

Mathematical Programming Gives Hard Bounds of the Dirichlet Problem for Partial Differential Equations

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Abstract: Differential equations, either deterministic or stochastic, play an indispensable role in modeling virtually every dynamics in physical and social sciences and devising efficient computational methods for differential equations is thus of paramount importance out of sheer necessity. The existing methods, such as finite difference, finite element and spectral methods, are designed to provide a good approximation of the solution, while approximation results do not provide any direct information about where and how far the true value is. We propose a novel numerical method based on mathematical programming for the Dirichlet problem for elliptic and parabolic partial differential equations without discretization. Our method is designed to provide hard upper and lower bounds of the solution by mathematical programming. The availability of hard bounds is of paramount significance as those hard bounds form a 100%-confidence interval in the context of probabilistic Monte Carlo methods. An optimization problem is formulated based upon the probabilistic representation of the solution and can be solved by semidefinite programming with the help of sum-of-square relaxation. Various theory-based techniques are developed to cope with difficult situations, such as finding a bounding polynomial function over the entire domain through a single implementation of the optimization problem. Numerical results are presented to support our theoretical developments and to illustrate the effectiveness of our methodology and techniques.

Keywords: *Elliptic partial differential equation, parabolic partial differential equation, polynomial programming, semidefinite programming, stochastic differential equation, sum-of-squares relaxation*

1 INTRODUCTION

Differential equations, either deterministic or stochastic, play an indispensable role in modeling virtually every dynamics in physical and social sciences, from fluid dynamics, celestial motion, financial asset price dynamics, to bridge design, to interactions between neurons, whenever a relation involving some continuously varying quantities and their rates of change in space and/or time is postulated. A complex structure of differential equations, such as time-inhomogeneity, high dimensionality, nonlinearity and randomness, makes almost all realistic problems impossible to solve analytically. Due to the wide range of applications, devising efficient computational methods for differential equations is thus of paramount importance out of sheer necessity.

Various numerical methods for partial differential equations have been studied in the literature, such as finite difference methods, finite element methods, finite volume methods, domain decomposition methods, spectral methods, etc. In all those existing methods, the error analysis is an essential requirement with rigorous mathematical footings. This is so because those methods are designed to provide an approximation of the solution, while approximation results do not provide any direct information about where and how far the true value is. Although the quality of approximations may be improved by increasing the computing effort in a systematic manner, such as a refinement of the grid, the theoretical error analysis is a necessary component with carefully stated assumptions for its validity.

Building on our recent discoveries (Kashima and Kawai (2011a,b, 2013)), in this paper, we present a novel methodology for the Dirichlet problem for elliptic and parabolic partial differential equations. Our method is substantially different from a variety of existing numerical methods on its approach level. Namely, our method does not directly work on given partial differential equations and associated initial-boundary-value conditions. Although given Dirichlet problems are purely *deterministic*, our method makes use of its representation in the form of *probabilistic* expectation. Nevertheless, unlike Monte Carlo methods for estimating a probabilistic expectation, our numerical method is again purely *deterministic*.

There are even further differences from the existing methods on the conceptual level as well as on the implementation level. First, on the conceptual level, our method is designed to make hard upper and lower bounds of the solution available. In the other words, our method yields two values (or functions), that are guaranteed in a rigorous manner to bound the solution from both above and below. In the meantime, the existing methods provide a good approximation of the solution supported by rigorous error analysis, which is essential as an approximation of the solution does not tell where and how far the true solution is. The availability of *hard* bounds is of paramount significance as those hard bounds form a 100%-confidence interval in the context of probabilistic Monte Carlo methods (which can never achieve a 100%-confidence).

The rest of the paper is organized as follows. Section 2 is devoted to problem setting and the probabilistic representation of the solution. Section 3 presents how the probabilistic representation can be translated into the deterministic optimization framework. In Section 4, we extend the theory of Section 2 and 3 to time-dependent parabolic partial differential equations. As the main aim of this paper is to introduce the novel methodology, we omit nonessential details in some instances in order to maintain the flow of the paper. Finally, Section 5 concludes this study and highlights future research directions.

