

Bounds on Linear PDEs via Semidefinite Optimization

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Abstract— Using recent progress on moment problems, and their connections with semidefinite optimization, we present in this paper a new methodology based on semidefinite optimization, to obtain a hierarchy of upper and lower bounds on both linear and certain nonlinear functionals defined on solutions of linear partial differential equations. We apply the proposed methods to examples of PDEs in one and two dimensions with very encouraging results. We also provide computational evidence that the semidefinite constraints are critically important in improving the quality of the bounds, that is without them the bounds are weak.

Contributions

Using recent progress on moment problems, and their connections with semidefinite optimization, we present in this paper a new methodology based on semidefinite optimization, to obtain a hierarchy of upper and lower bounds on both linear functionals, as well as the supremum and infimum functionals, for linear PDEs with coefficients that are polynomials of the variables. We apply the proposed methods to examples of PDEs in one and two dimensions with very encouraging results. We also provide computational evidence that the semidefinite constraints are critically important in improving the quality of the bounds, that is without them the bounds are weak. The numerical results further indicate fast convergence. The practicality and numerical stability of the proposed method depends on the numerical stability of semidefinite optimization codes, which are currently under intensive research. We hope that progress in semidefinite optimization codes will lead to improved performance for obtaining bounds on PDEs using the methods of the present paper.

I. INTRODUCTION

In many real-world applications of phenomena that are described by partial differential equations (PDEs) we are primarily interested in a functional of the solution of the PDE, as opposed to the solution itself. For example, we might be primarily interested in the average temperature rather than the entire distribution of temperature in a mechanical device; or we might be interested in the lift and drag of an aircraft wing, which is computed by surface integrals over the wing; or finally we might be interested in the average inventory and its variability in a supply chain network.

Given that analytical solutions of PDEs are very scarce, there is a large body of literature on numerical methods for solving PDEs. Excellent references can be found in Quarteroni and Valli [17], Strang and Fix [21], Brezzi and Fortin [7]. Such methods typically involve some discretization of the domain of the solution, and thus obtain an approximate solution by solving the resulting equations, and matching boundary values and initial conditions. Such approaches scale exponentially with the dimension, i.e., if we use $O(1/\epsilon)$ points in each dimension, the size of systems we need to solve is of the order of $(1/\epsilon)^d$ for d -dimensional PDEs and result in accuracy of $O(\epsilon)$.

Given the interest in a functional of the solution of the underlying PDE, and the computational burden for obtaining a solution within ϵ , it is desirable to obtain bounds on the functional at a decreased computational burden. An approach based on Lagrangean duality that performs computations using a coarse discretization, but provides bounds on the solution for a refined discretization is presented in Paire and Patera [13], Paraschivoiu, Paire and Patera [14] and Paire and Patera [15]. For other duality based methods see Brezzi and Fortin [7].

Moment Problems and Semidefinite Optimization

Problems involving moments of random variables arise naturally in many areas of mathematics, economics, and operations research. Recently, semidefinite optimization methods have been applied to several problems arising in probability theory, finance and stochastic optimization. Bertsimas [3] applies semidefinite optimization methods to find bounds for stochastic optimization problems arising in queueing networks. Bertsimas and Popescu [4] apply semidefinite optimization methods to find best possible bounds on the probability that a multidimensional random variable belongs in a set given a collection of its moments. In [5], Bertsimas and Popescu use these methods to find best possible bounds for pricing financial derivatives without assuming particular price dynamics. For a survey of this line of work, including several historical remarks on the origin of moment problems in the 20th century, see Bertsimas, Popescu and Sethuraman [6].

Semidefinite optimization is currently in the center of much research activity in the area of mathematical programming both from the point of view of new application areas (see for example the survey paper of Vandenberghe and Boyd [23]) as well as algorithmic development.

Structure of the Paper

The paper is structured as follows. We present in Section II the proposed approach. In Section III we present three examples that show how the method works and how it performs numerically. Finally, in Section IV we provide some concluding remarks.

II. THE PROPOSED METHOD

Suppose we are given the partial differential operators L and G operating on some distribution space \mathcal{A} :

$$L, G : \mathcal{A} \longrightarrow \mathcal{A},$$

and we are interested in finding

$$\int Gu(\mathbf{x}),$$

where $u \in \mathcal{A}$ (note also that $f \in \mathcal{A}$) satisfies the PDE,

$$Lu(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} = (x_1, \dots, x_d) \in \Omega \subset \mathcal{R}^d, \quad (1)$$

including the appropriate boundary conditions on $\partial\Omega$,

Eq. (1) is understood in the sense that both sides of the equation act in the same way on a given class of functions \mathcal{D} , i.e.,

$$Lu = f \iff \int (Lu)\phi = \int f\phi, \quad \forall \phi \in \mathcal{D},$$

where \mathcal{D} is taken to be some sufficiently nice class of test functions—typically a subset of the smooth functions \mathcal{C}^∞ .

