Finding the signature matrix of minimizing the Cayley transform by using computer algebra

Dexuan Zhang[1]*, Yongbin Li*[2] *and Haocheng Zhou*[3]
[1]zdxssss@126.com, [2]yongbinli@uestc.edu.cn and [3]657253957@qq.com
School of Mathematical Sciences
University of Electronic Science and Technology of China
Chengdu 611731
P.R. China

Abstract

Given an orthogonal matrix Q, we can choose a diagonal matrix D with diagonal entries such that $I + QD$ is nonsingular and then that the Cayley transform $\$(QD) = I + QD)(I - QD)^{-1}$ is well defined. Evan O'Dorney has proven the existence of the diagonal matrix D with diagonal entries ± 1 (called a signature matrix) to make sure every entry of $\$(QD)$ is less than or equal to 1 in absolute value. The remaining question is how to compute D directly. In this paper, we present a method for computing the signature matrix D based upon Gröbner basis and Real-Root-Classification in the case of $n = 2$. Our approach is helpful to develop the interest of learning computer algebra and using computer algebra systems in researching.

1 Introduction

The Cayley transform \$ of a real square matrix $A \in M_n(\mathbb{R})$ is defined as

$$\$(A) = (I - A)(I + A)^{-1} = (I + A)^{-1}(I - A),$$

where I is the identity matrix, provided that $I + A$ is nonsingular. The Cayley transform maps skew-symmetric matrices to orthogonal matrices and vice versa, see [4, 7] for the details. W.Kahan in [7] shows that for any matrix $A \in M_n(\mathbb{R})$ there is at least one diagonal matrix D with diagonal entries ± 1, called a *signature matrix*, such that $I + AD$ is nonsingular. Furthermore, given an orthogonal matrix Q, Evan O'Dorney in [4] proves the existence of a signature matrix D such that every entry of $\$(QD)$ is less than or equal to 1 in absolute value. For example, let

$$Q = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

we can choose

$$D = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

such that $I+QD$ is nonsingular and every entry of $\$(QD)$ is less than or equal to 1 in absolute value. The remaining question is how to find the above signature matrix D directly. In this paper, we present a method for computing D when $n=2$ based upon using Gröbner basis which was introduced and developed by Buchberger in [1] and Real-Root-Classification introduced and developed by Bican Xia and Lu Yang in [2, 3, 5, 6].Our method is helpful to enhance the interest of learning computer algebra and using computer algebra systems in researching.

2 Structuring the signature $D \in M_2(\mathbb{R})$

Let

$$Q = \begin{bmatrix} x1 & x2 \\ x3 & x4 \end{bmatrix},$$
$$D = \begin{bmatrix} u1 & 0 \\ 0 & u2 \end{bmatrix},$$
$$\$(QD) = \begin{bmatrix} z1 & z2 \\ z3 & z4 \end{bmatrix},$$

where $x_i, z_i, u_j \in \mathbb{R}$ for $1 \le i \le 4$ and $1 \le j \le 2$.

Consider $\$(QD) = (I+QD)(I-QD)^{-1}$ and $QQ^T = Q^TQ = I$. Simplifying the above matrix equations, we get the following polynomial equations,

$$\begin{aligned}
p1 &= u1x1z1 + u1x3z2 + u1x1 + z1 - 1 = 0, \\
p2 &= u2x2z1 + u2x4z2 + u2x2 + z2 = 0, \\
p3 &= u1x1z3 + u1x3z4 + u1x3 + z3 = 0, \\
p4 &= u2x2z3 + u2x4z4 + u2x4 + z4 - 1 = 0, \\
p5 &= x1x3 + x2x4 = 0, \\
p6 &= x1x2 + x3x4 = 0, \\
p7 &= x1x1 + x2x2 - 1 = 0, \\
p8 &= x3x3 + x4x4 - 1 = 0, \\
p9 &= x1x1 + x3x3 - 1 = 0, \\
p10 &= x2x2 + x4x4 - 1 = 0, \\
p11 &= u1u1 - 1 = 0, \\
p12 &= u2u2 - 1 = 0.
\end{aligned}$$

2.1 Computing the Gröbner Basis

The above polynomial equations can be simplified by using Maple's Gröbner package, and the syntax is as follows:

```
>with(Groebner):
>Basis([p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,p11,p12,z1,z4],
plex(z2,z3,z1,z4,x1,x2,x3,x4,u1,u2));
[u2^2-1,u1^2-1,x3^2+x4^2-1,u1*u2*x3+x2,-u1*u2*x4+x1,
z4,z1,u1*u2*x3+u2*z3+x4*z3,-u1*u2*x4+x3*z3+u1,z2+z3].
```

