A Ulm-like Cayley Transform Method for Inverse Eigenvalue Problems*

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Abstract. *We propose a Ulm-like Cayley transform method for solving inverse eigenvalue problems, which avoids solving approximate Jacobian equations comparing with other known methods. A convergence analysis of this method is provided and the quadratic convergence property is proved under the assumption of the distinction of the given eigenvalues. Numerical experiments are given in the last section and comparisons with the inexact Cayley transform method [1] are made.*

Keyword. *nonlinear equation, inverse eigenvalue problem, Moser's method, inexact Cayley transform method.*

1 Introduction

Over the years there has been considerable interest in deriving and analyzing the theory or algorithms for inverse eigenvalue problems (IEPs) which are defined as follows. Let $\mathbf{c} = (c_1, c_2, \ldots, c_n)^T \in \mathbb{R}^n$ and $\{A_i\}_{i=1}^n$ be a sequence of real symmetric $n \times n$ matrices. Define

$$A(\mathbf{c}) = \sum_{i=1}^{n} c_i A_i \tag{1.1}$$

and denote its eigenvalues by $\{\lambda_i(\mathbf{c})\}_{i=1}^n$ with the ordering $\lambda_1(\mathbf{c}) \leq \lambda_2(\mathbf{c}) \leq \cdots \leq \lambda_n(\mathbf{c})$. Let $\{\lambda_i^*\}_{i=1}^n$ be given with $\lambda_1^* \leq \lambda_2^* \leq \cdots \leq \lambda_n^*$. Then the IEP is to find a vector $\mathbf{c}^* \in \mathbb{R}^n$ such that

$$\lambda_i(\mathbf{c}^*) = \lambda_i^* \quad \text{for } i = 1, 2, \ldots, n. \tag{1.2}$$

The vector $\mathbf{c}^*$ is called a solution of the IEP.

This type of inverse problem arises in a variety of applications. See for instance the pole assignment problem [2, 33], the inverse Toeplitz eigenvalue problem [30, 34], the inverse Sturm-Liouville problem

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[19] , problems in applied mechanics and structure design [15, 16, 21], applied geophysics [29], applied physics [25], numerical analysis [27] and dynamics systems [9]. A good reference for these applications is a recent survey paper on structured inverse eigenvalue problems by Chu and Golub [7]. In many of these applications, the problem size n can be large. For example, large Toeplitz eigenvalue problems [30] and large discrete inverse Sturm-Liouville problems [7]. Our goal in this paper is to derive an efficient algorithm for solving large IEPs.

Recall that solving the IEP (1.2) is equivalent to solving the equation $\mathbf{f}(\mathbf{c}) = \mathbf{0}$ on $\mathbb{R}^n$, where the function $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ is defined by

$$\mathbf{f}(\mathbf{c}) = (\lambda_1(\mathbf{c}) - \lambda_1^*, \lambda_2(\mathbf{c}) - \lambda_2^*, \ldots, \lambda_n(\mathbf{c}) - \lambda_n^*)^T. \tag{1.3}$$

Then $\mathbf{c}^*$ is a solution of the IEP if and only if $\mathbf{c}^*$ is a solution of the equation $\mathbf{f}(\mathbf{c}) = \mathbf{0}$. Based on this equivalence, Newton's method can be applied to the IEP, and it converges quadratically [13, 36]. To overcome this drawback, different Newton-like methods have been proposed and studied [5, 6, 13, 36]. Instead of computing the exact eigenvectors of the matrix $A(\mathbf{c})$, Newton-like methods adopt the approximations to them in each outer iteration. Among these methods, the Cayley transform method [13] is particularly interesting which forms an approximate Jacobian equation by applying matrix exponentials and Cayley transforms. To alleviate the over-solving problem, Bai, Chan and Morini presented in [1] an inexact Cayley transform method for solving the nonlinear system $\mathbf{f}(\mathbf{c}) = 0$. Their method stops the inner iterations before convergence. Suitable inner tolerances for the approximate Jacobian equation (ii) was set in that paper and the super-linear convergence rate was obtained.

The purpose of the present paper is, motivated by Moser's method and Ulm's method (cf. [11, 14, 18, 19, 20, 26, 31, 32, 37]), to propose a deformed Cayley transform method for solving the IEP, which avoids solving the Jacobian equations in each outer iteration. Under the classical assumption that the given eigenvalues are distinct and the Jacobian matrix $J(\mathbf{c}^*)$ is nonsingular (which is also used in [1, 3]), we prove that this method converges quadratically.

Comparing with the inexact Cayley transform method in [1], the deformed Cayley transform method seems more stable, and reduces the difficulty though they have the same costs. Numerical experiments are given in the last section to illustrate the comparisons with the inexact Cayley transform method.

2 Ulm-like Cayley transform method

Let $[1, n]$ denote the set of n integers $1, 2, \ldots, n$. As usual, let $\mathbb{R}^{n\times n}$ denote the set of all real $n \times n$ matrices. Let $\|\cdot\|$ denote the 2-norm in $\mathbb{R}^n$. The induced 2-norm in $\mathbb{R}^{n\times n}$ is also denoted by $\|\cdot\|$, i.e.,

$$\|A\| := \sup_{\mathbf{x}\in\mathbb{R}^n,\ \mathbf{x}\neq\mathbf{0}} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|} \quad \text{for each } A \in \mathbb{R}^{n\times n}.$$

Let $\|\cdot\|_F$ denote the Frobenius norm in $\mathbb{R}^{n\times n}$. Then

$$\|A\| \le \|A\|_F \quad \text{for each } A \in \mathbb{R}^{n\times n}. \tag{2.1}$$