We will assume that the operators L and G are linear operators with coefficients that are polynomials of the variables. In Section II-E we discuss extensions for a nonlinear operator G . In particular,

$$Lu(\mathbf{x}) = \sum_{\boldsymbol{\alpha}} L_{\boldsymbol{\alpha}}(\mathbf{x}) \frac{\partial^{\boldsymbol{\alpha}} u(\mathbf{x})}{\partial \mathbf{x}^{\boldsymbol{\alpha}}},$$

$$Gu(\mathbf{x}) = \sum_{\boldsymbol{\alpha}} G_{\boldsymbol{\alpha}}(\mathbf{x}) \frac{\partial^{\boldsymbol{\alpha}} u(\mathbf{x})}{\partial \mathbf{x}^{\boldsymbol{\alpha}}},$$

where $\boldsymbol{\alpha} = (i_1, \dots, i_d)$ is a multi-index,

$$\frac{\partial^{\boldsymbol{\alpha}} u(\mathbf{x})}{\partial \mathbf{x}^{\boldsymbol{\alpha}}} = \frac{\partial^{\sum_k i_k} u(\mathbf{x})}{\partial x_1^{i_1} \dots \partial x_d^{i_d}},$$

and $L_{\boldsymbol{\alpha}}(\mathbf{x})$ and $G_{\boldsymbol{\alpha}}(\mathbf{x})$ are multivariate polynomials (we discuss extensions in Section II-F). We will restrict ourselves to the case where \mathcal{D} is separable, that is, it has a countable dense subset. This restriction is not as limiting as it might first appear. In particular, if the solution u has compact support, then we may also assume without loss of generality that every element of \mathcal{D} has compact support as well, and thus by the Stone–Weierstrass theorem, \mathcal{D} is separable. The condition that u have compact support may also be replaced by the (slightly) weaker condition that u have exponentially decaying tails.

Let $\mathcal{F} = \{\phi_1, \phi_2, \dots\}$ generate (in the basis sense) a dense subset of \mathcal{D} . Then, by the linearity of integration we have

$$\begin{aligned} Lu = f &\iff \int (Lu)\phi = \int f\phi, \quad \forall \phi \in \mathcal{D}, \\ &\iff \int (Lu)\phi_i = \int f\phi_i, \quad \forall \phi_i \in \mathcal{F}. \end{aligned}$$

We discuss different choices for the subset \mathcal{F} in Section II-F. One separable subspace around which this paper focuses is the subspace spanned by the monomials $\mathbf{x}^{\boldsymbol{\alpha}} = x_1^{i_1} \dots x_d^{i_d}$. Polynomials have the property that they are closed under action by polynomial coefficient differential operators.

The Adjoint Operator

The adjoint operator, L^* , is defined by the equation:

$$\int (Lu)\phi = \int u(L^*\phi), \quad \forall \phi \in \mathcal{D}.$$

Therefore, if we have both L and L^* , then equality in the original PDE becomes:

$$\begin{aligned} Lu = f &\iff \int (Lu)\phi = \int f\phi, \quad \forall \phi \in \mathcal{D}, \\ &\iff \int (Lu)\phi_i = \int f\phi_i, \quad \forall \phi_i \in \mathcal{F}, \\ &\iff \int u(L^*\phi_i) = \int f\phi_i, \quad \forall \phi_i \in \mathcal{F}. \quad (2) \end{aligned}$$

To illustrate the computation of the adjoint operator, we consider the one dimensional case. The general term of this operator is, up to a constant multiple:

$$x^a \frac{\partial^b}{\partial x^b}.$$

Using the notation $\tilde{\phi} = x^a \phi$, this term's contribution to the adjoint operator is as follows.

$$\begin{aligned} \int_{\Omega} x^a (\partial^b u) \phi &= \int_{\Omega} (\partial^b u) (x^a \phi) dx = \int_{\Omega} (\partial^b u) \tilde{\phi} dx \\ &= u^{(b-1)} \tilde{\phi} \Big|_{\partial\Omega} + \dots + (-1)^{k+1} u^{(b-k)} \tilde{\phi}^{(k-1)} \Big|_{\partial\Omega} + \dots \\ &\quad + (-1)^{b+1} u \tilde{\phi}^{(b-1)} \Big|_{\partial\Omega} + (-1)^b \int_{\Omega} u \partial^b \tilde{\phi} dx. \end{aligned}$$

Thus, while perhaps notationally tedious in higher dimensions, computing the adjoint of a linear partial differential operator with polynomial coefficients is essentially only as difficult as performing the chain rule for differentiation on polynomials, and in particular, it may be easily automated.

A. Linear Constraints

Let us define variables in an optimization sense

$$M_{\boldsymbol{\alpha}} = \int_{\Omega} \mathbf{x}^{\boldsymbol{\alpha}} u(\mathbf{x}) = \int_{\Omega} x_1^{i_1} \dots x_d^{i_d} u(\mathbf{x}),$$

together with variables related to the boundary $\partial\Omega$:

$$z_{\boldsymbol{\alpha}} = \int_{\partial\Omega} \mathbf{x}^{\boldsymbol{\alpha}} u(\mathbf{x}) = \int_{\partial\Omega} x_1^{i_1} \dots x_d^{i_d} u(\mathbf{x}).$$

The specific form of these variables depends on the nature of the boundary conditions we are given (see Section III for specific examples). We refer to the quantities M_{α} and z_{α} as moments, even though $u(\cdot)$ is not a probability distribution. We select as ϕ_i 's the family of monomials \mathbf{x}^{α} . Since, for the case we are considering, L , and thus L^* , are linear operators with coefficients that are polynomials in \mathbf{x} , then Eqs. (2) can be written as linear equations in terms of the variables $\mathbf{M} = (M_{\alpha})$ and $\mathbf{z} = (z_{\alpha})$.

B. Objective Function Value

Given that the operator G is also a linear operator with coefficients that are polynomials of the variables, then the functional $\int Gu$ can also be expressed as a linear function of the variables \mathbf{M} and \mathbf{z} . So if we minimize or maximize this particular linear function, we obtain upper and lower bounds on the value of the functional.

C. Semidefinite Constraints

Let us assume that the solution we are looking for is bounded from below, that is $u(\mathbf{x}) \geq u_0$. The constant u_0 is in fact unknown. In certain cases, u_0 is naturally known; for example if $u(\mathbf{x})$ is a probability distribution, then $u(\mathbf{x}) \geq 0$, i.e., $u_0 = 0$; or if $u(\mathbf{x})$ represents temperature, then again $u(\mathbf{x}) \geq 0$.