A new equations with the same solution is as follows.

$$
\begin{aligned}
&f1 = u2^2 - 1 = 0,\\
&f2 = u1^2 - 1 = 0,\\
&f3 = x3^2 + x4^2 - 1 = 0,\\
&f4 = u1u2x3 + x2 = 0,\\
&f5 = -u1u2x4 + x1 = 0,\\
&f6 = u1u2x3 + u2z3 + x4z3 = 0,\\
&f7 = -u1u2x4 + x3z3 + u1 = 0,\\
&\quad z1 = z4 = 0, z2 = -z3.
\end{aligned}
$$

2.2 Solving the Semi-algebraic System

In order to solve completely the above real algebraic system, we need to apply a Maple function, *RealRootClassification* which is based upon the early Maple's DISCOVERER package developed by Bican Xia and Lu Yang in [2, 3, 6].The function is an essential tool for studying the real solutions of parametric polynomial systems, see the overview of the subpackage RegularChains[SemiAlgebraicSetTools] in Maple 13 or more later for the details.

Here, we first start Maple and load some relative internal packages as follows. Based on the above result, the matrix D can be structured as follows.

```
> with(RegularChains):
> with(ParametricSystemTools):
> with(SemiAlgebraicSetTools):
> R:= PolynomialRing([u1,u2,,x1,x2,x3,x4,z1,z2,z3,z4]):
> infolevel[RegularChains]:= 1:
> RealRootClassification([f1, f2, f3, f4, f5, f6, f7], [], [], [],
[u1, u2, x1, x2, x3, z3], [x4], 1 .. n,R);
```

The result gives the range of $x4$.

```
                          FINAL RESULT:
 The system has given number of real solution(s) IF AND ONLY IF

                       [R[1]<0,0<R[2]]
  where
                          R[1]=x4-1
                          R[2]=x4+1

        PROVIDED THAT
                           x4-1<0
                           x4+1<0
```

$x4 = \pm 1$ will be consider later. We are going to add the condition $[R_1 < 0, 0 < R_2]$ in the next command.

```
> RealRootClassification([f1,f2,f3,f4,f5,f6,f7], [], [1-x4,x4+1], [],
[u1,u2,x1,x2,x3],[z3,x4], 1 .. n,R)

                          FINAL RESULT
       There is always given number of real solution(s)!
                         IF AND ONLY IF
                   x4 z3  - z3  + x4 + 1 = 0
                   x4 z3  + z3  + x4 - 1 = 0
```

It has two results and we are going to consider $x4z3^2 - z3^2 + x4 + 1 = 0$ in the next step. The others will be considered later.

```
> RealRootClassification([f1,f2,f3,f4,f5,f6,f7,x4*z3^2-z3^2+x4+1], [1-x4,x4+1],
[], [], [u1,u2,x3,x2,z3], [x4,x1], 1 .. n,R);
                         FINAL RESULT
       There is always given number of real solution(s)!
                         IF AND ONLY IF
                          x1-x4=0
                          x1+x4=0

       PROVIDED THAT
                            x1 <> 0
                          x1 - 1 <> 0
                          x1 + 1 <> 0
```

It has two results. $x1 = x4$ will be put into next step.

```
> RealRootClassification([f1,f2,f3,f4,f5,f6,f7,x4*z3^2-z3^2+x4+1,x4-x1], [1-x4, x4+1],
[], [], [u1,u2,x4,x1,z3], [x3,x2], 1 .. n,R);
                         FINAL RESULT:
 The system has given number of real solution(s) IF AND ONLY IF

                 [0<R[1], R[2]<0, (1)S[1]]
  where
                         R[1]=x2+1
                         R[2]=x2-1
  and
                         S[1]=x2+x3

               PROVIDED THAT
                            x2 <> 0
                          x2 + 1 <> 0
                          x2 - 1 <> 0
```