Let $\mathbf{c}= (c_1, c_2, \ldots, c_n)^T \in \mathbb{R}^n$ and let $\{A_i\}_{i=1}^n$ be a sequence of real symmetric $n \times n$ matrices. Let $A(\mathbf{c})$ be defined by (1.1), i.e.,

$$A(\mathbf{c}) = \sum_{i=1}^n c_i A_i,$$

Let $\lambda_1(\mathbf{c}) \le \lambda_2(\mathbf{c}) \le \cdots \le \lambda_n(\mathbf{c})$ be the eigenvalues of the matrix $A(\mathbf{c})$ and $\{\mathbf{q}_i(\mathbf{c})\}_{i=1}^n$ be the normalized eigenvectors corresponding to $\{\lambda_i(\mathbf{c})\}_{i=1}^n$. Define $J(\mathbf{c}) = ([J(\mathbf{c})]_{ij})$ by

$$[J(\mathbf{c})]_{ij} := \mathbf{q}_i(\mathbf{c})^T A_j \mathbf{q}_i(\mathbf{c}) \quad \text{for each } i, j \in [1, n]. \tag{2.2}$$

Let $\{\lambda_i^*\}_{i=1}^n$ be given with $\lambda_1^* \le \lambda_2^* \le \cdots \le \lambda_n^*$ and write $\boldsymbol{\lambda}^* = (\lambda_1^*, \lambda_2^*, \ldots, \lambda_n^*)^T$. Let $\mathbf{c}^*$ be the solution of the IEP, i.e.,

$$\lambda_i(\mathbf{c}^*) = \lambda_i^* \quad \text{for each } i \in [1, n].$$

As in [1, 3, 13], we assume that the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ are distinct. Then the eigenvalues of $A(\mathbf{c})$ are distinct too in some neighborhood of $\mathbf{c}^*$. It follows that the function $\mathbf{f}(\mathbf{c})$ is analytic in the same neighborhood and that $J(\mathbf{c})$ is the Jacobian matrix of $\mathbf{f}$ at $\mathbf{c}$ (cf. [1, 3]). This means Newton's method, which converges quadratically (cf. [23, 36]), involves solving a complete eigenproblem for the matrix $A(\mathbf{c})$. In [13], it was proved that if we only compute it approximately, we still have quadratic convergence. This results in the following Cayley transform method which forms approximate Jacobian equations by applying matrix exponentials and Cayley transforms.

Algorithm 1: Cayley transform method

1. Given $\mathbf{c}^0$, compute the orthonormal eigenvectors $\{\mathbf{q}_i(\mathbf{c}^0)\}_{i=1}^n$ of $A(\mathbf{c}^0)$. Let $P_0 = [\mathbf{p}_1^0, \ldots, \mathbf{p}_n^0] = [\mathbf{q}_1(\mathbf{c}^0), \ldots, \mathbf{q}_n(\mathbf{c}^0)]$.
2. For $k = 0, 1, \ldots$ until convergence, do:

   (a) Form the approximate Jacobian matrix J_k as follows:

   $$[J_k]_{ij} = (\mathbf{p}_i^k)^T A_j \mathbf{p}_i^k \quad \text{for each } i, j \in [1, n]. \tag{2.3}$$

   (b) Solve $\mathbf{c}^{k+1}$ from the approximate Jacobian equation

   $$J_k \mathbf{c}^{k+1} = \boldsymbol{\lambda}^*. \tag{2.4}$$

   (c) Form the skew-symmetric matrix Y_k:

   $$[Y_k]_{ij} = \frac{(\mathbf{p}_i^k)^T A(\mathbf{c}^{k+1}) \mathbf{p}_j^k}{\lambda_j^* - \lambda_i^*} \quad \text{for each } i, j \in [1, n] \quad \textit{and} \quad i \ne j. \tag{2.5}$$

   (d) Compute $P_{k+1} = [\mathbf{p}_1^{k+1}, \ldots, \mathbf{p}_n^{k+1}] = [\mathbf{v}_1^{k+1}, \ldots, \mathbf{v}_n^{k+1}]^T$ by solving

   $$(I + \tfrac{1}{2} Y_k) \mathbf{v}_j^{k+1} = \mathbf{h}_j^k \quad \text{for each } j \in [1, n], \tag{2.6}$$

   where $\mathbf{h}_j^k$ is the jth column of $H_k = (I - \frac{1}{2} Y_k) P_k^T$.

Note that in **Algorithm 1**, systems (2.4) and (2.6) are solved exactly. However, if n is large, one may solve these systems by iterative methods. One could expect that it requires only a few iterations to solve (2.6) iteratively. This is due to the fact that, as $\{\mathbf{c}_k\}$ converges to $\mathbf{c}^*$, $\|P_k\|$ converges to zero (cf. [1, 13]). Consequently, the coefficient matrix on the left-hand side of (2.6) approaches the identity matrix in the limit, and therefore (2.6) can be solved efficiently by iterative methods. On the other hand, as for the approximate Jacobian equation (2.4), iterative methods may bring the over-solving problem in the sense that the last few iterations before convergence are usually insignificant as far as the convergence of the outer iteration is concerned. This over-solving of the inner iterations will cause a waste of time and does not improve the efficiency of the whole method. To alleviate the over-solving problem and improve the efficiency in solving the IEP, Bai, Chan and Morini proposed in [1] the following inexact Cayley transform method where system (2.4) is solved approximately rather than exactly.