We consider the vector $\mathbf{F}(\mathbf{x}) = [\mathbf{x}^{\alpha}]$ and the semidefinite matrix $\mathbf{F}(\mathbf{x})\mathbf{F}(\mathbf{x})'$. Then the matrices

$$\int_{\Omega} (u(\mathbf{x}) - u_0)\mathbf{F}(\mathbf{x})\mathbf{F}(\mathbf{x})', \quad \int_{\partial\Omega} (u(\mathbf{x}) - u_0)\mathbf{F}(\mathbf{x})\mathbf{F}(\mathbf{x})'$$

are also positive semidefinite. This leads to semidefinite constraints involving the variables (\mathbf{M}, u_0) and (\mathbf{z}, u_0) .

Note that this is an extension to multiple dimensions of the classical moment problem (see Akhiezer [2]). The problem is to determine, given some sequence of numbers, whether it is a valid moment sequence, that is to say, whether the numbers given are indeed the moments of a nonnegative function or distribution. In one dimension, if $u(x) \geq 0$, and we define $m_i = \int_{-\infty}^{+\infty} x^i u(x) dx$, then the sequence of moments $\{m_i\}$ is valid if and only if the matrix

$$M_{2n} = \begin{pmatrix} m_0 & m_1 & \cdots & m_n \\ m_1 & m_2 & \cdots & m_{n+1} \\ \vdots & & \ddots & \vdots \\ m_n & & & m_{2n} \end{pmatrix}$$

is positive semidefinite for every n . In the case where $u(x)$ has support $[0, \infty)$, we need to add the additional constraint, that the matrix

$$M_{2n+1} = \begin{pmatrix} m_1 & m_2 & \cdots & m_{n+1} \\ m_2 & m_3 & \cdots & m_{n+2} \\ \vdots & & \ddots & \vdots \\ m_{n+1} & & & m_{2n+1} \end{pmatrix}$$

also be positive semidefinite.

In multiple dimensions, it is generally unknown which are the exact necessary and sufficient conditions for M_{α}

and z_{α} to be a valid moment sequence, when we are working over a general domain. For a wide class of domains, however, Schmüdgen [20] finds such conditions. We review his work briefly, and use it to derive the necessary and sufficient conditions for M_{α} and z_{α} to be a moment sequence.

An Operator Approach

Given a closed subset Ω of \mathcal{R}^d , a sequence of numbers M_{α} defines a valid moment sequence if there exists a measure μ such that

$$M_{\alpha} = \int_{\Omega} \mathbf{x}^{\alpha} d\mu.$$

We define the linear operator

$$Hf = \int_{\Omega} f(\mathbf{x}) d\mu.$$

It is obviously necessary that $Hf \geq 0$, whenever $f \geq 0$ on Ω . A classical theorem says that it is also sufficient:

Theorem 1 (Haviland [11]) If $\Omega \subseteq \mathcal{R}^n$ is closed, then M_{α} defines a valid moment sequence if and only if the linear operator H is nonnegative on all polynomials that are nonnegative on Ω .

Theorem 1 implies that the problem of finding necessary and sufficient conditions for M_{α} and z_{α} to be a moment sequence, reduces to checking the nonnegativity of the image of a polynomial that is nonnegative on Ω . In one dimension, we know that any polynomial that is nonnegative may be written as the sum of squares. Since the square of a polynomial may be written as a quadratic form, the nonnegativity of the operator reduces to matrix semidefiniteness conditions. The Motzkin polynomial in \mathcal{R}^3 ,

$$P(x, y, z) = x^4 y^2 + x^2 y^4 + z^6 - 3x^2 y^2 z^2,$$

is an example that shows that in higher dimensions, the sum of squares decomposition of a nonnegative polynomial is not in general possible (see Reznick [18] for details). However, Schmüdgen [20] gives a representation of all polynomials that are nonnegative over a compact finitely generated semialgebraic set Ω , as defined in the theorem below. This leads to necessary and sufficient conditions for a moment sequence to be valid on Ω .

Theorem 2 (Schmüdgen [20]) Suppose $\Omega := \{\mathbf{x} \in \mathcal{R}^n : f_i(\mathbf{x}) \geq 0, 1 \leq i \leq r\}$ is closed and bounded, where $f_i(\mathbf{x})$ are polynomials. Then a polynomial $g(\mathbf{x}) > 0$ on Ω if and only if it is expressible as a sum of terms of the form

$$h_I^2(\mathbf{x}) \prod_{k \in I} f_k(\mathbf{x}),$$

for $I \subset \{1, \dots, r\}$, and h_I some polynomial.

Theorems 1 and 2 lead to the following result.

Theorem 3: Given $\mathbf{M} = [M_{\alpha}]$, there exists a distribution $u(\mathbf{x})$ such that

$$M_{\alpha} = \int_{\Omega} (u(\mathbf{x}) - u_0) \mathbf{x}^{\alpha},$$

for a closed and bounded domain Ω of the form

$$\Omega = \{\mathbf{x} \in \mathcal{R}^d : f_1(\mathbf{x}) \geq 0, \dots, f_r(\mathbf{x}) \geq 0\},$$

if and only if for all subsets $I \subseteq \{1, \dots, r\}$ the following matrices are positive semidefinite:

$$\int_{\Omega} (u(\mathbf{x}) - u_0) \mathbf{F}(\mathbf{x}) \mathbf{F}(\mathbf{x})' \prod_{i \in I} f_i(\mathbf{x}), \quad (3)$$

where $I \subseteq \{1, \dots, r\}$.

