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Semidefinite Optimization Estimating Bounds on Linear Functionals Defined on Solutions of Linear ODEs

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Abstract. In this paper, semidefinite optimization method is proposed to estimate bounds on linear functionals defined on solutions of linear ordinary differential equations (ODEs) with smooth coefficients. The method can get upper and lower bounds by solving two semidefinite programs, not solving ODEs directly. Its convergence theorem is proved. The theorem shows that the upper and lower bounds series of linear functionals discussed can approach their exact values infinitely. Numerical results show that the method is effective for the estimation problems discussed. In addition, in order to reduce calculation amount, Cheybeshev polynomials are applied to replace Taylor polynomials of smooth coefficients in computing process.

AMS subject classifications: 35A24, 37C10, 90C22

Key words: Semidefinite optimization, bound, linear functional, ordinary differential equation.

1 Introduction

Semidefinite optimization is a very efficient optimization method [1]. It has been successfully used to solve many important problems, including combinatorial optimization [2,3], filter design [4], eigenvalue optimization [5] and mobile communication optimization [6]. Recently, the method was applied to deal with moment problem [7–9], polynomial global optimization [7, 10–17] and bounds on linear functionals defined on solutions of linear differential equations [18] with polynomial coefficients. Instead of finding out the solutions of linear differential equations, D. Bertsimas and C. Caramanis [18] presented semidefinite optimization to estimate bounds on linear functionals defined on solutions of linear differential equations with polynomial coefficients. The numerical results show

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that the method is very efficient for the related problems. The method can easily obtain good upper and lower bounds of the functionals discussed under a small amount computational burden. At this regard, the discretization-based approaches cannot provide guaranteed bounds on functionals defined on solutions of the differential equations.

In this paper, we will propose semidefinite optimization method for estimating bounds on linear functionals defined on solutions of ODEs with general smooth coefficients. The primal problem is first transformed into a series of approximate problems with polynomial coefficients. Then semidefinite optimization method is applied to solve these approximate problems. Convergence theorem of the proposed method is proved. Two numerical examples are given to show the effectiveness of our estimation method. Our approach generalizes the one in [18] in terms of ODEs case, which can estimate bounds on linear functionals defined on solutions of ODEs with general smooth coefficients, including ODEs with polynomial coefficients.

The rest of this paper is organized as follows. In Section 2, we propose semidefinite optimization method for estimating bounds on the linear functionals defined on solutions of ODEs with smooth coefficients. In Section 3, we prove that the approach is convergent for the problems discussed. Numerical experiments are performed in Section 4. We end the paper with some conclusions and discussions in Section 5.

2 Semidefinite optimization

Suppose that L and G are two linear differential operators operating on some distribution space $\mathcal{A}$, in which the space $\mathcal{F}=Span\{1,x,x^2,\cdots,x^i,\cdots\}$ is dense. Their orders are r_1 and r_2 $(r_2\leq r_1)$, respectively.

We define L and G as follows:

$$Lu(x)=\sum_{s\leq r_1}L_s(x)\frac{d^s u(x)}{dx^s}, \tag{2.1a}$$

$$Gu(x)=\sum_{s\leq r_2}G_s(x)\frac{d^s u(x)}{dx^s}, \tag{2.1b}$$

where $L_s(x)$ and $G_s(x)$ are all in $\mathbb{C}^\infty[0,1]$.

Primal Problem: Computing

$$\int_0^1 Gu(x), \tag{2.2}$$

where $u(x)\in\mathcal{A}$ satisfies the following differential equation

$$Lu(x)=f(x),\quad x\in[0,1], \tag{2.3}$$

with some appropriate boundary conditions at $x=0$ and $x=1$. In (2.3), we also suppose $f(x)\in\mathcal{A}$.

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Expand $L_s(x)$ and $G_s(x)$ as Taylor polynomials at $x=0$ with orders k and l $(l\leq k)$, respectively, that is,

$$L_s(x)\approx L_s^A(x)=\sum_{i=0}^{k}a_i^{L_s}x^i,\quad G_s(x)\approx G_s^A(x)=\sum_{i=0}^{l}a_i^{G_s}x^i.$$

We define two differential operators L^A and G^A as follows,

$$L^A=\sum_{s\leq r_1}L_s^A(x)\frac{d^s}{dx^s}=\sum_{s\leq r_1}\Big(\sum_{i=0}^{k}a_i^{L_s}x^i\Big)\frac{d^s}{dx^s},\tag{2.4a}$$

$$G^A=\sum_{s\leq r_2}G_s^A(x)\frac{d^s}{dx^s}=\sum_{s\leq r_2}\Big(\sum_{i=0}^{l}a_i^{G_s}x^i\Big)\frac{d^s}{dx^s}.\tag{2.4b}$$

Then Primal Problem can be approximated by the following problem:

Approximate Problem: Computing

$$\int_0^1 G^Au(x),\tag{2.5}$$

where $u(x)$ satisfies

$$L^Au(x)=f(x),\qquad x\in[0,1],\tag{2.6}$$

with the appropriate boundary conditions at $x=0$ and $x=1$.