Algorithm 2: Inexact Cayley transform method

1. Given $\mathbf{c}^0$, compute the orthonormal eigenvectors $\{\mathbf{q}_i(\mathbf{c}^0)\}_{i=1}^n$ and the eigenvalues $\{\lambda_i(\mathbf{c}^0)\}_{i=1}^n$ of $A(\mathbf{c}^0)$. Let $P_0 = [\mathbf{p}_1^0, \ldots, \mathbf{p}_n^0] = [\mathbf{q}_1(\mathbf{c}^0), \ldots, \mathbf{q}_n(\mathbf{c}^0)]$ and $\boldsymbol{\rho}^0 = (\lambda_1(\mathbf{c}^0), \ldots, \lambda_n(\mathbf{c}^0))^T$.
2. For $k = 0, 1, 2$ until convergence do:
   (a) Same as (a) in **Algorithm 1**
   (b) Solve $\mathbf{c}^{k+1}$ inexactly from the approximate Jacobian equation
   $$J_k \mathbf{c}^{k+1} = \boldsymbol{\lambda}^* + \mathbf{r}^k, \tag{2.7}$$
   until the residual $\mathbf{r}^k$ satisfies
   $$\|\mathbf{r}^k\| \leq \frac{\|\boldsymbol{\rho}^k - \boldsymbol{\lambda}^*\|^\beta}{\|\boldsymbol{\lambda}^*\|^\beta}, \quad \beta \in (1, 2]. \tag{2.8}$$
   (c) Same as (c) in **Algorithm 1**
   (d) Same as (d) in **Algorithm 1**
   (e) Compute $\boldsymbol{\rho}^{k+1} = (\rho_1^{k+1}, \ldots, \rho_n^{k+1})^T$ by
   $$\rho_i^{k+1} = (\mathbf{p}_i^{k+1})^T A(\mathbf{c}^{k+1}) \mathbf{p}_i^{k+1} \quad \text{for each } i = 1, 2, \ldots, n. \tag{2.9}$$

Under the assumption that the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ are distinct and the Jacobian matrix $J(\mathbf{c}^*)$ is invertible, the inexact Cayley transform method converges locally with convergence rate β [1]. In each outer iteration of the inexact Cayley transform method, an approximate Jacobian equation is required to solve. This still can be costly sometimes especially when $\mathbf{c}^k$ is close to the solution $\mathbf{c}^*$. Furthermore, as we know, system (2.7) will involves the stability problem or the preconditioning problem in some cases.

Recall that Moser's method [18, 26, 31] to solve operator equations in Banach spaces is defined as follows. Let X, Y be (real or complex) Banach spaces, and $D \subseteq X$ be an open subset. Consider the general operator equation:
$$f(x) = 0, \tag{2.10}$$
where $f : D \subseteq X \longrightarrow Y$ is a nonlinear operator with continuous Fréchet derivative f'. Given $x_0 \in D$ and $B_0 \in \mathcal{L}(Y, X)$, Moser's method has the following form:
$$\begin{cases} x_{k+1} = x_k - B_k f(x_k) \\ B_{k+1} = 2B_k - B_k f'(x_k) B_k \end{cases} \quad \text{for each } k = 0, 1, \ldots.$$

The convergence rate of Moser's method is $(1 + \sqrt{5})/2 = 1.61\cdots$ (see [26]). However, quadratic convergence rate can be obtained when the sequence $\{B_k\}$ generated by
$$B_{k+1} = 2B_k - B_k f'(x_{k+1}) B_k \quad \text{for each } k = 0, 1, \ldots.$$

This is Ulm's method introduced in [35] and has been further studied in [11, 14, 18, 20, 31, 32, 37]. Compared with Newton's method, the advantage of Moser's method and Ulm's method is that Jacobian equations are avoided to solve. Motivated by Moser's method and Ulm's method, we propose the following deformed Cayley transform method for solving the IEP, which also avoids solving the approximate Jacobian equations.

Algorithm 3: Ulm-like Cayley transform method

1. Given $\mathbf{c}^0 \in \mathbb{R}^n$ and $B_0 \in \mathbb{R}^{n\times n}$ be such that
$$\|I - B_0 J(\mathbf{c}^0)\| \le \mu, \tag{2.11}$$
where μ is a positive constant. Compute the orthonormal eigenvectors $\{\mathbf{q}_i(\mathbf{c}^0)\}_{i=1}^n$ of $A(\mathbf{c}^0)$. Let $P_0 = [\mathbf{p}_1^0, \dots, \mathbf{p}_n^0] = [\mathbf{q}_1(\mathbf{c}^0), \dots, \mathbf{q}_n(\mathbf{c}^0)]$ and $J_0 = J(\mathbf{c}^0)$.
2. For $k = 0, 1, 2, \dots$ until convergence, do:
   (a) Compute $\mathbf{c}^{k+1}$ by
$$\mathbf{c}^{k+1} = \mathbf{c}^k - B_k(J_k\mathbf{c}^k - \boldsymbol{\lambda}^*). \tag{2.12}$$
   (b) Same as (c) in **Algorithm 1**.
   (c) Same as (d) in **Algorithm 1**.
   (d) Form the approximate Jacobian matrix J_{k+1} as follows:
$$[J_{k+1}]_{ij} = (\mathbf{p}_i^{k+1})^T A_j \mathbf{p}_i^{k+1} \quad \text{for each } i, j \in [1, n]. \tag{2.13}$$
   (e) Compute the matrix B_{k+1} by
$$B_{k+1} = 2B_k - B_k J_{k+1} B_k. \tag{2.14}$$