2 PROBABILISTIC REPRESENTATION OF THE DIRICHLET PROBLEM FOR THE ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

Define an open bounded subset D of \mathbb{R}^d , with its boundary ∂D and closure $\bar{D} := D \cup \partial D$. We are interested in the function $u(\mathbf{x})$ at position $\mathbf{x} \in D$ satisfying the elliptic partial differential equation

$$\mathcal{A}u(\mathbf{x}) := \langle a(\mathbf{x}), \nabla u(\mathbf{x}) \rangle + \frac{1}{2} \text{trace} \left[b(\mathbf{x})^\top \text{Hess}(u(\mathbf{x})) b(\mathbf{x}) \right] = -g(\mathbf{x}), \quad \mathbf{x} \in D, \quad (1)$$

with the boundary condition

$$u(\mathbf{x}) = \varphi(\mathbf{x}), \quad \mathbf{x} \in \partial D, \quad (2)$$

that is, the Dirichlet problem for an elliptic partial differential equation. Above and hereafter, we denote by ∇ and $\text{Hess}(\cdot)$ the gradient operator and the Hessian operator, respectively.

The elliptic partial differential equation (1) is called the Poisson equation if no advection $a(\mathbf{x}) \equiv 0$ and unit diagonal diffusion $b(\mathbf{x}) \equiv \mathbb{I}_d$ (the identity matrix in $\mathbb{R}^{d \times d}$), or the Laplace equation if moreover no heat source $g(\mathbf{x}) \equiv 0$. We assume, for the sake of simplicity, that coefficients $a(\mathbf{x}) : D \rightarrow \mathbb{R}^d$ and $b(\mathbf{x}) : D \rightarrow \mathbb{R}^{d \times d}$ are

continuous functions and that at least one diagonal entry of $b(\mathbf{x})$ is strictly positive for every $\mathbf{x} \in \overline{D}$. For each point $\mathbf{x} \in D$, the matrix $b(\mathbf{x})$ may represent thermal conductivity at the position \mathbf{x} , that is, the rate of thermal energy transfer per unit area and per unit temperature gradient. The function $g(\mathbf{x})$ is bounded and may represent the internal heat generation or absorption when it is positive or negative, respectively. Without loss of physical relevance, we can assume that the boundary temperature $\varphi(\mathbf{x})$ is non-negative and bounded over ∂D .

It is well known (Doob (1955); Dynkin (1965)) that the solution $u(\mathbf{x})$ can be expressed in a probabilistic manner under suitable smoothness conditions. Let $\{W_t : t \geq 0\}$ be the standard Brownian motion in \mathbb{R}^d starting from the origin. Define the time-homogeneous diffusion process $\{X_t : t \geq 0\}$ by

$$dX_t = a(X_t)dt + b(X_t)dW_t. \quad (3)$$

We denote by $\mathbb{P}_{s,\mathbf{x}}$ the probability measure under which $X_s = \mathbf{x}$ almost surely. Existence and uniqueness of the weak solution of $\{X_t : t \geq 0\}$ are readily guaranteed by the condition imposed on the coefficients $a(\mathbf{x})$ and $b(\mathbf{x})$. We denote by $\mathbb{E}_{s,\mathbf{x}}[\cdot]$ the expectation associated with the probability measure $\mathbb{P}_{s,\mathbf{x}}$. Define the $\mathbb{P}_{s,\mathbf{x}}$ -stopping time

$$\tau_D := \inf \{t > s : X_t \in D^c, X_s = \mathbf{x} \in \overline{D}\}, \quad (4)$$

the time of first exit from the domain D with initial state $X_s = \mathbf{x}$. Under the probability measure $\mathbb{P}_{s,\mathbf{x}}$, it holds true that $\tau_D \geq s$ almost surely. Since the domain D is bounded and the diffusion coefficient $b(\mathbf{x})$ has at least one strictly positive diagonal element over the domain, the expectation of the first exit time from the domain is finite, that is, $\mathbb{E}_{0,\mathbf{x}}[\tau_D] < +\infty$. Then, if the domain D is sufficiently nice, it is well known that the solution to the elliptic partial differential equation (1) with the boundary condition (2) is given by

$$u(\mathbf{x}) = \mathbb{E}_{0,\mathbf{x}} \left[\varphi(X_{\tau_D}) + \int_0^{\tau_D} g(X_t)dt \right], \quad \mathbf{x} \in \overline{D}. \quad (5)$$