Assume that the solution of the Eq. (2.3) is bounded from below, that is, $u(x)\geq u_0$ for all $x\in[0,1]$. We define the following moments on the solution $u(x)$

$$m_i=\int_0^1(u(x)-u_0)x^i,\quad i=0,1,2,\cdots,\tag{2.7}$$

even though $u(x)$ may not be a probability distribution.

By the linearity of integration and $u(x)\in\mathcal{A}$, we have

$$\begin{aligned}L^Au(x)=f(x)&\Longleftrightarrow\int_0^1(L^Au(x))\varphi_i=\int_0^1f(x)\varphi_i,&&\forall\varphi_i\in\mathcal{A},\\&\Longleftrightarrow\int_0^1(L^Au(x))x^i=\int_0^1f(x)x^i,&&i=0,1,2,\cdots,\end{aligned}\tag{2.8a}$$

in which $\varphi_i=x^i$, $i=0,1,\cdots$, are called the test functions.

We consider the general term x^kd^j/dx^j of the linear differential operators L^A and G^A in (2.4a) and (2.4b).

By (2.7), (2.8a) and integration by parts, we get

$$\begin{aligned}\int_0^1\Big(x^k\frac{d^ju(x)}{dx^j}\Big)x^idx&=\int_0^1x^{k+i}u^{(j)}(x)dx=\int_0^1x^{k+i}du^{(j-1)}(x)\\&=x^{k+i}u^{(j-1)}(x)\big|_0^1-(k+i)x^{k+i-1}u^{(j-2)}(x)\big|_0^1+\cdots\end{aligned}$$

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$$+(-1)^j(k+i)(k+i-1)\cdots(k+i-j+1)\int_0^1 x^{k+i-j}u(x)$$
$$=u^{(j-1)}(1)-(k+i)u^{(j-2)}(1)+\cdots+(-1)^j(k+i)(k+i-1)\cdots(k+i-j+1)m_{k+i-j}. \quad (2.9)$$

From the equality (2.9), we know that the integral $\int_0^1 x^k u^{(j)}(x)dx$ can be represented by the moments m_{k+i-j}, boundary values $u^{(k)}(0)$ and $u^{(k)}(1)$, $k=0,1,\cdots,j-1$. Therefore, the integral $\int_0^1 (L^A u(x))x^i$ can be expressed by the moments m_j, $j=0,1,\cdots,i+k$, unknown $u^{(j)}(0)$ and $u^{(j)}(1)$, $j=0,1,\cdots,r_1-1$, that is,

$$\int_0^1 (L^A u(x))x^i=\sum_{j=0}^{i+k}\alpha_j m_j+\sum_{j=0}^{r_1-1}\beta_j u^{(j)}(0)+\sum_{j=0}^{r_1-1}\gamma_j u^{(j)}(1), \quad (2.10)$$

where α_j, β_j, γ_j are constants.

Similarly, the integral $\int_0^1 G^A u(x)$ in (2.5) can be written as the following linear combination on m_j, $j=0,1,\cdots,l$, unknown $u^{(j)}(0)$ and $u^{(j)}(1)$, $j=0,1,\cdots,r_2-1$,

$$\int_0^1 G^A u(x)=\sum_{j=0}^{l}a_j m_j+\sum_{j=0}^{r_2-1}b_j u^{(j)}(0)+\sum_{j=0}^{r_2-1}c_j u^{(j)}(1)\triangleq v^{(l)}, \quad (2.11)$$

where a_j, b_j, c_j are constants.

By the equivalency (2.7) and (2.10), the differential equation (2.4b) can be written as a series of linear equations whose variables are m_j, $j=0,1,\cdots,i+k$, unknown $u^{(j)}(0)$ and $u^{(j)}(1)$, $j=0,1,\cdots,r_1-1$, that is,

$$\sum_{j=0}^{i+k}\alpha_j m_j+\sum_{j=0}^{r_1-1}\beta_j u^{(j)}(0)+\sum_{j=0}^{r_1-1}\gamma_j u^{(j)}(1)=\xi_i, \quad i=0,1,\cdots, \quad (2.12)$$

where

$$\xi_i=\int_0^1 f(x)x^i.$$

For $x\in[0,1]$, we have the following semidefinite constraints by the method in [18]

$$Q_0\succeq 0, \quad Q_1\succeq 0, \quad Q_0-Q_1\succeq 0, \quad Q_1-Q_2\succeq 0,$$

in which

$$Q_0=\begin{pmatrix} m_0 & m_1 & \cdots & m_{i+k} \\ m_1 & m_2 & \cdots & m_{i+k+1} \\ \vdots & \vdots & \ddots & \vdots \\ m_{i+k} & m_{i+k+1} & \cdots & m_{2(i+k)} \end{pmatrix},$$

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$$Q_1=\begin{pmatrix} m_1 & m_2 & \cdots & m_{i+k+1} \\ m_2 & m_3 & \cdots & m_{i+k+2} \\ \vdots & \vdots & \ddots & \vdots \\ m_{i+k+1} & m_{i+k+2} & \cdots & m_{2(i+k+1)} \end{pmatrix},$$

$$Q_2=\begin{pmatrix} m_2 & m_3 & \cdots & m_{i+k+2} \\ m_3 & m_4 & \cdots & m_{i+k+3} \\ \vdots & \vdots & \ddots & \vdots \\ m_{i+k+2} & m_{i+k+3} & \cdots & m_{2(i+k+2)} \end{pmatrix}.$$

Q_i, $i=0,1,2$, are only dependent on the interval $[0,1]$ (see [18]).