Remark 2.1. *Note that* (2.6) *implies*
$$P_{k+1} = P_k(I + \tfrac{1}{2}Y_k)(I - \tfrac{1}{2}Y_k)^{-1} \quad \textit{for each } k = 0, 1, \dots. \tag{2.15}$$
Since P_0 is an orthogonal matrix and $\{Y_k\}$ are skew-symmetric matrices, we see that the matrix $\{P_k\}$ generated by (2.6) *must be orthogonal, i.e.,*
$$P_k^T P_k = P_k P_k^T = I \quad \textit{for each } k = 0, 1, \dots. \tag{2.16}$$
To maintain the orthogonality of P_k, that would mean that (2.6) *cannot be solved inexactly. However, we will see in Section 3 that $\|Y_k\|$ converges to zero (see* (3.10), (3.15) *and* (3.35)*). Consequently, the matrix on the left-hand side of* (2.6) *approaches the identity matrix in the limit. Therefore we can expect to solve* (2.6) *accurately by iterative methods using just a few iterations.*

Remark 2.2. *The main difference of the deformed Cayley transform method and the inexact Cayley transform method is that the step of solving the approximate Jacobian equation* (2.4) *in the inexact Cayley transform method is replaced by computing the product of matrices, which has the same computational cost as solving the approximate Jacobian equation. However, computing the product of matrices is simpler than solving equations and has no unstability problem caused by ill-conditioning in solving equations. Therefore, the deformed Cayley transform method reduces significantly the difficulty of the problem. In particular, the parallel computation techniques can be applied in the deformed Cayley transform method to improve the computational efficiency.*

3 Convergence analysis

In this section, we carry on the convergence analysis of the deformed Cayley transform method. Let $\{\lambda_i^*\}_{i=1}^n$ be given with $\lambda_1^* \leq \lambda_2^* \leq \cdots \leq \lambda_n^*$. Let $\mathbf{c}^*$ be the solution of the IEP and let $Q_* = [q_1(\mathbf{c}^*), \ldots, q_n(\mathbf{c}^*)]$ be the orthogonal matrix of the eigenvectors of $A(\mathbf{c}^*)$. Then the matrix Q_* satisfies

$$Q_*^T A(\mathbf{c}^*) Q_* = \wedge_*, \tag{3.1}$$

where $\wedge_* = \mathrm{diag}(\lambda_1^*, \ldots, \lambda_n^*)$. As the standard assumption in [1, 3], we assume that the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ are distinct and that the Jacobian matrix $J(\mathbf{c}^*)$ is nonsingular. Let $\mathbf{c}^k$ be the kth iteration of the method, $\{\lambda_i(\mathbf{c}^k)\}_{i=1}^n$ and $\{\mathbf{q}_i(\mathbf{c}^k)\}_{i=1}^n$ be the eigenvalues and normalized eigenvectors of $A(\mathbf{c}^k)$ respectively, i.e.,

$$A(\mathbf{c}^k)\mathbf{q}_i(\mathbf{c}^k) = \lambda_i(\mathbf{c}^k)\mathbf{q}_i(\mathbf{c}^k) \quad \text{and} \quad \mathbf{q}_i(\mathbf{c}^k)^T \mathbf{q}_j(\mathbf{c}^k) = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$$

Below, we will prove that if B_0 approximates $J(\mathbf{c}^0)^{-1}$ and the initial guess $\mathbf{c}^0$ is closed to the solution $\mathbf{c}^*$, then the sequence $\{\mathbf{c}^k\}$ generated by the deformed Cayley transform method converges locally to $\mathbf{c}^*$ with root-convergence rate 2. For this purpose, we need the following four lemmas. The first two lemmas have been presented in [3]; while the third one has been presented in [13, Corollary 3.1].

Lemma 3.1. *Suppose that $\{\lambda_i^*\}_{i=1}^n$ are distinct. Then there exist positive numbers δ_0 and ρ_0 such that the following assertion holds for each $\mathbf{c} \in \mathbf{B}(\mathbf{c}^*, \delta_0)$.*

$$\| \mathbf{q}_i(\mathbf{c}) - \mathbf{q}_i(\mathbf{c}^*) \| \leq \rho_0 \| \mathbf{c} - \mathbf{c}^* \| \quad \textit{for each } i \in [1, n]. \tag{3.2}$$

Lemma 3.2. *Let $\{\boldsymbol{\omega}_i\}_{i=1}^n \subset \mathbb{R}^n$ be unit vectors approximating $\mathbf{q}_i(\mathbf{c}^*)$. Let $J_{\boldsymbol{\omega}}$ be the matrix defined by $[J_{\boldsymbol{\omega}}]_{ij} = (\boldsymbol{\omega}_i)^T A_j \boldsymbol{\omega}_i$ for each $i, j \in [1, n]$. Then*

$$\| J_{\boldsymbol{\omega}}\mathbf{c}^* - J(\mathbf{c}^*)\mathbf{c}^* \| \leq 2n \cdot \max_i |\lambda_i^*| \cdot \max_i \| \boldsymbol{\omega}_i - q_i(\mathbf{c}^*) \|^2 . \tag{3.3}$$

Lemma 3.3. *There exist two positive numbers δ_1 and ρ_1 such that, for any orthogonal matrix P with $\|P - Q_*\| < \delta_1$, the skew-symmetric matrix X defined by $e^X = P^T Q_*$ satisfies*

$$\|X\| \leq \rho_1 \|P - Q_*\|. \tag{3.4}$$

Let $\{P_k\}$ be defined by (2.15). Define

$$E_k := P_k - Q_* \quad \text{for each } k = 0, 1, \ldots. \tag{3.5}$$

Then we have the following key lemma.

