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

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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 $\pm 1$ (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 \cite{4,7} for the details. W.Kahan in \cite{7} shows that for any matrix $A \in M_n(\mathbb{R})$ there is at least one diagonal matrix $D$ with diagonal entries $\pm 1$, called a signature matrix, such that $I + AD$ is nonsingular. Furthermore, given an orthogonal matrix $Q$, Evan O’Dorney in \cite{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

\[
Q = \begin{bmatrix} x_1 & x_2 \\ x_3 & x_4 \end{bmatrix},
\]

\[
D = \begin{bmatrix} u_1 & 0 \\ 0 & u_2 \end{bmatrix},
\]

\[
(QD) = \begin{bmatrix} z_1 & z_2 \\ z_3 & z_4 \end{bmatrix},
\]

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

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

\[
p_1 = u_1x_1z_1 + u_1x_3z_2 + u_1x_1 + z_1 - 1 = 0,
\]

\[
p_2 = u_2x_2z_1 + u_2x_4z_2 + u_2x_2 + z_2 = 0,
\]

\[
p_3 = u_1x_1z_3 + u_1x_3z_4 + u_1x_3 + z_3 = 0,
\]

\[
p_4 = u_2x_2z_3 + u_2x_4z_4 + u_2x_4 + z_4 - 1 = 0,
\]

\[
p_5 = x_1x_3 + x_2x_4 = 0,
\]

\[
p_6 = x_1x_2 + x_3x_4 = 0,
\]

\[
p_7 = x_1x_1 + x_2x_2 - 1 = 0,
\]

\[
p_8 = x_3x_3 + x_4x_4 - 1 = 0,
\]

\[
p_9 = x_1x_1 + x_3x_3 - 1 = 0,
\]

\[
p_{10} = x_2x_2 + x_4x_4 - 1 = 0,
\]

\[
p_{11} = u_1u_1 - 1 = 0,
\]

\[
p_{12} = u_2u_2 - 1 = 0.
\]

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:

\[
> \text{with(Groebner):}
\]

\[
> \text{Basis([p1,p2,p3,p4,p5,p6,p7,p8,p9,p10,p11,p12,z1,z4],}
\]

\[
\text{plex(z2,z3,z1,z4,x1,x2,x3,x4,u1,u2)});
\]

\[
[u^2-1,u^1-1,x^3-2+x^4-2-1,u1*u2*x3+x2,-u1*u2*x4+x1,
\]

\[
z4,z1,u1*u2*x3+u2*z3+x4*z3,-u1*u2*x4+x3*z3+u1,z2+z3].
\]
A new equations with the same solution is as follows.

\[
\begin{align*}
    f_1 &= u_2^2 - 1 = 0, \\
    f_2 &= u_1^2 - 1 = 0, \\
    f_3 &= x_3^2 + x_4^2 - 1 = 0, \\
    f_4 &= u_1 u_2 x_3 + x_2 = 0, \\
    f_5 &= -u_1 u_2 x_4 + x_1 = 0, \\
    f_6 &= u_1 u_2 x_3 + u_2 z_3 + x_4 z_3 = 0, \\
    f_7 &= -u_1 u_2 x_4 + x_3 z_3 + u_1 = 0, \\
    z_1 &= z_4 = 0, z_2 = -z_3.
\end{align*}
\]

2.2 Solving the Semi-algebraic System

In order to solve completely the above real algebraic system, we need to apply a Maple function, \textit{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 \textit{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.

\[
\begin{align*}
    &\texttt{> with(RegularChains):} \\
    &\texttt{> with(ParametricSystemTools):} \\
    &\texttt{> with(SemiAlgebraicSetTools):} \\
    &\texttt{> \texttt{R:= PolynomialRing([u1,u2,,x1,x2,x3,x4,z1,z2,z3,z4]):}} \\
    &\texttt{> \texttt{infolevel[RegularChains]:= 1:}} \\
    &\texttt{> \texttt{RealRootClassification([f1, f2, f3, f4, f5, f6, f7], [], [], [],}} \\
    &\texttt{[u1, u2, x1, x2, x3, z3], [x4], 1 .. n,R);} \\
\end{align*}
\]

The result gives the range of \(x_4\).

\textbf{FINAL RESULT:}

The system has given number of real solution(s) \textbf{IF AND ONLY IF}

\[ [R[1]<0,0<R[2]] \]

where

\[
\begin{align*}
    &R[1]=x_4-1 \\
    &R[2]=x_4+1
\end{align*}
\]

\textbf{PROVIDED THAT}

\[
\begin{align*}
    &x_4-1<0 \\
    &x_4+1<0
\end{align*}
\]

\(x_4 = \pm 1\) 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
\[ x_4 z_3 - z_3 + x_4 + 1 = 0 \]
\[ x_4 z_3 + z_3 + x_4 - 1 = 0 \]

It has two results and we are going to consider \( x_4 z_3^2 - z_3^2 + x_4 + 1 = 0 \) 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
\[ x_1-x_4=0 \]
\[ x_1+x_4=0 \]

PROVIDED THAT
\[ x_1 <> 0 \]
\[ x_1 - 1 <> 0 \]
\[ x_1 + 1 <> 0 \]

It has two results. \( x_1 = x_4 \) 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
\[ R[1]=x_2+1 \]
\[ R[2]=x_2-1 \]

and
\[ S[1]=x_2+x_3 \]

PROVIDED THAT
\[ x_2 <> 0 \]
\[ x_2 + 1 <> 0 \]
\[ x_2 - 1 <> 0 \]

Now we get the range of \( x_2 \). \( u_1 \) and \( u_2 \) 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 $f3 = x3^2 + x4^2 + 1 = 0$.

$$-1 < x4 \leq 0$$

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

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

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:

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

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

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

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 [3] 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 $Q = \begin{bmatrix} x_1 & -x_2 \\ x_2 & x_1 \end{bmatrix}$ where $x_1^2 + x_2^2 = 1$, even $Q = \begin{bmatrix} \frac{1-t^2}{(1+t^2)^2} & -\frac{2t}{(1+t^2)^2} \\ \frac{2t}{(1+t^2)^2} & \frac{-2t}{(1+t^2)^2} \end{bmatrix}$ the number of variables is less, but the output becomes more complicated and the computation cost is higher.

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References