In fact, the above constraints can be simplified to

$$Q_0-Q_1\succeq 0,\quad Q_1-Q_2\succeq 0,\quad Q_1\succeq 0. \tag{2.13}$$

Now, we present semidefinite optimization method for estimating the bound on the integral (2.2) in Primal Problem with smooth coefficients $L_s(x)$ and $G_s(x)$ in the space $\mathbb{C}^\infty[0,1]$.

Algorithm 2.1.

Step 1 Transform Primal Problem into Approximate Problem according to the above analysis. Let $i:=1$, $k:=1$, $l:=1$ and give a tolerance ϵ;

Step 2 Generate linear constraints (2.12);

Step 3 Generate the semidefinite constraints (2.13);

Step 4 Construct the following semidefinite Programs (I)

$$\max/\min v^{(l)},\quad s.t.\ (2.12)\ \text{and}\ (2.13),$$

in which the decision variables are m_j, $j=0,1,\cdots,2(i+k+2)$, unknown $u^{(j)}(0)$ and $u^{(j)}(1)$, $j=0,1,\cdots,r_1-1$;

Step 5 Apply SeDuMi 1.1R3 [19] to solve the Programs (I). Then get upper and lower bounds on $v^{(l)}$. Let $i:=i+1$;

Step 6 Decide whether the iteration goes on or not. If $|m_j^{(i+1)}-m_j^{(i)}|$, $j=0,1,\cdots,i+k$, where $m_j^{(i)}$ means moment m_j when the highest degree of the test functions in Algorithm 2.1 is i, and $m_j^{(i+1)}$ has similar meaning, are less than the given tolerance ϵ, then we stop the iteration, output $v^{(l)}$ and all decision variables, or increase $k:=k+1$ and $l:=l+1$ by turns, go to Step 2.

Remark 2.1. Obviously, if the interval $[0,1]$ is replaced by the general interval $[a,b]\subset\mathbb{R}$, Algorithm 2.1 can also work well.

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Remark 2.2. If $L_s(x)$ and $G_s(x)$ in (2.1a) and (2.1b) are all in the polynomial ring $\mathbb{R}[x]$, then Algorithm 2.1 is just the proposed method in [18] for ODEs with polynomial coefficients. If $L_s(x)\in\mathbb{C}^\infty[0,1]$, $s=0,1,\cdots,r_1$, but $G_s(x)\in\mathbb{R}[x]$, $s=0,1,\cdots,r_2$ $(r_2\leq r_1)$, and vice versa, then Algorithm 2.1 still work well. Similarly, Theorem 2 in Section 3 holds still for these cases.

Remark 2.3. There are two programs in Step 4 of Algorithm 2.1. They are maximize and minimize programs, respectively. In one iteration, we have to solve them, respectively. Upper bounds are gotten by solving the former, and lower bounds are just the opposite.

Remark 2.4. Generally, lower bound u_0 is unknown. We can first set a small value to u_0. When the iterative number is large, if $|m_j^{\max}-m_j^{\min}|$, $j=0,1,\cdots,i+k$, where $m_j^{\max}$ and $m_j^{\min}$ are the two moment m_j's gotten by solving maximize and minimize programs in the Programs (I), respectively, are small enough, then for $x\in[0,1]$, $u(x)\geq u_0$ holds, or a smaller value will be given to u_0.

Remark 2.5. Before iterative computing is performed, we usually set two appropriate positive integers to k and l, respectively. This means that solving the Programs (I) need not start from $k=1$ and $l=1$.

Remark 2.6. The semidefinite constraints only depend on the interval $[0,1]$ and not on the operators L^A and G^A. In the semidefinite constraints, there are some moments $m_{i+k+1},\cdots,$ $m_{2(i+k+2)}$ which are not appearing in the linear constraints. They are extension moments (see [9] or [18] for details).

Remark 2.7. In Algorithm 2.1, in order to reduce calculation amount under the same precision, we may expand the coefficients $L_s(x)$ and $G_s(x)$ as Chebyshev polynomials, instead of Taylor polynomials.

3 Convergence analysis

We first introduce a theorem which is a special case of Theorem 3 in [18] when $x\in[0,1]$.