Lemma 3.4. *Suppose that the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ is distinct and the Jacobian matrix $J(\mathbf{c}^*)$is invertible. Then there exist positive numbers δ_2 and ρ_2 such that, for any $k = 1, 2, ...$, if $\|\mathbf{c}^{k+1} - \mathbf{c}^*\| \leq \delta_2$ and $\|E_k\| \leq \delta_2$ then*

$$\|E_{k+1}\| \leq \rho_2(\|\mathbf{c}^{k+1} - \mathbf{c}^*\| + \|E_k\|^2). \tag{3.6}$$

Proof. Let $k = 1, 2, ...$ and consider the matrix X_k defined by $e^{X_k} = P_k^T Q_*$. Since P_k is orthogonal, it follows from (3.1) that

$$e^{X_k} \wedge_* e^{-X_k} = P_k^T A(\mathbf{c}^*) P_k. \tag{3.7}$$

Note that

$$e^X = I + X + O(\|X\|^2) \quad \text{for each matrix } X. \tag{3.8}$$

Combining this and (3.7), we have that

$$\wedge_* + X_k \wedge_* - \wedge_* X_k = P_k^T A(\mathbf{c}^*) P_k + O(\|X_k\|^2),$$

Let $i, j = 1, ...n$ with $i \neq j$. Then the above equality implies that

$$[X_k]_{ij} = \frac{1}{\lambda_j^* - \lambda_i^*} (\mathbf{p}_i^k)^T A(\mathbf{c}^*) \mathbf{p}_j^k + O(\|X_k\|^2).$$

By the definition of Y_k in (2.5), one has that

$$[X_k]_{ij} - [Y_k]_{ij} = \frac{1}{\lambda_j^* - \lambda_i^*} (\mathbf{p}_i^k)^T (A(\mathbf{c}^*) - A(\mathbf{c}^{k+1})) \mathbf{p}_j^k + O(\|X_k\|^2).$$

As $A(\cdot)$ is Lipschitz continuous, it follows that

$$|[X_k]_{ij} - [Y_k]_{ij}| = O(\|\mathbf{c}^{k+1} - c^*\| + \|X_k\|^2).$$

Consequently,

$$\|X_k - Y_k\| \leq \|X_k - Y_k\|_F = O(\|\mathbf{c}^{k+1} - \mathbf{c}^*\| + \|X_k\|^2) \tag{3.9}$$

and so $\|Y_k\| = O(\|\mathbf{c}^{k+1} - \mathbf{c}^*\| + \|X_k\|)$. Let $C > 0$ be such that

$$\|Y_k\| \leq C(\|\mathbf{c}^{k+1} - \mathbf{c}^*\| + \|X_k\|) \quad \text{for each } k. \tag{3.10}$$

Take $0 < \delta_2 < \min\left\{\delta_1, \frac{1}{(1+\rho_1)C}\right\}$, where δ_1 and ρ_1 are the positive numbers determined by Lemma 3.3. Assume that $\|\mathbf{c}^{k+1} - \mathbf{c}^*\| < \delta_2$ and $\|E_k\| < \delta_2$. Then $\|E_k\| < \delta_1$ and Lemma 3.3 is applicable to getting

$$\|X_k\| \leq \rho_1 \|E_k\|. \tag{3.11}$$

Thus (3.10) entails that

$$\|Y_k\| \leq C(\|\mathbf{c}^{k+1} - \mathbf{c}^*\| + \rho_1 \|E_k\|) \leq C(1 + \rho_1)\delta_2 \leq 1.$$

Consequently

$$\left\| \left(I - \tfrac{1}{2} Y_k\right)^{-1} \right\| \leq \frac{1}{1 - \frac{1}{2}\|Y_k\|} \leq 2. \tag{3.12}$$

Below we will show that there exists $\rho_2 > 0$ such that (3.6) holds. Granting this, the proof is complete. To this end, we note by (3.5) and (2.15) that

$$E_{k+1} = P_k[(I + \tfrac{1}{2}Y_k)(I - \tfrac{1}{2}Y_k)^{-1} - e^{X_k}] = P_k[(I + \tfrac{1}{2}Y_k) - e^{X_k}(I - \tfrac{1}{2}Y_k)](I - \tfrac{1}{2}Y_k)^{-1}.$$

Applying (3.8) to x_k, one has

$$\begin{aligned} E_{k+1} &= P_k[(I + \tfrac{1}{2}Y_k) - [I + X_k + O(\|X_k\|^2)](I - \tfrac{1}{2}Y_k)](I - \tfrac{1}{2}Y_k)^{-1} \\ &= P_k[Y_k - X_k + \tfrac{1}{2}X_k Y_k + O(\|X_k\|^2)](I - \tfrac{1}{2}Y_k)^{-1}. \end{aligned} \tag{3.13}$$

Since P_k is orthogonal, it follows that

$$\|E_{k+1}\| \leq \left[\|Y_k - X_k\| + O(\|X_k\| \cdot \|Y_k\| + \|X_k\|^2)\right] \|(I - \tfrac{1}{2}Y_k)^{-1}\|. \tag{3.14}$$

Thus (3.6) is seen to hold by (3.9)-(3.12). $\square$

Now we present the main result of this paper which shows that the deformed Cayley transform method converges quadratically.

Theorem 3.1. *Suppose that $\{\lambda_i^*\}_{i=1}^n$ are distinct and that the Jacobian matrix $J(\mathbf{c}^*)$ is invertible. Then there exist $\tau \in (0,1]$, $\delta \in (0,\tau)$ and $\mu \in [0,\delta]$ such that, for each $\mathbf{c}^0 \in \mathbf{B}(\mathbf{c}^*,\delta)$ and $B_0 \in \mathbb{R}^{n\times n}$ satisfying* (2.11)*, the sequence $\{\mathbf{c}^k\}$ generated by* **Algorithm 3** *with initial point $\mathbf{c}^0$ converges to $\mathbf{c}^*$, and the following estimates hold for each $k = 0, 1, \ldots$.*

$$\|\mathbf{c}^k - \mathbf{c}^*\| \le \tau \left(\frac{\delta}{\tau}\right)^{2^k}, \tag{3.15}$$