Examples of domains for which the above result applies include the unit ball in \mathcal{R}^d , which can be written as

$$B = \{\mathbf{x} \in \mathcal{R}^d : 1 - x_1^2 - \dots - x_d^2 \geq 0\},$$

and the unit hypercube,

$$C = \{\mathbf{x} \in \mathcal{R}^d : x_i \geq 0, 1 - x_i \geq 0, 1 \leq i \leq d\}.$$

We next make the connection to semidefinite constraints explicit. While all the results can be easily generalized to d -dimensions, for notational simplicity we consider $d = 2$, assume that $u_0 = 0$ and use Ω as the unit hypercube C in two dimensions. Note that in this case there are four functions,

$$f_1(x_1, x_2) = x_1, \quad f_2(x_1, x_2) = 1 - x_1,$$

$$f_3(x_1, x_2) = x_2, \quad f_4(x_1, x_2) = 1 - x_2,$$

defining the set Ω . Thus, there are $2^4 = 16$ possible subsets I of $\{1, 2, 3, 4\}$. Each of these subsets gives rise to a particular semidefinite constraint as follows. Denoting the moment sequence as $\{m_{i,j}\}$, for $I = \emptyset$, we have that

$$\begin{pmatrix} m_{0,0} & m_{1,0} & m_{0,1} & m_{1,1} & \cdots \\ m_{1,0} & m_{2,0} & m_{1,1} & m_{2,1} & \cdots \\ m_{0,1} & m_{1,1} & m_{0,2} & m_{1,2} & \cdots \\ m_{1,1} & m_{2,1} & m_{1,2} & m_{2,2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \succeq \mathbf{0}.$$

For $I = \{2\}$, we obtain

$$\begin{pmatrix} m_{0,0} - m_{1,0} & m_{1,0} - m_{2,0} & m_{0,1} - m_{1,1} & \cdots \\ m_{1,0} - m_{2,0} & m_{2,0} - m_{3,0} & m_{1,1} - m_{2,1} & \cdots \\ m_{0,1} - m_{1,1} & m_{1,1} - m_{2,1} & m_{0,2} - m_{1,2} & \cdots \\ m_{1,1} - m_{2,1} & m_{2,1} - m_{3,1} & m_{1,2} - m_{2,2} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \succeq \mathbf{0}.$$

Proceeding in this way, we obtain 16 semidefinite constraints. Note that these are only necessary constraints, because we only check the semidefiniteness of the truncated matrices. If Ω is the unit ball in d dimensions, we have exactly two semidefinite constraints.

D. The Overall Formulation

As we mentioned, the variables are the moments $M_{\alpha} = \int_{\Omega} \mathbf{x}^{\alpha} u(\mathbf{x})$, the boundary moments $z_{\alpha} = \int_{\partial\Omega} \mathbf{x}^{\alpha} u(\mathbf{x})$ and the bound u_0 , which might be naturally known. The semidefinite optimization consists of linear

equality constraints generated by the adjoint operator for different test functions \mathbf{x}^{α} , and of the semidefinite constraints that express the fact that the variables M_{α} and z_{α} are in fact moments. Subject to these constraints, we maximize and minimize a linear function of the variables that expresses the given linear functional. The overall steps of the formulation process are then summarized as follows:

- (i) Compute the adjoint operator L^* .
- (ii) Generate the n^{th} equality constraint by requiring that

$$\int u(L^* \phi_n) = \int f \phi_n.$$

- (iii) Generate the desired semidefinite constraints; note that these only depend on the domain Ω and not on the operator L .

- (iv) Compute upper and lower bounds on the given functional by solving a semidefinite optimization problem over the intersection of the positive semidefinite cone and the equality constraints.

E. The Maximum and Minimum Operator

Suppose that the given functional is

$$Gu = \min_{\mathbf{x} \in \Omega} u(\mathbf{x}).$$

Then, we will formulate the objective function

$$\min u_0.$$

This approach gives a lower bound on the minimum of $u(\mathbf{x})$ over Ω . However, if we maximize $\max u_0$ we do not obtain a true upper bound on the minimum of $u(\mathbf{x})$ over Ω , only an approximation.

Similarly, if we are interested in

$$\max_{\mathbf{x} \in \Omega} u(\mathbf{x})$$

we solve $\max v_0$ such that $u(\mathbf{x}) \leq v_0$, which leads to semidefinite constraints involving \mathbf{M} , \mathbf{z} and v_0 . This approach gives an upper bound on v_0 , while minimizing v_0 only leads to an approximation.

Note that here the semidefinite constraints are absolutely crucial. This is because the additional variable u_0 is introduced linearly, and because of the linearity of integration, cannot possibly be calculated by the family of linear constraints. Rather, the linear constraints link it to the variables of the optimization, and then it is constrained by the semidefinite constraints.

F. Using Trigonometric Moments

Instead of choosing polynomials as test functions, we could choose other classes of test functions. Polynomials are particularly convenient as they are closed under differentiation. While this property is not a necessary condition for the proposed method to work, it significantly limits the proliferation of variables we introduce. When the linear operator has coefficients that are not polynomials, other bases might be more appropriate.

The trigonometric functions $\{\sin(nx), \cos(nx)\}$ are also closed under differentiation (again we can form products in higher dimensions, just as with monomials). Using trigonometric functions as a basis of our test functions provides a straightforward way for us to deal with linear operators with trigonometric coefficients. This is an important point, as Section III-D reveals, namely, that the choice of test function basis ought to depend on the coefficients of the linear operator. In Section III-D, we present an example of the use of the method with trigonometric test functions.

III. EXAMPLES

In this section, we illustrate our approach with three examples: (a) a simple homogeneous ordinary differential equation, (b) a more interesting ODE: Bessel's equation, and (c) a two-dimensional partial differential equation known as Helmholtz's equation. In all three examples, we take the solution to have support on the unit interval for the ODEs, and on the unit square for the PDE.