Theorem 3.1. *Given* $\mathbf{M}=\{m_i,i=0,1,2,\cdots\}$, *there exists a function* $u(x)\geq u_0$ *such that*

$$m_i=\int_0^1(u(x)-u_0)x^i,\quad \forall i=0,1,2,\cdots,$$

if and only if for all subsets $I\subseteq\{1,2\}$, *and all* $n\geq 0$, *the matrix obtained from the expression*

$$\int_0^1(u(x)-u_0)\mathbf{F}_n(x)\mathbf{F}_n(x)^T\prod_{i\in I}f_i(x),$$

in which $\mathbf{F}_n(x)=[1\ x\ x^2\ \cdots\ x^n]^T$, $f_1(x)=x$ *and* $f_2(x)=1-x$, *be replacing* $\int_0^1(u(x)-u_0)x^i$ *by* m_i, *which is positive semidefinite.*

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Now, we give the following lemma:

Lemma 3.1. *Assume $u^*(x)$ is the unique solution of the differential equation*

$$\sum_{s\le r_1} L_s(x)\frac{d^s u(x)}{dx^s} = f(x), \quad x\in[0,1], \tag{3.1}$$

with some appropriate boundary conditions at $x=0$ and $x=1$. In (3.1), $f(x)$ and $L_s(x)$, $s=0,1,\cdots,r_1$, are all in $\mathbb{C}^\infty[0,1]$, and every $L_s(x)$ can be expanded as the following Taylor polynomials at $x=0$

$$L_s(x) = \sum_{i=0}^{\infty} a_i^{L_s} x^i, \quad x\in[0,1]. \tag{3.2}$$

Suppose a series of differential equations

$$\sum_{s\le r_1}\Big(\sum_{i=0}^{k} a_i^{L_s} x^i\Big)\frac{d^s u(x)}{dx^s} = f(x), \quad k=0,1,2,\cdots, \tag{3.3}$$

with the same boundary conditions just like the above exist a unique series of solutions $\{\tilde{u}_k(x), k=0,1,2,\cdots\}$ in the space $\mathbb{C}^\infty[0,1]$. Then we have the following conclusion

$$\lim_{k\to\infty}\tilde{u}_k(x) = u^*(x). \tag{3.4}$$

Proof. Let

$$R_k^{L_s}(x) = L_s(x) - \sum_{i=0}^{k} a_i^{L_s} x^i.$$

It is obvious that $R_k^{L_s}(x)\in\mathbb{C}^\infty[0,1]$. By (3.2), we have

$$\lim_{k\to\infty} R_k^{L_s}(x) = 0. \tag{3.5}$$

Denote

$$H_k(x) = \sum_{s\le r_1} L_s(x)\frac{d^s u(x)}{dx^s} - \sum_{s\le r_1}\Big(\sum_{i=0}^{k} a_i^{L_s} x^i\Big)\frac{d^s u(x)}{dx^s}. \tag{3.6}$$

Then

$$H_k(x) = \sum_{s\le r_1}\Big(L_s(x) - \sum_{i=0}^{k} a_i^{L_s} x^i\Big)\frac{d^s u(x)}{dx^s} = \sum_{s\le r_1} R_k^{L_s}(x)\frac{d^s u(x)}{dx^s}. \tag{3.7}$$

For $u(x)\in\mathbb{C}^\infty[0,1]$, there exists a positive real number M_0 satisfying

$$\left|\frac{d^j u(x)}{dx^j}\right| \le M_0, \quad x\in[0,1], \quad j=0,1,\cdots,r_1. \tag{3.8}$$

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By (3.7) and (3.8), we have

$$|H_k(x)| \le \sum_{s\le r_1} |R_k^{L_s}(x)| \cdot \left| \frac{d^s u(x)}{dx^s} \right| \le M_0 \sum_{s\le r_1} |R_k^{L_s}(x)|. \tag{3.9}$$

The fact that

$$\lim_{k\to\infty} H_k(x) = 0 \tag{3.10}$$

can be deduced easily from (3.5) and (3.9). Then, by (3.10) and (3.6), we get

$$\lim_{k\to\infty} \sum_{s\le r_1} \left(\sum_{i=0}^{k} a_i^{L_s} x^i \right) \frac{d^s u(x)}{dx^s} = \sum_{s\le r_1} L_s(x) \frac{d^s u(x)}{dx^s}.$$

Therefore, the conclusion (3.4) holds because the solution of the Eq. (3.1) with some appropriate boundary conditions exists and is unique. □

The following theorems show Algorithm 2.1 is convergent.

Theorem 3.2. *If the conditions in Lemma 3.1 hold and the linear differential operator G in* (2.2) *can be written as*

$$G = \sum_{s\le r_2} G_s(x) \frac{d^s}{dx^s},$$

where $G_s(x)$, $s=0,1,\cdots,r_2$, $(r_2 \le r_1)$, are all polynomials, then

$$\lim_{k\to\infty} \int_0^1 G\tilde{u}_k(x) = \int_0^1 Gu^*(x).$$

Furthermore, applying Algorithm 2.1 to solve the semidefinite Programs (I) with the test functions $\varphi_i = x^i$, $i=0,1,\cdots,N$, we can get two upper and lower bounds series $\{\rho_{kN}, k=0,1,\cdots\}$ and $\{\xi_{kN}, k=0,1,\cdots\}$ of the integral $\int_0^1 Gu(x)$, respectively, where, for two fixed positive integers k and N, ρ_{kN} and ξ_{kN} are the optimal values of the maximization and minimization programs in the Programs (I), respectively. Then the two series satisfy

$$\lim_{k\to\infty} \lim_{N\to\infty} \rho_{kN} = \lim_{k\to\infty} \int_0^1 G\tilde{u}_k(x) = \int_0^1 Gu^*(x), \tag{3.11a}$$

$$\lim_{k\to\infty} \lim_{N\to\infty} \xi_{kN} = \lim_{k\to\infty} \int_0^1 G\tilde{u}_k(x) = \int_0^1 Gu^*(x). \tag{3.11b}$$