$$\|I - B_k J_k\| \le \tau \left(\frac{\delta}{\tau}\right)^{2^k}. \tag{3.16}$$

Proof. Let $\delta_0, \rho_0 \in (0,+\infty)$ be the constants determined by Lemma 3.1 such that $H_1\|J(\mathbf{c}^*)^{-1}\|\delta_0 < 1$ where

$$H_1 := 2n\rho_0 \cdot \max_j \|A_j\|. \tag{3.17}$$

Let $\delta_2 \in (0,\varepsilon_1]$ and $\rho_2 \in (0,+\infty)$ be the constants determined by Lemma 3.4. Moreover, we write for simplicity,

$$\bar\rho = \frac{\|J(\mathbf{c}^*)^{-1}\|}{1 - H_1\|J(\mathbf{c}^*)^{-1}\|\delta_0} \quad \text{and} \quad H_2 = 4n\bar\rho \cdot \max_i |\lambda_i^*|. \tag{3.18}$$

Set

$$\tau = \min\left\{\frac{1}{1+H_2},\ \frac{\sqrt{n}\rho_0}{\rho_2(1+n\rho_0^2)},\ \frac{1}{(1+4\bar\rho H_1)^2}\right\}. \tag{3.19}$$

Clearly

$$\tau \le 1. \tag{3.20}$$

Take δ and μ such that

$$0 < \delta < \min\left\{\delta_0,\ \delta_2,\ \tau,\ \frac{\delta_2}{\sqrt{n}\rho_0},\ \frac{1}{\bar\rho H_1}\right\} \quad \text{and} \quad 0 \le \mu \le \delta. \tag{3.21}$$

Then, one has by the definition of $\bar\rho$ that

$$\delta < \frac{1}{\bar\rho H_1} = \frac{1 - H_1\|J(\mathbf{c}^*)^{-1}\|\delta_0}{H_1\|J(\mathbf{c}^*)^{-1}\|} < \frac{1}{H_1\|J(\mathbf{c}^*)^{-1}\|}.$$

Thus for any matrix A,

$$\|A - J(\mathbf{c}^*)\| \le H_1\delta \Longrightarrow A^{-1} \text{ exists and } \|A^{-1}\| \le \bar\rho. \tag{3.22}$$

Below we shall show that τ, δ and μ are as desired. To do this, let $k = 0, 1, \ldots$ and consider the following conditions:

$$\|E_k\| \le \sqrt{n}\rho_0\tau \left(\frac{\delta}{\tau}\right)^{2^k}; \tag{3.23}$$

$$\|J_k - J(\mathbf{c}^*)\| \le H_1\tau \left(\frac{\delta}{\tau}\right)^{2^k} \quad \text{and} \quad \|J_k^{-1}\| \le \bar\rho; \tag{3.24}$$

$$\|I - B_k J_k\| \le \tau \left(\frac{\delta}{\tau}\right)^{2^k} \quad \text{and} \quad \|\mathbf{c}^k - \mathbf{c}^*\| \le \tau \left(\frac{\delta}{\tau}\right)^{2^k}; \tag{3.25}$$

$$\|B_k\| \le 2\bar{\rho} \quad \text{and} \quad \|\mathbf{c}^{k+1} - \mathbf{c}^*\| \le \tau \left(\frac{\delta}{\tau}\right)^{2^{k+1}}. \tag{3.26}$$

Then we have the following implications:

$$(3.23) \Longrightarrow (3.24) \tag{3.27}$$

and

$$[(3.23) + (3.25)] \Longrightarrow (3.26). \tag{3.28}$$

To prove the first implication, we suppose that (3.23) holds. Note that

$$\|\mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)\| \le \|P_k - Q_*\| = \|E_k\| \le \sqrt{n}\rho_0\tau \left(\frac{\delta}{\tau}\right)^{2^k} \quad \text{for each } i \in [1, n]. \tag{3.29}$$

Then, for any i, $j \in [1, n]$,

$$\begin{aligned} |\,[J_k]_{ij} - [J(\mathbf{c}^*)]_{ij}\,| &= |\,[\mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)]^T A_j \mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)^T A_j [\mathbf{q}_i(\mathbf{c}^*) - \mathbf{p}_i^k]\,| \\ &\le 2 \parallel A_j \parallel \cdot \parallel \mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*) \parallel \\ &\le 2\sqrt{n}\rho_0 \parallel A_j \|\tau \left(\frac{\delta}{\tau}\right)^{2^k}, \end{aligned}$$

which together with the definition of H_1 gives

$$\|J_k - J(\mathbf{c}^*)\| \le \|J_k - J(\mathbf{c}^*)\|_F \le 2n^{\frac{3}{2}}\rho_0 \cdot \max_j \|A_j\|\tau \left(\frac{\delta}{\tau}\right)^{2^k} \le H_1\tau \left(\frac{\delta}{\tau}\right)^{2^k}.$$

Thus, the first inequality of (3.24) is proved; while the second inequality follows from (3.22) because $\|J_k - J(\mathbf{c}^*)\| \le H_1\delta$ (noting that $\delta < \tau$). Therefore, the implication (3.27) is proved.