In deriving this probabilistic representation (5), the problem description (1) and (2) comes into play in a very interesting manner. Under $\mathbb{P}_{0,\mathbf{x}}$, the Ito formula yields

$$u(X_{\tau_D \wedge s}) = u(\mathbf{x}) + \int_0^{\tau_D \wedge s} \mathcal{A}u(X_t)dt + \int_0^{\tau_D \wedge s} \langle \nabla u(X_t), b(X_t)dW_t \rangle, \quad s > 0,$$

provided that the solution $u(\mathbf{x})$ is twice differentiable. With the help of the optional stopping theorem, we get

$$u(\mathbf{x}) = \mathbb{E}_{0,\mathbf{x}} \left[u(X_{\tau_D}) - \int_0^{\tau_D} \mathcal{A}u(X_t)dt \right] = \mathbb{E}_{0,\mathbf{x}} \left[\varphi(X_{\tau_D}) + \int_0^{\tau_D} g(X_t)dt \right],$$

where the conditions (1) and (2) replace the unknown solution $u(\mathbf{x})$ inside the expectation with the given input data $\varphi(\mathbf{x})$ and $g(\mathbf{x})$.

3 FROM PROBABILISTIC REPRESENTATION TO DETERMINISTIC OPTIMIZATION FRAMEWORK

We begin this section with the main theoretical base.

Theorem 1. *Suppose there exist functions f_U and f_L in $C^2(D; \mathbb{R}) \cap C(\overline{D}; \mathbb{R})$ such that*

$$f_U(\mathbf{x}) \geq \varphi(\mathbf{x}), \quad \mathbf{x} \in \partial D, \quad (6)$$

$$\mathcal{A}f_U(\mathbf{x}) + g(\mathbf{x}) \leq 0, \quad \mathbf{x} \in D. \quad (7)$$

$$f_L(\mathbf{x}) \leq \varphi(\mathbf{x}), \quad \mathbf{x} \in \partial D, \quad (8)$$

$$\mathcal{A}f_L(\mathbf{x}) + g(\mathbf{x}) \geq 0, \quad \mathbf{x} \in D. \quad (9)$$

Then, it holds that for $\mathbf{x} \in \overline{D}$,

$$f_L(\mathbf{x}) \leq u(\mathbf{x}) \leq f_U(\mathbf{x}).$$

Based upon Theorem 1, we wish to minimize the upper bound and maximize the lower bound of $u(\mathbf{x}_0)$ at a certain point $\mathbf{x}_0 \in D$ under the given constraints in the following way;

$$\left| \begin{array}{l} \min \quad f_U(\mathbf{x}_0) \\ \text{s.t.} \quad f_U(\mathbf{x}) \geq \varphi(\mathbf{x}), \quad \mathbf{x} \in \partial D, \\ \quad \quad \mathcal{A} f_U(\mathbf{x}) + g(\mathbf{x}) \leq 0, \quad \mathbf{x} \in D, \\ \quad \quad f_U \in C^2(D; \mathbb{R}) \cap C(\bar{D}; \mathbb{R}), \end{array} \right| \text{ and } \left| \begin{array}{l} \max \quad f_L(\mathbf{x}_0) \\ \text{s.t.} \quad f_L(\mathbf{x}) \leq \varphi(\mathbf{x}), \quad \mathbf{x} \in \partial D, \\ \quad \quad \mathcal{A} f_L(\mathbf{x}) + g(\mathbf{x}) \geq 0, \quad \mathbf{x} \in D, \\ \quad \quad f_L \in C^2(D; \mathbb{R}) \cap C(\bar{D}; \mathbb{R}). \end{array} \right| \quad (10)$$

Those optimization problems over the class $C^2(D; \mathbb{R}) \cap C(\bar{D}; \mathbb{R})$ are way beyond the current numerical techniques, as the class is too broad. Nevertheless, the problems are within our reach when we restrict our attention to the smaller class of polynomial functions of fixed polynomial degree. Let us remark, despite its obviousness, that the restriction to polynomial functions makes the feasible region smaller in general. The resultant optimization problem is thus not as sharp as the original one.