Proof. By $\tilde{u}_k(x) \in C^\infty[0,1]$, $\tilde{u}^*(x) \in C^\infty[0,1]$ and (3.4), we have

$$\lim_{k\to\infty} \frac{d^s \tilde{u}_k(x)}{dx^s} = \frac{d^s u^*(x)}{dx^s}. \tag{3.12}$$

Because $G_s(x) \in \mathbb{C}^\infty[0,1]$, there exists a positive real number M_1 satisfying

$$|G_s(x)| \le M_1. \tag{3.13}$$

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Let

$$\eta_k = \int_0^1 Gu^*(x) - \int_0^1 G\tilde{u}_k(x).$$

We get

$$\begin{aligned}\lim_{k\to\infty}|\eta_k| &= \lim_{k\to\infty}\Big|\int_0^1 G(u^*(x)-\tilde{u}_k(x))\Big| \\ &= \lim_{k\to\infty}\Big|\sum_{s\le r_2}\int_0^1 G_s(x)\frac{d^s(u^*(x)-\tilde{u}_k(x))}{dx^s}\Big| \\ &\le \lim_{k\to\infty}\sum_{s\le r_2}\int_0^1 |G_s(x)|\cdot\Big|\frac{d^s(u^*(x)-\tilde{u}_k(x))}{dx^s}\Big| \\ &\le M_1\sum_{s\le r_2}\lim_{k\to\infty}\int_0^1\Big|\frac{d^s(u^*(x)-\tilde{u}_k(x))}{dx^s}\Big| = 0,\end{aligned}$$

by (3.12) and (3.13). Then

$$\lim_{k\to\infty}\eta_k = 0,$$

that is,

$$\lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x) = \int_0^1 Gu^*(x). \tag{3.14}$$

For a fixed positive integer k, which is the index in $\tilde{u}_k(x)$, we apply Algorithm 2.1 to solve the Programs (I), and get the upper and lower bounds series $\{\rho_{kN},\ N=0,1,\cdots\}$ and $\{\xi_{kN},\ N=0,1,\cdots\}$, respectively. By Theorem 3.1, we get

$$\lim_{N\to\infty}\rho_{kN} = \int_0^1 G\tilde{u}_k(x), \quad \lim_{N\to\infty}\xi_{kN} = \int_0^1 G\tilde{u}_k(x).$$

Therefore, by using the conclusion (3.14), we have

$$\lim_{k\to\infty}\lim_{N\to\infty}\rho_{kN} = \lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x) = \int_0^1 Gu^*(x), \tag{3.15a}$$

$$\lim_{k\to\infty}\lim_{N\to\infty}\xi_{kN} = \lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x) = \int_0^1 Gu^*(x). \tag{3.15b}$$

Thus, we complete the proof. □

Theorem 3.3. *If the conditions in Lemma 3.1 hold and the linear differential operator G in* (2.2) *can be written as*

$$G = \sum_{s\le r_2} G_s(x)\frac{d^s}{dx^s}, \tag{3.16}$$

where $r_2 \le r_1$ and $G_s(x) \in \mathbb{C}^\infty[0,1]$, $s=0,1,\cdots,r_2$, which can be expanded as the following Taylor polynomials at $x=0$

$$G_s(x) = \sum_{i=0}^{\infty} b_i^{G_s}x^i = \lim_{l\to\infty}\sum_{i=0}^{l} b_i^{G_s}x^i, \quad x\in[0,1], \quad s=0,1,\cdots,r_2. \tag{3.17}$$

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Then

$$\lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x)=\int_0^1 Gu^*(x). \tag{3.18}$$

Furthermore, applying Algorithm 2.1 to solve the semidefinite Programs (I) with the test functions $\varphi_i=x^i$, $i=0,1,\cdots,N$, *we can get upper and lower bounds series* $\{\delta_{klN},\ k=0,1,\cdots\}$ *and* $\{\omega_{klN},\ k=0,1,\cdots\}$ *of the integral* $\int_0^1 Gu(x)$, *respectively, where, for three fixed positive integers* k, l *and* N *which are the indexes in* $\tilde{u}_k(x)$, (3.17) *and the test function* ϕ_N, *respectively,* δ_{klN} *and* ω_{klN} *are the optimal values of the maximization and minimization programs in the Programs (I), respectively. Then the two series satisfy*

$$\lim_{k\to\infty}\lim_{l\to\infty}\lim_{N\to\infty}\delta_{klN}=\lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x)=\int_0^1 Gu^*(x), \tag{3.19a}$$

$$\lim_{k\to\infty}\lim_{l\to\infty}\lim_{N\to\infty}\omega_{klN}=\lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x)=\int_0^1 Gu^*(x). \tag{3.19b}$$

Proof. By (3.16) and (3.17), we have

$$Gu(x)=\sum_{s\le r_2}\Big(\sum_{i=0}^{\infty}b_i^{G_s}x^i\Big)\frac{d^su(x)}{dx^s}.$$