To verify the second implication, suppose that (3.23) and (3.25) hold. Then (3.24) holds by (3.27) and so $\|J_k^{-1}\| \le \bar{\rho}$. Furthermore,

$$\|B_k J_k\| \le 1 + \|I - B_k J_k\| \le 1 + \tau \left(\frac{\delta}{\tau}\right)^{2^k}.$$

Therefore,

$$\|B_k\| \le \|B_k J_k\| \cdot \|J_k^{-1}\| \le \left[1 + \tau \left(\frac{\delta}{\tau}\right)^{2^k}\right] \bar{\rho} \le (1+\tau)\bar{\rho} \le 2\bar{\rho} \tag{3.30}$$

(noting that $\tau \le 1$ by (3.20)). As for the estimate of $\|\mathbf{c}^{k+1} - \mathbf{c}^*\|$, we note that $\boldsymbol{\lambda}^* = J(\mathbf{c}^*)\mathbf{c}^*$. Thus, (2.12) implies

$$\begin{aligned} \mathbf{c}^{k+1} - \mathbf{c}^* &= \mathbf{c}^k - \mathbf{c}^* + B_k J_k \mathbf{c}^k - J(\mathbf{c}^*)\mathbf{c}^* \\ &= (I - B_k J_k)(\mathbf{c}^k - \mathbf{c}^*) + B_k(J_k\mathbf{c}^* - J(\mathbf{c}^*)\mathbf{c}^*). \end{aligned} \tag{3.31}$$

Since $\max_i \|\mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)\| \le \sqrt{n}\rho_0\tau \left(\frac{\delta}{\tau}\right)^{2^k}$ by (3.29), it follows from Lemma 3.2 that

$$\|J_k\mathbf{c}^* - J(\mathbf{c}^*)\mathbf{c}^*\| \le 2n \cdot \max_i |\lambda_i^*| \cdot \max_i \|\mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)\|^2 \le 2n^2\rho_0^2 \cdot \max_i |\lambda_i^*|\tau^2 \left(\frac{\delta}{\tau}\right)^{2^{k+1}}. \tag{3.32}$$

By (3.25) and using (3.30) and (3.32), we conclude from (3.31) that

$$\begin{aligned}\|\mathbf{c}^{k+1}-\mathbf{c}^*\| &\leq \|I-B_kJ_k\|\cdot\|\mathbf{c}^k-\mathbf{c}^*\|+\|B_k\|\cdot\|J_k\mathbf{c}^*-J(\mathbf{c}^*)\mathbf{c}^*\| \\ &\leq \tau^2\left(\frac{\delta}{\tau}\right)^{2^{k+1}}+4n^2\rho_0^2\bar{\rho}\cdot\max_i|\lambda_i^*|\tau^2\left(\frac{\delta}{\tau}\right)^{2^{k+1}} \\ &= (1+H_2)\tau^2\left(\frac{\delta}{\tau}\right)^{2^{k+1}},\end{aligned} \tag{3.33}$$

where the last inequality holds because of the definition of H_2. Thus, by the definition of τ,

$$\|\mathbf{c}^{k+1}-\mathbf{c}^*\|\leq\tau\left(\frac{\delta}{\tau}\right)^{2^{k+1}}. \tag{3.34}$$

This together with (3.30) completes the proof of the second implication.

Below we will show that (3.15), (3.16) and

$$\|E_k\|\leq\sqrt{n}\rho_0\tau\left(\frac{\delta}{\tau}\right)^{2^k} \tag{3.35}$$

hold for each $k\geq 0$. We will proceed by mathematical induction. Clearly, (3.15) and (3.16) for $k=0$ are trivial by assumptions (noting that $\mu\leq\delta$). Moreover, by Lemma 3.1,

$$\|E_0\|\leq\|E_0\|_F\leq\sqrt{n}\cdot\max_i\|\mathbf{q}_i(\mathbf{c}^0)-\mathbf{q}_i(\mathbf{c}^*)\|\leq\sqrt{n}\rho_0\|\mathbf{c}^0-\mathbf{c}^*\|\leq\sqrt{n}\rho_0\delta. \tag{3.36}$$

Thus (3.35) is true for $k=0$.

Now assume that (3.15), (3.16) and (3.35) hold for all $k\leq m-1$. Then, recalling that $\delta\leq\tau$, one has that

$$\|E_{m-1}\|\leq\sqrt{n}\rho_0\tau\left(\frac{\delta}{\tau}\right)^{2^k}\leq\delta_2$$

Moreover, by implication (3.28) (with $k=m-1$), one has that (3.15) holds for $k=m$ and

$$\|B_{m-1}\|\leq 2\bar{\rho}. \tag{3.37}$$

Hence

$$\|\mathbf{c}^m-\mathbf{c}^*\|\leq\tau\left(\frac{\delta}{\tau}\right)^{2^m}<\delta, \tag{3.38}$$

Applying Lemma 3.4, we obtain

$$\|E_m\|\leq\rho_2(\|\mathbf{c}^m-\mathbf{c}^*\|+\|E_{m-1}\|^2)\leq\rho_2(1+n\rho_0^2)\tau^2\left(\frac{\delta}{\tau}\right)^{2^m}\leq\sqrt{n}\rho_0\tau\left(\frac{\delta}{\tau}\right)^{2^m}. \tag{3.39}$$

Thus (3.15) and (3.35) are seen to hold for $k=m$. To show that (3.16) holds for $k=m$, using implication (3.27) (with $k=m-1$, m), one gets that

$$\|J_{m-1}-J(\mathbf{c}^*)\|\leq H_1\tau\left(\frac{\delta}{\tau}\right)^{2^{m-1}}\quad\text{and}\quad\|J_m-J(\mathbf{c}^*)\|\leq H_1\tau\left(\frac{\delta}{\tau}\right)^{2^m}.$$

Hence

$$\|J_m-J_{m-1}\|\leq\|J_m-J(\mathbf{c}^*)\|+\|J_{m-1}-J(\mathbf{c}^*)\|\leq 2H_1\tau\left(\frac{\delta}{\tau}\right)^{2^{m-1}}. \tag{3.40}$$

Recalling that $B_k = 2B_{k-1} - B_{k-1}J_kB_{k-1}$ for each $k = 1, 2, \ldots$, we have

$$I - B_mJ_m = (I - B_{m-1}J_m)^2 = (I - B_{m-1}J_{m-1} - B_{m-1}(J_m - J_{m-1}))^2. \tag{3.41}$$