A. Example 1: $u'' + 3u' + 2u = 0$

We consider the linear ODE with constant coefficients

$$u'' + 3u' + 2u = 0 \quad (4)$$

with the boundary conditions $u'(0) = -2e^2$ and $u'(1) = -2$, and $\Omega = [0, 1]$. In this case, we can easily find the solution $u(x) = e^2 \cdot e^{-2x}$. Let us apply the proposed method. For simplicity of the exposition we use the fact that $u(x) \geq 0$.

We can compute the adjoint operator directly by integration by parts:

$$\int_0^1 (u'' + 3u' + 2u)\phi = u'\phi \Big|_0^1 - u\phi' \Big|_0^1 + 3u\phi \Big|_0^1 + \int_0^1 (u\phi'' - 3u\phi' + 2u\phi).$$

We use $\phi_i(x) = x^i$, $i = 0, \dots, n$ and let

$$m_i = \int_0^1 x^i u(x) dx.$$

Together with the two unknown boundary conditions $u(0)$ and $u(1)$, we have $n + 1$ variables m_i , $i = 0, \dots, n$ for a total of $n + 3$ variables. The linear equality constraints generated by the adjoint equations are:

$$\begin{aligned} \phi = 1 : & \Rightarrow 3(u(1) - u(0)) + 2m_0 = u'(0) - u'(1), \\ \phi = x : & \Rightarrow 2u(1) + u(0) - 3m_0 + 2m_1 = -u'(1), \\ \phi = x^2 : & \Rightarrow u(1) + 2m_0 - 6m_1 + 2m_2 = -u'(1), \\ & \vdots \\ \phi = x^n : & \Rightarrow (3 - n)u(1) + n(n - 1)m_{n-2} \\ & \quad - 3n \cdot m_{n-1} + 2m_n = -u'(1). \end{aligned}$$

Variable	LB	UB
m_0	3.1939	3.1951
m_1	1.0969	1.1619
m_2	0.5975	0.5997
m_3	0.3957	0.3961
m_4	0.2916	0.3179
m_5	0.2580	0.8809

TABLE I

UPPER AND LOWER BOUNDS FOR THE ODE (4) FOR $N = 14$, USING SDPA. THE TOTAL COMPUTATION TIME WAS LESS THAN 15 SECONDS FOR ALL TWELVE SDPs.

Since we assume that the solution has support on $[0, 1]$, we apply Proposition 3 to derive the two semidefinite constraints:

$$\begin{pmatrix} m_0 & m_1 & \cdots & m_n \\ m_1 & m_2 & \cdots & m_{n+1} \\ \vdots & & \ddots & \vdots \\ m_n & & & m_{2n} \end{pmatrix} \succeq \mathbf{0},$$

$$\begin{pmatrix} m_0 - m_1 & m_1 - m_2 & \cdots & m_n - m_{n+1} \\ m_1 - m_2 & m_2 - m_3 & \cdots & m_{n+1} - m_{n+2} \\ \vdots & & \ddots & \vdots \\ m_n - m_{n+1} & & & m_{2n} - m_{2n+1} \end{pmatrix} \succeq \mathbf{0}.$$

Subject to these constraints, we maximize and minimize each of the m_i , $0 \leq i \leq n$ in order to obtain values for m_i .

We applied two semidefinite optimization packages to solve the resulting SDPs: the optimization package SDPA version 5.00 by Fujisawa, Kojima and Nakata [10] and the Matlab based package SeDuMi version 1.03, by Sturm [22]. The semidefinite optimizations were run on a Sparc 5.

In Table I, we report the results from SDPA using monomials up to $N = 14$. As SDPA exhibited some numerical instability, we replaced the equality constraints $\mathbf{a}'\mathbf{x} = b$ with $-\varepsilon + b \leq \mathbf{a}'\mathbf{x} \leq b + \varepsilon$ with $\varepsilon = 0.001$.

We observe that because of the perturbation we introduced the bounds are only accurate up to the second decimal point. We see, as we would expect, that the performance begins to deteriorate as we ask for higher order moments.

In Table II, we report results using SeDuMi with $N = 60$. SeDuMi successfully solved for the first 45 moments, such that the upper and lower bounds agreed to 5 decimal points.

In order to test the ability of our method to find the minimum of $u(x)$, we reversed the sign of the boundary values for this linear ODE, to obtain an ODE with a solution that is no longer nonnegative:

$$u(x) = -e^2 e^{-2x}.$$

By implementing the method we outlined to compute the minimum of $u(x)$ in the previous section, and using SeDuMi, we obtain the exact value for the minimum of the function $u(x)$ to be $u_0 = -7.389$.

Variable	LB	UB
m_0	3.1945	3.1945
m_1	1.0973	1.0973
m_2	0.5973	0.5973
m_3	0.3959	0.3959
m_4	0.2918	0.2918
m_5	0.2295	0.2295
m_6	0.1884	0.1884
m_7	0.1595	0.1595
m_8	0.1382	0.1382
m_9	0.1218	0.1218
m_{10}	0.1088	0.1088
\vdots	\vdots	\vdots
m_{20}	0.0524	0.0524
\vdots	\vdots	\vdots
m_{30}	0.0344	0.0344
\vdots	\vdots	\vdots
m_{40}	0.0256	0.0256

TABLE II

UPPER AND LOWER BOUNDS FOR THE ODE (4) FOR $N = 60$, USING SeDuMi. THE TOTAL COMPUTATION TIME WAS UNDER FIVE MINUTES.