It is obvious that there exists a positive real number M_2 satisfying

$$|b_i^{G_s}x^i|\le M_2,\quad x\in[0,1],\quad s=0,1,\cdots,r_2.$$

Denote

$$R_l^{G_s}(x)=G_s(x)-\sum_{i=0}^{l}b_i^{G_s}x^i.$$

Then $R_l^{G_s}(x)\in\mathbb{C}^\infty[0,1]$ and by (3.17), it is obvious that

$$\lim_{l\to\infty}R_l^{G_s}(x)=0.$$

Denote

$$G_{(l)}u(x)=\sum_{s\le r_2}\Big(\sum_{i=0}^{l}b_i^{G_s}x^i\Big)\frac{d^su(x)}{dx^s}, \tag{3.20a}$$

$$\lambda_{kl}=\int_0^1 G_{(l)}u^*(x)-\int_0^1 G_{(l)}\tilde{u}_k(x). \tag{3.20b}$$

We have

$$Gu(x)=\lim_{l\to\infty}G_{(l)}u(x).$$

By (3.14), we get

$$\lim_{k\to\infty}|\lambda_{kl}|=0.$$

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Furthermore,

$$\lim_{l\to\infty}\lim_{k\to\infty}|\lambda_{kl}|=0. \tag{3.21}$$

The following equality holds by (3.20b) and (3.21)

$$\lim_{k\to\infty}\lim_{l\to\infty}|\lambda_{kl}|=\lim_{l\to\infty}\lim_{k\to\infty}|\lambda_{kl}|=0. \tag{3.22}$$

Then

$$\begin{aligned}\lim_{k\to\infty}\left|\int_0^1 G(u^*(x)-\tilde{u}_k(x))\right| &= \lim_{k\to\infty}\left|\int_0^1 (\lim_{l\to\infty}G_{(l)})(u^*(x)-\tilde{u}_k(x))\right| \\ &= \lim_{k\to\infty}\lim_{l\to\infty}\left|\int_0^1 G_{(l)}(u^*(x)-\tilde{u}_k(x))\right| \\ &= \lim_{k\to\infty}\lim_{l\to\infty}|\lambda_{kl}|=0.\end{aligned}$$

Therefore,

$$\lim_{k\to\infty}\int_0^1 G\tilde{u}_k(x)=\int_0^1 Gu^*(x).$$

For two fixed positive integers k and l which are the indexes in $\tilde{u}_k(x)$ and $G_{(l)}u(x)$, respectively, we apply Algorithm 2.1 to solve the Programs (I), and get the upper and lower bounds series $\{\delta_{klN},\ N=1,2,\cdots\}$ and $\{\omega_{klN},\ N=1,2,\cdots\}$, respectively. By Theorem 3.1, we get

$$\lim_{N\to\infty}\delta_{klN}=\int_0^1 G_{(l)}\tilde{u}_k(x),\quad \lim_{N\to\infty}\omega_{klN}=\int_0^1 G_{(l)}\tilde{u}_k(x).$$

The equality that

$$\lim_{k\to\infty}\lim_{N\to\infty}\int_0^1 G_{(l)}\tilde{u}_k(x)=\int_0^1 G_{(l)}u^*(x) \tag{3.23}$$

can be deduced easily from the conclusion (3.11a). So, by (3.22) and (3.23), we get

$$\begin{aligned}\lim_{k\to\infty}\lim_{l\to\infty}\lim_{N\to\infty}\delta_{klN}&=\int_0^1 Gu^*(x),\\ \lim_{k\to\infty}\lim_{l\to\infty}\lim_{N\to\infty}\omega_{klN}&=\int_0^1 Gu^*(x).\end{aligned}$$

So, we complete the proof of the theorem. □

4 Numerical experiments

In this section, two numerical examples will be given to illustrate that Algorithm 2.1 is effective.

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Example 4.1. Computing

$$\int_0^1 x^i u(x), \tag{4.1}$$

where $u(x)$ satisfies

$$u'\cos x+u\sin x=1, \quad x\in[0,1], \tag{4.2}$$

with boundary condition $u(0)=1$.

The exact solution of the Eq. (4.2) is

$$u(x)=\sin x+\cos x.$$

Let $d_1=0.9974$, $d_2=-0.1563$, $h_1=1.0005$, $h_2=-0.5040$, $h_3=0.0440$. Chebyshev polynomial with degree 3 of $\sin x$ and Chebyshev polynomial with degree 4 of $\cos x$ are as follows

$$\sin x\approx y_1(x)=d_1x+d_2x^3, \tag{4.3a}$$

$$\cos x\approx y_2(x)=h_1+h_2x^2+h_3x^4, \tag{4.3b}$$

respectively. $|\sin x-y_1(x)|$ and $|\cos x-y_2(x)|$ are all less than 8×10^{-4} for $x\in[0,1]$. We apply the two polynomials to replace $\sin x$ and $\cos x$ in (4.2), respectively. Then we get the following problem:

Approximate Problem: Computing (4.1), where $u(x)$ satisfies

$$(h_1+h_2x^2+h_3x^3)u'+(d_1x+d_2x^3)u=1, \quad x\in[0,1], \tag{4.4}$$

with boundary condition $u(0)=1$.

