly in terms of the number of iterations.

| Problems | MFPC | MFPC-BB | AFPC-BB |
|----------|------|---------|---------|
| n  | r  | p | FR | # iter | error | # iter | error | # iter | error |
| 100 | 10 | 579 | 1.6494 | 140 | 4.99e-3 | 75 | 4.95e-3 | 31 | 4.76e-3 |
| 200 | 10 | 1221 | 1.6011 | 187 | 4.99e-3 | 105 | 4.97e-3 | 37 | 4.88e-3 |
| 500 | 10 | 5124 | 0.9670 | 632 | 4.99e-3 | 499 | 4.99e-3 | 66 | 4.90e-3 |

Table 1: Comparison of MFPC, MFPC-BB and AFPC-BB, without using continuation technique.

In Figure 1 and Figure 2, we plot the relative error $\|A(X^k) - b\|_2/\|b\|_2$ and approximation error $\|X^k - X_{opt}\|_F$ versus the iteration number of these three methods on recovering a randomly generated $500 \times 500$ Gram matrix with rank 10 respectively. We terminate these three algorithms when the relative error (16) is below $5 \times 10^{-3}$. We observe that in both cases AFPC-BB converges much faster than MFPC-BB and MFPC. The comparison of MFPC-BB and MFPC clearly shows that the Barzilai-Borwein technique is quite effective in accelerating the convergence of the MFPC algorithm.

In Table 2 we report the performance of the AFPC-BB algorithm with continuation technique on randomly generated Gram matrix completion problems. We use PROPACK to compute partial eigenvalues and eigenvectors. We set the regularization parameter in problem (15) to be $\bar{\mu} = 10^{-4}\|A^* b\|$ and $\mu_1 = 1/4\|A^* b\|$. The update strategy for $\mu_k$ is $\max(1/4\mu_{k-1}, \bar{\mu})$ whenever the stopping criterion is satisfied with $\epsilon = 10^{-3}$.

As indicated in the table, it takes the AFPC-BB algorithm fewer than 300 iterations on the average and less than 15 minutes to solve all problems in our experiments. In addition, for most of these problems, $FR$ is larger than 1. Especially, $FR$ is up to 4.5923 for the problem with $n = 1000, r = 50$. To our best knowledge, nobody has considered solving matrix completion problems.
Table 2: Numerical results for AFPC-BB on random Gram matrix completion problems.

| Problems | Results |
|----------|---------|
| n  | r  | p  | FR  | # iter | time | error |
| 100 | 10 | 579 | 1.6494 | 76 | 1.48e+0 | 9.64e-4 |
| 500 | 10 | 3309 | 1.4974 | 80 | 2.35e+1 | 9.90e-4 |
| 1000 | 10 | 10621 | 0.9372 | 165 | 1.41e+2 | 9.95e-4 |
| 1000 | 50 | 10621 | 4.5923 | 120 | 1.10e+2 | 9.89e-4 |
| 1500 | 10 | 25573 | 0.5848 | 271 | 6.04e+2 | 9.96e-4 |
| 1500 | 50 | 25573 | 2.8849 | 156 | 4.59e+2 | 9.83e-4 |

problems in this situation yet. It is rather surprising that the original random Gram matrix with low rank can be recovered given only such a small number of affine constraints.

5.2. Exact rational sum of squares certificates

The numerical Gram matrix $W$ returned by the AFPC-BB algorithm satisfies

$$f(x) \approx m_d(x)^T \cdot W \cdot m_d(x), \quad W \succeq 0.$$  

(17)