B. The Bessel Equation

In this section we consider Bessel's differential equation

$$x^2 u'' + x u' + (x^2 - p^2) u = 0.$$

The Bessel function and its variants appear in one form or another in a wide array of engineering applications, and applied mathematics. Furthermore, while there are integral and series representations, the Bessel function is not expressible in closed form. The series representation of the Bessel function, which can be found in, e.g. Watson [24], is:

$$J_p(x) := \sum_{k=0}^{\infty} \frac{(-1)^k (x/2)^{2k+p}}{k!(k+p)!}.$$

Also, over the appropriate range, the Bessel function is neither nonnegative, nor convex.

In order to avoid numerical difficulties from large constant factors, we solve a modified version of Bessel's equation:

$$x^2 u'' + x u' + (49x^2 - p^2) u = 0. \quad (5)$$

The solution is $u(x) = J_p(7x)$. Assuming we are given the value of the derivatives on the boundary, using the monomials as the test functions, we obtain the adjoint equations:

$$\begin{aligned} \phi = 1 : & \Rightarrow -u(1) + (1 - p^2)m_0 + 49m_2 = u'(1), \\ \phi = x : & \Rightarrow -2u(1) + (4 - p^2)m_1 + 49m_3 = u'(1), \\ \phi = x^2 : & \Rightarrow -3u(1) + (9 - p^2)m_2 + 49m_4 = u'(1), \\ & \vdots \\ \phi = x^n : & \Rightarrow -(n+1)u(1) + ((n+1)^2 - p^2)m_n \\ & \quad + 49m_{n+2} = u'(1). \end{aligned}$$

N	Minimum	Maximum
20	-0.3087	0.4986
24	-0.3101	0.5068
30	-0.3111	0.5081
40	-0.3142	0.5046

TABLE III

APPROXIMATIONS FOR THE MAXIMUM AND THE MINIMUM OF THE SOLUTION OF EQ. (5) USING SeDuMi.

Variable	LB	UB
m_1	0.1766	0.1766
m_2	0.0903	0.0903
m_3	0.0583	0.0583
m_4	0.0438	0.0438
m_5	0.0361	0.0361

TABLE IV

UPPER AND LOWER BOUNDS FOR EQ. (5) FOR $N = 24$ USING SeDuMi.

In what follows, we choose $p = 1$. We used SeDuMi to compute the moments, and also to compute the max and min. Recall from the discussion in Section II-E that while we are able to obtain bounds for the moments, our method can only compute *approximations* to the max and min of the solution. In the case of the Bessel function, the approximations we obtain of the minimum are greater than the actual value, and the approximations for the maximum are less than the actual value. The true values are: $\min = -0.347$ and $\max = 0.583$. In Table III we report the results from using SeDuMi.

SeDuMi reported severe numerical instabilities for the computation of the maximum for the cases $N = 30$ and $N = 40$.

Next, we use these results to translate the function so that it is nonnegative, and so that we can compute the moments of the translated function. We use $u(x) - u_0 \geq 0$ with $u_0 = -0.4$. Again using SeDuMi, we obtain very accurate bounds to the moments. We give the first few in Table IV. We would expect by linearity, and indeed the results show, that just having a lower bound on the function is enough to find accurate results on the moments of the function.

C. The Helmholtz Equation

In this section we consider the two dimensional PDE

$$\Delta u + k^2 u = f \quad (6)$$

over $\Omega = [0, 1]^2$. To compute the adjoint operator we need to use Stokes's formula:

$$\int_{\Omega} d\omega = \int_{\partial\Omega} \omega.$$

Recall that in two dimensions we have:

$$\omega = f dx + g dy \iff d\omega = \left(\frac{\partial g}{\partial x} - \frac{\partial f}{\partial y} \right) dx dy,$$

and thus computing the adjoint operator, we have:

$$\begin{aligned} \int_{\Omega} \left(\frac{\partial^2 u}{\partial x^2} \right) \phi \, dx dy &= \int_{\Omega} \left(\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \cdot \phi \right) - \frac{\partial u}{\partial x} \frac{\partial \phi}{\partial x} \right) \, dx dy \\ &= \int_{\partial\Omega} \frac{\partial u}{\partial x} \cdot \phi \, dy - \int_{\Omega} \left(\frac{\partial}{\partial x} \left(u \frac{\partial \phi}{\partial x} \right) - u \frac{\partial^2 \phi}{\partial x^2} \right) \, dx dy \\ &= \int_{\partial\Omega} \left(\frac{\partial u}{\partial x} \cdot \phi - u \frac{\partial \phi}{\partial x} \right) \, dy + \int_{\Omega} u \frac{\partial^2 \phi}{\partial x^2} \, dx dy. \end{aligned}$$

By a similar process for the $\frac{\partial^2 u}{\partial y^2}$ term, we obtain

$$\begin{aligned} \int_{\Omega} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f \right) \phi \, dx dy &= \int_{\Omega} \left(f \phi + \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \, dx dy \\ &+ \int_{\partial\Omega} \left(\frac{\partial u}{\partial x} \cdot \phi - u \frac{\partial \phi}{\partial x} \right) \, dy - \int_{\partial\Omega} \left(\frac{\partial u}{\partial y} \cdot \phi - u \frac{\partial \phi}{\partial y} \right) \, dx. \end{aligned}$$

Again we consider the family of monomials,

$$\mathcal{F} = \{x^i \cdot y^j\}, \quad \text{for } i, j \in \mathcal{N} \cup \{0\}.$$