In this example, $u(x)\geq0$ for all $x\in[0,1]$. We set zero to u_0.

Let

$$m_j=\int_0^1 x^j u(x), \quad j=0,1,2,\cdots.$$

We generate linear equality constraints. By (4.4), we have

$$\int_0^1 x^i((h_1+h_2x^2+h_3x^4)u'+(d_1x+d_2x^3)u)=\int_0^1 x^i. \tag{4.5}$$

Then we get

$$i=0 \quad \Rightarrow(h_1+h_2+h_3)u(1)+(d_1-2d_2)m_1+(d_2-4h_3)m_3=1+h_1, \tag{4.6a}$$

$$i=1 \quad \Rightarrow(h_1+h_2+h_3)u(1)-h_1m_0+(d_1-3h_2)m_2+(d_2-5h_3)m_4=\frac{1}{2},\cdots, \tag{4.6b}$$

$$i=N \quad \Rightarrow(h_1+h_2+h_3)u(1)-Nh_1m_{N-1}+(d_1-(N+2)h_2)m_{N+1}$$
$$+(d_2-(N+4)h_1)m_{N+3}=\frac{1}{N+1},\cdots, \tag{4.6c}$$

by (4.5) and boundary condition $u(0)=1$.

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Table 1: Upper and lower bounds for Example 4.1 for $N=50$.

UN-Ob	LLFoS	ULFoS	ELFoS	*Errors*
m_0	1.301208	1.301208	1.301168	0.000040
m_1	0.682963	0.682963	0.682941	0.000022
m_2	0.462387	0.462387	0.462377	0.000010
m_3	0.348839	0.348839	0.348836	0.000003
m_4	0.279725	0.279725	0.279727	0.000002
m_5	0.233397	0.233397	0.233300	0.000003
m_6	0.200093	0.200093	0.199998	0.000095
m_7	0.175057	0.175057	0.174962	0.000095
m_8	0.155559	0.155559	0.155464	0.000095
m_9	0.139951	0.139951	0.139856	0.000095
m_{10}	0.127178	0.127178	0.127083	0.000095
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
m_{20}	0.066315	0.066315	0.066319	0.000004
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
m_{30}	0.044831	0.044831	0.044834	0.000002
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
m_{40}	0.033855	0.033855	0.033857	0.000002

In these linear constraints, unknown variables are m_i, $i=0,1,\cdots,u(1)$.

For $x\in[0,1]$, the semidefinite constraints are the same as (2.13). So, for solving Example 4.1, we construct the following semidefinite programs

$$\max/\min m_i, \quad \text{s.t. } (4.6a)-(4.6c) \text{ and } (2.13).$$

Let $\epsilon=10^{-8}$ and $N=50$. We applied SeDuMi 1.1R3 to solve the above programs. Numerical results are listed in Table 1. In Table 1, UN-Ob, LLFoS, ULFoS and ELFoS mean unknown variables or objective functions in max/min programs, lower bounds, upper bounds and exact values on linear functionals defined on solution of the differential equation (4.2), respectively. *Errors* mean $|ULFoS-ELFoS|$. These signs in Table 2 have the same meanings. From Table 1, we can see that Algorithm 2.1 is effective since the numerical results of lower and upper bounds are accurate to several decimal points of the exact values. We also solve the max/min programs when $N=49$. Numerical results show that $|m_j^{(50)}-m_j^{(49)}|$, $j=0,1,\cdots,50$, are all less than 10^{-9}. The following example is similar.

Example 4.2. Computing

$$\int_0^1 Gu(x), \tag{4.7}$$

where the operator G is

$$G=x^2\frac{d}{dx}+3, \tag{4.8}$$

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and $u(x)$ satisfies

$$-u''+u'\cos x+(e^{-\sin x}-\sin x)u=1,\quad x\in[0,1], \tag{4.9}$$

with boundary conditions $u'(0)=1$ and $u'(1)=e^{\sin x}\cos 1$.

The exact solution of the Eq. (4.9) is $u(x)=e^{\sin x}$.

Let $q_0=1.0000$, $q_1=-1.9973$, $q_2=0.5000$, $q_3=0.1563$, $q_4=-0.1250$, $q_5=0.0583$. Chebyshev polynomial with degree 5 of $e^{-\sin x}-\sin x$ is as follows

$$e^{-\sin x}-\sin x\approx y_3(x)=q_0+q_1x+q_2x^2+q_3x^3+q_4x^4+q_5x^5. \tag{4.10}$$

$|e^{-\sin x}-\sin x-y_3(x)|$ is less than 3×10^{-3} for $x\in[0,1]$. We apply (4.3b) and (4.10) to replace $\cos x$ and $e^{-\sin x}-\sin x$ in the differential equation (4.9), respectively. Then we get

Approximate Problem: Computing (4.7), where $u(x)$ satisfies

$$-u''+(h_1+h_2x^2+h_3x^3)u'+(q_0+q_1x+q_2x^2+q_3x^3+q_4x^4+q_5x^5)u=1 \tag{4.11}$$

with boundary conditions $u'(0)=1$ and $u'(1)=e^{\sin x}\cos 1$.