Now we get the range of $x2$. $u1$ and $u2$ are as the following

```
> RealRootClassification([f1,f2,f3,f4,f5,f6,f7,x4*z3^2-z3^2+x4+1,x4-x1],
[1-x4,1+x4,1-x2,1+x2],[], [], [u2,x2,x3,x4,x1,z3], [u1], 1 .. n,R);
                         FINAL RESULT:
       There is always given number of real solution(s)!
                         IF AND ONLY IF
                           u1 + 1 = 0

                PROVIDED THAT
                            x2 <> 0
                          x2 + 1 <> 0
                          x2 - 1 <> 0
                         0.032 seconds

> RealRootClassification([f1,f2,f3,f4,f5,f6,f7,x4*z3^2-z3^2+x4+1,x4-x1,u1+1],
 [1-x4,1+x4,1-x2,1+x2],[], [], [u1,x2,x3,x4,x1,z3], [u2], 1 .. n,R);
                         FINAL RESULT:
       There is always given number of real solution(s)!
                         IF AND ONLY IF
                           u2 + 1 = 0

                PROVIDED THAT
                            x2 <> 0
                          x2 + 1 <> 0
                          x2 - 1 <> 0
```

Under the condition of $x1 = x4$ and $x4z3^2 - z3^2 + x4 + 1 = 0$, we get $u1 = -1$ and $u2 = -1$.

$$D = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

The range of $x4$ is determined by $x4z3^2 - z3^2 + x4 + 1 = 0$ and $f3 = x3^2 + x4^2 + 1 = 0$.

$$-1 < x4 \leqslant 0$$

Put $u1, u2$ into the set of equations and we get the final result:

$$u1 = -1, u2 = -1, z3 = \pm\sqrt{\frac{1+x4}{1-x4}}, x1 = x4, x2 = -x3, x3 = \pm\sqrt{1-x4^2}, -1 < x4 \leqslant 0$$

We also can use the similar process to solve the problem under the condition of $x1 = -x4$ and $x4z3^2 + z3^2 + x4 - 1 = 0$. The results are as follows:

$$u1 = 1, u2 = 1, z3 = \pm\sqrt{\frac{1-x4}{1+x4}}, x1 = x4, x2 = -x3, x3 = \pm\sqrt{1-x4^2}, 0 \leqslant x4 < 1$$

$$u1 = 1, u2 = -1, z3 = \pm\sqrt{\frac{1+x4}{1-x4}}, x1 = -x4, x2 = x3, x3 = \pm\sqrt{1-x4^2}, -1 < x4 \leqslant 0$$

$$u1 = -1, u2 = 1, z3 = \pm\sqrt{\frac{1-x4}{1+x4}}, x1 = -x4, x2 = -x3, x3 = \pm\sqrt{1-x4^2}, 0 \leqslant x4 < 1$$

When $x4 = \pm 1$, the following result is easy to get.

```
solve([f1,f2,f3,f4,f5,f6,f7,f8,f9,f10,f11,f12,z1,z4],
[z1,z2,z3,z4,x1,x2,x3,x4,u1,u2]);
[[z1=0,z2=0,z3=0,z4=0,x1=1,x2=0,x3=0,x4=1,u1=1,u2=1],
 [z1=0,z2=0,z3=0,z4=0,x1=-1,x2=0,x3=0,x4=1,u1=-1,u2=1],
 [z1=0,z2=0,z3=0,z4=0,x1=1,x2=0,x3=0,x4=-1,u1=1,u2=-1],
 [z1=0,z2=0,z3=0,z4=0,x1=-1,x2=0,x3=0,x4=-1,u1=-1,u2=-1]].
```

In short, we can prove that every entry of $\$(QD)$ is less than or equal to 1 in absolute value by calculating $z1, z2, z3, z4$.

3 Summary

With the help of computer algebra system, we can compute the signature matrix D and show that every entry of $\$(QD)$ is less than or equal to 1 in absolute value by using Gröbner basis and Real-Root-Classification when $n = 2$. In other words, we get the main result of [4] in the mechanical theorem proving. In practical computation, our method is difficult when $n \geq 3$. The main difficulty in our method is how to effectively compute the Gröbner basis and a triangular decomposition of a zero-dimensional polynomial system. For instance, when we write the orthogonal matrix $Q = \begin{bmatrix} x1 & -x2 \\ x2 & x1 \end{bmatrix}$ where $x_1^2 + x_2^2 = 1$, even $Q = \begin{bmatrix} \frac{1-t^2}{(1+t^2)^2} & \frac{-2t}{(1+t^2)^2} \\ \frac{2t}{(1+t^2)^2} & \frac{1-t^2}{(1+t^2)^2} \end{bmatrix}$ the number of variables is less, but the output becomes more complicated and the computation cost is higher.

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