In addition to the variables

$$m_{i,j} = \int_0^1 \int_0^1 x^i y^j u(x, y) \, dx dy,$$

we also introduce the boundary moment variables:

$$b_i^{x=1} = \int_0^1 u(x=1, y) y^i \, dy, \quad d_i^{x=1} = \int_0^1 \partial_x u(x=1, y) y^i \, dy$$

$$b_i^{x=0} = \int_0^1 u(x=0, y) y^i \, dy, \quad d_i^{x=0} = \int_0^1 \partial_x u(x=0, y) y^i \, dy$$

$$b_i^{y=1} = \int_0^1 u(x, y=1) x^i \, dx, \quad d_i^{y=1} = \int_0^1 \partial_y u(x, y=1) x^i \, dx$$

$$b_i^{y=0} = \int_0^1 u(x, y=0) x^i \, dx, \quad d_i^{y=0} = \int_0^1 \partial_y u(x, y=0) x^i \, dx.$$

Then the adjoint relationship above yields:

$$\phi = 1 : \Rightarrow \quad d_0^{x=1} - d_0^{x=0} + d_0^{y=1} - d_0^{y=0} + m_{0,0} = \int_{\Omega} f \, dx dy$$

$$\phi = x^i : \Rightarrow \quad d_0^{x=1} + i(i-1)m_{i-2,0} + d_i^{y=1} - d_i^{y=0} + m_{i,0} = \int_{\Omega} f \cdot x^i \, dx dy$$

$$\phi = y^j : \Rightarrow \quad d_j^{x=1} - d_j^{x=0} + d_0^{y=1} + j(j-1)m_{0,j-2} + m_{0,j} = \int_{\Omega} f \cdot y^j \, dx dy$$

$$\phi = x^i y^j : \Rightarrow \quad d_j^{x=1} + i(i-1)m_{i-2,j} + d_i^{y=1} + j(j-1)m_{i,j-2} + m_{i,j} = \int_{\Omega} f \cdot x^i y^j \, dx dy.$$

Note that either the $\{d_i^x, d_j^y\}$, or the $\{b_i^x, b_j^y\}$, are given as boundary values. In order to compare with the exact

Variable	Value
$m_{0,0}$	2.9525
$m_{1,0}$	1.7183
$m_{1,1}$	1.0000
$m_{2,0}$	1.2342
$m_{2,1}$	0.7183
$m_{2,2}$	0.5159
$m_{3,0}$	0.9681
$m_{3,1}$	0.5634
$m_{3,2}$	0.4047
$m_{3,3}$	0.3175

TABLE V

EXACT RESULTS FOR THE SOLUTION OF THE PDE (6).

Var	LB	UB	LB	UB	LB	UB
	$N=5$	$N=5$	$N=10$	$N=10$	$N=20$	$N=20$
$m_{0,0}$	0.0000	$+\infty$	0.0000	$+\infty$	0.0000	$+\infty$
$m_{1,0}$	0.0000	4.3142	0.0000	4.0822	0.0000	3.8694
$m_{1,1}$	0.7559	1.0881	0.8557	1.0419	0.9400	1.0120
$m_{2,0}$	0.0000	4.6790	0.0000	4.6790	0.0000	4.6790
$m_{2,1}$	0.0545	1.0563	0.1417	1.0059	0.1749	0.9753
$m_{2,2}$	0.0000	0.9447	0.0000	0.9087	0.0000	0.9087
$m_{3,0}$	0.0000	4.8743	0.0000	4.4932	0.0000	4.4414
$m_{3,1}$	0.1692	0.6806	0.4015	0.6063	0.5025	0.5758
$m_{3,2}$	0.0000	0.6383	0.0000	0.6105	0.0000	0.5989
$m_{3,3}$	0.0000	0.5291	0.1684	0.3640	0.2573	0.3296

TABLE VI

UPPER AND LOWER BOUNDS FROM LINEAR OPTIMIZATION FOR $N=5$, $N=10$, $N=20$. FOR THE CASES $N=5, 10$ WE ONLY RUN UP TO

$$m_{2,2}.$$

solution, we selected the boundary conditions such that $f(x, y) = 3e^{x+y}$.

In order for the $m_{i,j}$ to be a valid moment sequence, we need to impose 16 semidefinite matrix constraints. Similarly, we need to impose two semidefinite constraints for all boundary variables. In order to illustrate the power of the semidefinite constraints, we run our optimization problem in two different stages. First, we provide the results of solving the linear optimization problem generated by the adjoint equation, using the commercial software AMPL. Next, we enforce the semidefinite constraints. The true results, as computed by Maple 6.0, are reported in Table V. Solving a linear optimization problem, ignoring the semidefinite constraints and only imposing nonnegativity constraints on the variables, we obtain the bounds in Table VI for $N=5, 10, 20$.

We then add the semidefinite constraints and use SDPA to solve the corresponding semidefinite optimization problems. SDPA gave very tight bounds; however, there were nevertheless some numerical instabilities, which required us to change the desired accuracy in the search parameters, in order to obtain answers that made sense. In Table VII we report upper and lower bounds for $N=5, 10, N=20$. Note that when we use monomials up to degree N , there are in fact N^2 such monomials.

Var	LB	UB	LB	UB	LB	UB
	$N = 5$	$N = 5$	$N = 10$	$N = 10$	$N = 20$	$N = 20$
$m_{0,0}$	2.7687	5.5689	2.9113	2.9809	2.9377	2.9599
$m_{1,0}$	1.8377	2.2006	1.6955	1.7276	1.7106	1.7199
$m_{1,1}$	0.9679	1.0089	0.9851	1.0026	0.9988	1.0005
$m_{2,0}$	1.0860	1.8173	1.2058	1.2437	1.2261	1.2353
$m_{2,1}$	0.6089	0.7626	0.7019	0.7169	0.7177	0.7185
$m_{2,2}$	0.3192	0.5456	0.5010	0.5107	0.5148	0.5161
$m_{3,0}$	0.5263	1.8191	0.9411	1.0000	0.9601	0.9683
$m_{3,1}$	0.5296	0.6076	0.5485	0.5653	0.5623	0.5639
$m_{3,2}$	0.2021	0.4069	0.4009	0.4068	0.4036	0.4046
$m_{3,3}$	0.1025	0.3495	0.3139	0.3191	0.3163	0.3179

TABLE VII

UPPER AND LOWER BOUNDS FOR EQ. (6) FOR $N = 5, 10$ USING SDPA. THE COMPUTATION OF EACH BOUND TOOK LESS THAN 0.5 SECONDS FOR $N = 5$, 3-5 SECONDS FOR $N = 10$, AND 1-3 MINUTES FOR $N = 20$.