Then by (3.37), (3.40) and using the inductional assumption (3.16) (with $k = m-1$), we have that

$$\begin{aligned} \|I - B_mJ_m\| &\leq (\|I - B_{m-1}J_{m-1}\| + \|B_{m-1}\| \cdot \|J_m - J_{m-1}\|)^2 \\ &\leq \left[\tau\left(\frac{\delta}{\tau}\right)^{2^{m-1}} + 4\bar{\rho}H_1\tau\left(\frac{\delta}{\tau}\right)^{2^{m-1}}\right]^2 \\ &= (1 + 4\bar{\rho}H_1)^2\tau^2\left(\frac{\delta}{\tau}\right)^{2^m}. \end{aligned} \tag{3.42}$$

Note by (3.19) that $\tau(1 + 4\bar{\rho}H_1)^2 \leq 1$. It follows that

$$\|I - B_mJ_m\| \leq \tau\left(\frac{\delta}{\tau}\right)^{2^m}, \tag{3.43}$$

that is (3.16) holds for $k = m$ and completes the proof. □

4 Numerical experiments

In this section, we illustrate by numerical experiments the convergence performance of the deformed Cayley transform method on the inverse Toeplitz eigenvalue problem [1, 3, 30, 34]. For comparisons, the inexact Cayley transform method [1] is also tested. Our aim is to show that the outer iteration number required for convergence of the deformed Cayley transform method is comparable to that of the inexact Cayley transform method [1] with large β. We use Toeplitz matrices as our A_i in (1.1):

$$A_1 = I, \quad A_2 = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix}, \ldots, A_n = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & \ddots & \ddots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \ddots & \ddots & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

Thus $A(c)$ is a symmetric Toeplitz matrix with the first column equals to c. All our tests were done in Matlab.

In [30], very large inverse Toeplitz eigenvalue problem were solved on parallel architectures. Here we consider three problem sizes: $n = 100$, 200 and 300. For each value of n, we constructed ten n-by-n test problems. For each test problem, we first generate $\mathbf{c}^*$ with entries randomly chosen between 0 and 10. Then we compute the eigenvalues $\{\lambda_i^*\}_{i=1}^n$ of $A(\mathbf{c}^*)$ as the prescribed eigenvalues. Since both algorithms are locally convergent, the initial guess $\mathbf{c}^0$ is formed by chopping the components of $\mathbf{c}^*$ to two decimal places for $n = 30$, three decimal places for $n = 200$ and five decimal places for $n = 300$. For both algorithms, the stopping tolerance for the outer (Newton) iterations is 10^{-10}.

The linear systems (2.6) and (2.7) are all solved iteratively by the QMR method (cf. [1, 12]) using the Matlab-provided QMR function. At the $(k+1)$th iteration, we use $\mathbf{v}_j^k$ as the initial guess of the inverse power equations (2.6), and $\mathbf{c}^k$ as the initial guess of the Jacobian equation (2.7). The stopping tolerance for the systems (2.7) is as given in the equations. We also set the maximum number of iterations allowed to 400 for all inner iterations. To speed up the convergence, we use the Matlab-provided Modified ILU (MILU) preconditioner: LUINC(A, [drop-tolerance, 1, 1, 1]) which is one of the most versatile pre-conditioners for unstructured matrices [8, 17]. The drop tolerance we use here is 0.01 for all the three problem sizes.

The following table gives the total numbers of outer iterations averaged over the ten test matrices respectively when $n = 100$, 200 and 300. Note by (2.11) that B_0 is an approximation of J_0^{-1}. Here, we take $B_0 = J_0^{-1}$ for the deformed Cayley transform method. Since Algorithm 2 converges with convergence rate $1+\varepsilon$, we present the outer iterations of Algorithm 2 with large ε. From this table, we can see that the outer iteration number of Algorithm 3 required for convergence is comparable to that of Algorithm 2 with large ε. Moreover, it should be noted that Algorithm 3 avoids the solvation of the approximate Jacobian equation in each outer iteration. This will be very attractive when the Jacobian equation (2.7) is difficult to solve .

Table 1: Averaged total numbers of outer iterations of Algorithms 2 and 3

n	Algorithm ICTM				Algorithm 2
	ε=0.5	ε=0.6	ε=0.8	ε=1	
100	5.0	5.0	5.0	5.0	5.5
200	5.2	4.6	4.6	4.6	4.0
300	3.2	3.2	3.2	3.2	3.1

To further illustrate the convergence performance of Algorithm 3, we give the convergence history this method for different initial guess B_0. Recall that B_0 satisfies $\|I - B_0 J_0\| \leq \mu$. The following table gives the averaged total numbers of outer iterations of Algorithm 3 with different μ. From this table, we can see that, for Algorithm 3, the numbers of outer iterations, where B_0 is an approximation to J_0^{-1}, is comparable to the one where $B_0 = J_0^{-1}$.

Table 2: Averaged total numbers of outer iterations of Algorithm 3 with different μ

	$\mu = 1e-1$	$\mu = 1e-2$	$\mu = 1e-3$	$\mu = 1e-4$	$\mu = 0$
100	6.0	5.5	5.5	5.5	5.5
200	4.2	4.0	4.0	4.0	4.0
300	3.4	3.1	3.1	3.1	3.1

From this table, we can see that for the Deform Cayley transform method, the convergence performance in the case when B_0 is an approximation to $J(\mathbf{c}^0)^{-1}$ is comparable to the one when $B_0 = J(\mathbf{c}^0)^{-1}$ especially for $\mu = 1e-2$, $1e-3$ and $1e-4$.

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