In this example, we let $u_0=0$. In fact, $u(x)\geq 1$ for all $x\in[0,1]$.

Let

$$m_j=\int_0^1 x^j u(x),\quad j=0,1,2,\cdots. \tag{4.12}$$

We generate linear equality constraints. By (4.11), we have

$$\int_0^1 x^i(-u''+(h_1+h_2x^2+h_3x^3)u'+(q_0+q_1x+q_2x^2+q_3x^3+q_4x^4+q_5x^5)u)=\int_0^1 x^i. \tag{4.13}$$

Then we have

$$\begin{aligned}
i=0\quad &\Rightarrow q_0m_0+(q_1-2h_2)m_1+q_2m_2+(q_3-4h_3)m_3+q_4m_4+q_5m_5\\
&\quad+(h_1+h_2+h_3)u(1)=e^{\sin 1}\cos 1, &(4.14a)\\
i=1\quad &\Rightarrow -h_1m_0+q_0m_1+(q_1-3h_2)m_2+q_2m_3+(q_3-5h_3)m_4+q_4m_5\\
&\quad+q_5m_6+(h_1+h_2+h_3+1)u(1)-u(0)=e^{\sin 1}\cos 1+\frac{1}{2},\cdots, &(4.14b)\\
i=N\quad &\Rightarrow -N(N-1)m_{N-2}-Nh_1m_{N-1}+q_0m_N+[q_1-(N+2)h_2]m_{N+1}+q_2m_{N+2}\\
&\quad+[q_3-(N+4)h_3]m_{N+3}+q_4m_{N+4}+q_5m_{N+5}+(h_1+h_2+h_3+N)u(1)\\
&\quad=e^{\sin 1}\cos 1+\frac{1}{N+1},\cdots, &(4.14c)
\end{aligned}$$

by (4.13), boundary conditions $u'(0)=1$ and $u'(1)=e^{\sin x}\cos 1$.

In above linear constraints, unknown variables are m_i, $i=0,1,\cdots$, $u(0)$ and $u(1)$.

The semidefinite constraints are the same as (2.13) for $x\in[0,1]$.

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Table 2: Upper and lower bounds for Example 4.1 for $N=50$.

LFoS	LLFoS	ULFoS	ELFoS	Errors
$\int_0^1 Gu(x)$	2.664893	2.664893	2.665011	0.000118
$u(0)$	0.999854	0.999854	1.000000	0.000146
$u(1)$	2.319768	2.319768	2.319777	0.000009
m_0	1.631814	1.631814	1.631864	0.000050
m_1	0.929146	0.929146	0.929152	0.000006
m_2	0.658212	0.658212	0.658210	0.000008
m_3	0.511281	0.511281	0.511277	0.000004
m_4	0.418444	0.418444	0.418439	0.000005
m_5	0.354302	0.354202	0.354297	0.000005
m_6	0.307205	0.307205	0.307271	0.000066
m_7	0.271298	0.271298	0.271294	0.000004
m_8	0.242876	0.242876	0.242872	0.000004
m_9	0.219851	0.219851	0.219848	0.000003
m_{10}	0.200818	0.200818	0.200815	0.000003
⋮	⋮	⋮	⋮	⋮
m_{20}	0.107648	0.107648	0.107646	0.000002
⋮	⋮	⋮	⋮	⋮
m_{30}	0.073533	0.073533	0.073531	0.000002
⋮	⋮	⋮	⋮	⋮
m_{40}	0.055836	0.055836	0.055835	0.000001

By (4.8) and (4.12), the integral $\int_0^1 Gu(x)$ in (4.7) can be written as

$$\int_0^1 Gu(x) = 3m_0 - 2m_1 + u(1).$$

Now, we construct the following semidefinite programs

$$\max / \min 3m_0 - 2m_1 + u(1), \quad \text{s.t. (4.14a)} - \text{(4.14c) and (2.13)},$$

for solving Example 4.2.

Let $\epsilon = 10^{-8}$ and $N=50$. We applied SeDuMi 1.1R3 to solve above programs. Numerical results are reported in Table 2. From Table 2, we can see that Algorithm 2.1 is effective since the numerical results of lower and upper bounds are accurate to several decimal points of the exact values. In addition, we also see that the errors of $\int_0^1 Gu(x)$ and $u(0)$ are more than 10^{-4}. In order to decrease these errors, we can replace $e^{-\sin x} - \sin x$ and $\cos x$ with approximate polynomials with higher degree.

5 Conclusions and discussions

In this paper, we propose semidefinite optimization method to estimate bounds on linear functionals defined on solutions of linear ODEs with smooth coefficients, and prove that

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the approach is convergent. The numerical results show that the proposed method are effective for the problems discussed. In [18], the authors also propose semidefinite optimization method for linear partial differential equations (PDEs) whose coefficients are all polynomials. Because unknown variables grow exponentially with dimension, solving the semidefinite programming constructed on PDEs case is very difficult, and must draw support from the commercial software AMPL (see [18]). Theoretically, our method can be generalized to linear PDEs case, but the same computing issue will be run into.

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