Variable	LB	UB
m_0	0.1128	3.1239
m_1	0.6730	1.0954
m_2	0.0000	0.0294
m_3	0.4471	0.7192
m_4	0.0127	0.0130
m_5	0.3349	0.5390
m_6	0.0072	0.0073
m_7	0.2678	0.4310
m_8	0.0046	0.0047
m_9	0.2231	0.3591
m_{10}	0.0032	0.0032

TABLE VIII

UPPER AND LOWER BOUNDS FOR THE ODE (7) FOR $N = 20$ USING SeDuMi.

We notice that the tightness of the bounds is nearly as dramatic as in the one dimensional case. Moreover, the bounds using semidefinite optimization are significantly tighter than the ones obtained using linear optimization. This observation is significant and emphasizes the importance of the semidefinite constraints. For example, without the semidefinite constraints, the upper bound on $m_{0,0}$ is $+\infty$, whereas we obtain very tight bounds for $N = 10$ using the semidefinite constraints.

D. Trigonometric Test Functions

In this section we illustrate the use of trigonometric test functions. We consider the differential equation

$$u'' + 2u' + \sin(2\pi x)u = 10 \sin x - 20 \cos x + (10 - 10 \sin x) \sin(2\pi x). \quad (7)$$

Note that if we attempted to use a polynomial basis we would encounter a proliferation of variables, since the polynomials are not closed by action of the adjoint (which has a $\sin(2\pi x)$ term). We use the family of functions

$$\phi_{2n}(x) := \sin(2\pi n x), \quad \phi_{2n+1}(x) := \cos(2\pi n x).$$

We define the variables:

$$m_{2n} := \int_{\Omega} u(x) \phi_{2n}(x) dx$$

$$m_{2n+1} := \int_{\Omega} u(x) \phi_{2n+1}(x) dx.$$

The adjoint equations become:

$$\phi_1 = 1 : \Rightarrow 2u(1) - 2u(0) + m_2 = \int_{\Omega} f dx,$$

$$\phi_{2n} = \sin(2\pi n x) : \Rightarrow 2\pi n(u(0) - u(1)) + \frac{1}{2}m_{2(n-1)+1}$$

$$- \frac{1}{2}m_{2(n+1)+1} - 4\pi^2 n^2 m_{2n} - 4\pi n m_{2n+1} = \int_{\Omega} f \phi_{2n} dx$$

$$\phi_{2n+1} = \cos(2\pi n x) : \Rightarrow 2u(1) - 2u(0) + \frac{1}{2}m_{2(n+1)}$$

$$- \frac{1}{2}m_{2(n-1)} - 4\pi^2 n^2 m_{2n+1} - 4\pi n m_{2n} = \int_{\Omega} f \phi_{2n+1} dx.$$

Note that for the semidefinite constraints products $\cos(2\pi n x) \cdot \sin(2\pi m x)$ appear, which can be rewritten as follows:

$$\sin(2\pi n x) \cdot \cos(2\pi m x) = \frac{1}{2}(\sin(2\pi(n+m)x) + \operatorname{sgn}(n-m) \sin(2\pi|n-m|x))$$

$$\sin(2\pi n x) \cdot \sin(2\pi m x) = \frac{1}{2}(\cos(2\pi(n-m)x) - \cos(2\pi(n+m)x))$$

$$\cos(2\pi n x) \cdot \cos(2\pi m x) = \frac{1}{2}(\cos(2\pi(n-m)x) + \cos(2\pi(n+m)x)).$$

Using SeDuMi we report in Table VIII upper and lower bounds for this ODE using trigonometric test functions. We see that the bounds are much tighter for the even moments. While the bounds are not as tight as in the earlier cases, nevertheless they do give an indication that the proposed method may have further applications than polynomial moments.

E. Insights From The Computations

In this section we summarize the major insights from the computations we performed.

(i) In both one and two dimensions, the proposed method gave strong bounds in reasonable times.

(ii) Perhaps the most encouraging finding is that the semidefinite constraints significantly improve over the bounds from the linear constraints.

(iii) The software packages we used exhibited some numerical difficulties.

(iv) Our experiments with trigonometric moments indicate that the proposed method is not restrictive to PDEs with polynomial coefficients, but can accommodate more general coefficients by appropriately changing the underlying basis.

IV. CONCLUDING REMARKS

We have presented a method for providing bounds on functionals defined on solutions of PDEs using semidefinite optimization methods.

The algorithm proposed in this paper uses N elements of our chosen function family (for example polynomials), and uses $O(N^d)$ variables. Compared to traditional discretization methods, the proposed method provides bounds, as opposed to approximate solutions by solving a semidefinite optimization problem on $O(N^d)$ variables. The computational results at least for one or two dimensions indicate that we obtain relatively tight bounds even with small to moderate N , which is encouraging.

Despite a lot of progress in recent years, the current state of the art of semidefinite optimization codes, especially with respect to stability of the numerical calculations is not yet at the level of linear optimization codes. This is one of the major limitations of the proposed method, as it relies on the semidefinite optimization codes. Moreover, we use general purpose semidefinite codes even though we have a very particular formulation with a lot of structure. The hope is that progress in the area of numerical methods for semidefinite optimization codes will improve the ability of the proposed method as well.

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