In order to derive an exact SOS decomposition of $f$, we need to start with an approximate Gram matrix with high accuracy. Although first-order methods are often the only practical option for large-scale problems, it has also been observed that the sequence $\{X^k\}$ computed by the AFPC-BB algorithm converges quite slowly to an optimal solution $W^*$. Therefore, we apply the structure-preserving Gauss-Newton iterations (see [20, 21]) to refine the Gram matrix $W$ with low rank returned by the AFPC-BB algorithm: we choose a rank $r$ which is less than or equal to the rank of $W$ and compute the truncated $L^TDL$ decomposition of $W$ to obtain an approximate SOS decomposition

$$f(x) \approx \sum_{i=1}^{r} \left( \sum_{\alpha} c_{i,\alpha} x^\alpha \right)^2,$$

then apply standard Gauss-Newton iteration to compute $\Delta c_{i,\alpha} x^\alpha$ such that

$$f(x) = \sum_{i=1}^{r} \left( \sum_{\alpha} c_{i,\alpha} x^\alpha + \Delta c_{i,\alpha} x^\alpha \right)^2 + O\left( \sum_{i=1}^{r} \left( \sum_{\alpha} \Delta c_{i,\alpha} x^\alpha \right)^2 \right).$$  

(18)

The matrix $W$ is updated accordingly to $W + \Delta W$ and the iteration is stopped when the backward error

$$\theta = \| f(x) - m_d(x)^T \cdot W \cdot m_d(x) \|_2$$  

(19)

is less than the given tolerance $\epsilon$. If $\theta$ remains greater than $\epsilon$ after several Gauss-Newton iterations, we may increase the precision or use different $r$ and try Gauss-Newton iterations again. After converting the refined matrix $W$ into a rational matrix, we use the orthogonal projection technique in [20, 21] to construct an exact rational SOS decomposition for the nonnegative polynomial $f$.

It is interesting to notice that the AFPC-BB algorithm provides a low-rank Gram matrix to seed Gauss-Newton iterations while most of the SDP solvers GloptiPoly [18], SOSTOOLS [40], YALMIP [29], SeDuMi [46], SDPT3 [48] and SparsePOP [50] usually return a Gram matrix with
maximum rank (see [22, Theorem 2.1]). For example, we consider a randomly generated Gram matrix completion problem with $n = 200$, $r = 5$, which is created in the same way described at the beginning of Section 5. The smallest 10 singular values of the numerical Gram matrix computed by SeDuMi are

$$3.527, 2.779, 2.445, 1.369, 1.184, 0.964, 0.627, 0.101, 0.485, 0.161, 0.069.$$  

However, the rank of the numerical Gram matrix returned by the AFPC-BB algorithm is 14. We notice that by applying Gauss-Newton iterations to the low-rank Gram matrix computed by AFPC-BB, it is usually much easy to recover an exact SOS decomposition of the nonnegative polynomial.

In [31], we have used the MFPC-BB algorithm to successfully recover the exact sums of squares of nonnegative polynomials in [21].

In the following two tables, we compare the performance of the AFPC-BB algorithm and the SDP solver SeDuMi for recovering low rank Gram matrices from affine constraints on the same randomly generated examples. We also show the effectiveness of Gauss-Newton iterations run in Maple with Digits = 14 in refining the numerical Gram matrix. These tables report the number of affine constraints $p$, the degree of freedom ratio $FR$, the backward error $\theta$, the rank of the Gram matrix and the running time in seconds. Table 4 also shows the smallest singular value $\sigma_n$ of numerical Gram matrices returned by SeDuMi. We set $\epsilon = 5 \times 10^{-4}$ in the AFPC-BB algorithm, which is small enough to guarantee very good recoverability.

| Examples | AFPC-BB | Gauss-Newton iteration |
|----------|---------|------------------------|
| n r p FR  | rank $\theta$ time | rank $\theta$ time |
| 50 5 255 0.9412 | 9 6.874 4.06e-1 | 5 1.443e-5 4.08e+0 |
| 100 5 579 0.8463 | 9 0.860 1.75e+0 | 5 1.935e-9 2.98e+1 |
| 150 5 896 0.8259 | 13 2.758 7.09e+0 | 5 4.023e-8 6.28e+1 |
| 200 5 1221 0.8108 | 14 3.629 1.07e+1 | 5 4.030e-5 4.69e+2 |
| 300 5 1932 0.7712 | 14 22.315 2.32e+1 | 5 1.379e-9 5.61e+2 |
| 400 5 2610 0.7624 | 15 12.515 6.23e+1 | 5 5.825e-5 1.22e+3 |
| 500 5 5124 0.4859 | 17 24.829 5.33e+1 | 5 1.479e-5 7.92e+3 |

Table 3: Exact SOS certificates via AFPC-BB and Gauss-Newton iterations.

| Examples | SDP | Gauss-Newton iteration |
|----------|-----|------------------------|
| n r p FR | $\sigma_n$ time | rank $\theta$ time |
| 50 5 255 0.9412 | 0.701 1.03e+0 | 6 3.769e-8 1.59e+1 |
| 100 5 579 0.8463 | 0.042 7.77e+0 | 7 2.438e-10 6.88e+1 |
| 150 5 896 0.8259 | 0.069 1.24e+1 | 7 1.883e-10 2.23e+2 |
| 200 5 1221 0.8108 | 0.069 6.58e+1 | 7 4.666e-9 8.21e+2 |
| 300 5 1932 0.7712 | 0.442 2.84e+2 | 7 5.679e-10 1.30e+3 |
| 400 5 2610 0.7712 | 0.114 3.94e+2 | 8 9.249e-10 5.00e+3 |
| 500 5 5124 0.4859 | 0.001 2.14e+3 | — — — |

Table 4: Approximate SOS certificates via SDP and Gauss-Newton iterations.

As indicated in Table 4, using the AFPC-BB algorithm, we can compute numerical low-rank Gram matrices very efficiently. Moreover, for each example, we can use Gauss-Newton iterations
to refine the Gram matrix returned by AFPC-BB to relatively high accuracy, e.g. $10^{-5}$. By rounding every entry of the refined matrix to the nearest integer, we can easily recover a rational Gram matrix with rank 5 which gives the exact SOS representation of the nonnegative polynomial.

As indicated in Table 4 for the same examples, numerical Gram matrices returned by SeDuMi have full rank for the given tolerance $10^{-3}$, while the rank of matrices returned by AFPC-BB are relatively small. We seed the numerical Gram matrices returned by SeDuMi to Gauss-Newton iterations, the ranks of the refined matrices are always larger than 5 in order to guarantee the convergence of the Gauss-Newton iterations. Furthermore, we are not yet able to recover exact SOS decompositions even though backward errors $\theta$ have been reduced to the order of $10^{-10}$.

From Table 5 it is also interesting to notice, if we decrease the degree of freedom ratio $FR$ by choosing a sparse monomial vector $m_d(x)$, it is possible to recover the exact SOS representation of the nonnegative polynomial from the numerical low-rank Gram matrix returned by the AFPC-BB algorithm, without running Gauss-Newton iterations.

| Problems | AFPC-BB | Rational SOS |
|----------|---------|--------------|
| n r p FR | # iter  | time | error | time |
| 50 5 608 0.3947 | 45 | 4.38e-1 | 5.84e-4 | 1.09e-1 |
| 150 5 1703 0.4345 | 217 | 5.91e-1 | 9.96e-4 | 8.12e-1 |
| 300 5 3544 0.4204 | 327 | 2.11e+1 | 9.77e-4 | 3.45e+0 |
| 400 10 10078 0.3924 | 151 | 2.46e+1 | 9.52e-4 | 1.14e+1 |
| 500 20 24240 0.4047 | 142 | 4.48e+1 | 4.70e-4 | 4.65e+1 |
| 1000 10 27101 0.3673 | 436 | 3.70e+2 | 4.97e-4 | 1.38e+2 |
| 1000 50 95367 0.5114 | 395 | 6.56e+2 | 9.99e-5 | 1.41e+3 |
| 1500 10 45599 0.3280 | 554 | 1.00e+3 | 4.99e-4 | 3.10e+2 |

Table 5: Exact SOS certificates via AFPC-BB.

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