To describe this more precisely, we take an illustrative example. Consider the system (1) and (2) in \mathbb{R}^2 with no advection $a(\mathbf{x}) \equiv 0$, a diagonal unit diffusion $b(\mathbf{x}) \equiv \mathbb{I}_2$ (the identity matrix in $\mathbb{R}^{2 \times 2}$), constant source $g(\mathbf{x}) \equiv 1/2$, zero boundary condition $\varphi(\mathbf{x}) \equiv 0$, and square domain

$$D = (-1, +1) \times (-1, +1).$$

Note that under $\mathbb{P}_{0,\mathbf{x}}$, $\{X_t : t \geq 0\}$ is the standard Brownian motion in \mathbb{R}^2 starting from \mathbf{x} . This is a simple diffusion model for the temperature in a square plate with uniform external heating and the edge of the plate being kept at an ice-cold temperature. With the notation $\mathbf{x} := [x, y]^\top$, the solution is available in closed form as

$$u(x, y) = \frac{1-x^2}{2} - \frac{16}{\pi^3} \sum_{\substack{k=1 \\ k \text{ odd}}}^{+\infty} \left[\frac{\sin(k\pi(1+x)/2)}{k^3 \sinh(k\pi)} \left(\sinh\left(k\pi \frac{1+y}{2}\right) + \sinh\left(k\pi \frac{1-y}{2}\right) \right) \right], \quad (11)$$

through the separation of variables. This solution is indeed smooth enough to be a classical solution. (Hereafter, we expand the arguments of the state \mathbf{x} to (x, y) for better display.)

Next, we restrict the bounding function f_U to the class of polynomial functions of the form

$$f_U(x, y) = \sum_{\substack{k_x + k_y \leq N \\ k_x \geq 0, k_y \geq 0}} c_{k_x, k_y} x^{k_x} y^{k_y}, \quad (x, y) \in \mathbb{R}^2, \quad (12)$$

of a *fixed* polynomial degree N . After a suitable sum-of-squares relaxation, the optimization problem, both minimization and maximization components, can be rewritten in full as semidefinite programming under a set of linear equalities and semidefinite constraints. Such problem conversion can be automatically executed by YALMIP (Löfberg (2004, 2009)) and the resulting optimization problems can be solved with the well-established semidefinite programming solver SDPT3 (Toh et al. (1999)). (See Kashima and Kawai (2011a,b, 2013) for more details.)

With fixed polynomial degree $N = 6$ in (12), we solve the optimization problems to tighten the bounds $f_L(0, 0) \leq u(0, 0) \leq f_U(0, 0)$, that is, $(x_0, y_0) = (0, 0)$ in the objective function of (10). According to the analytic solution (11), we know $u(0, 0) = 0.294685413126$, while our optimization approach yields the following bounds

$$0.292893217993127 = f_L^*(0, 0) \leq u(0, 0) \leq f_U^*(0, 0) = 0.300000000917426. \quad (13)$$

To compare with $u(0.5, 0.5) = 0.181144632438$ due to (11), we reset $(x_0, y_0) = (0.5, 0.5)$ in the objective function of (10) and get the following bounds

$$0.179384286494441 = f_L^*(0.5, 0.5) \leq u(0.5, 0.5) \leq f_U^*(0.5, 0.5) = 0.186125348287387. \quad (14)$$

(Note that the polynomial functions f_U^* and f_L^* in (14) are not identical to those in (13).)

The objective in the optimization problems (10) for the bounds (13) are $\min f_U(0, 0)$ and $\max f_L(0, 0)$, while those for the bounds (14) are $\min f_U(0.5, 0.5)$ and $\max f_L(0.5, 0.5)$. Solving the optimization problems, such as (10), however, yields the *functions* $f_U(x, y)$ and $f_L(x, y)$, not only the *values* $f_U(x_0, y_0)$ and $f_L(x_0, y_0)$ at a prescribed single point (x_0, y_0) . In fact, those optimized polynomial functions $f_U^*(x, y)$ and $f_L^*(x, y)$ are of direct practical value as well. Although this is a straightforward consequence of Theorem 1, we state it for the sake of completeness, in a general framework.

Corollary 1. Let $f_U^*(\mathbf{x})$ and $f_L^*(\mathbf{x})$ be the optimal solutions of the optimization problems (10). Then, it holds that for every $\mathbf{x} \in \bar{D}$,

$$f_L^*(\mathbf{x}) \leq u(\mathbf{x}) \leq f_U^*(\mathbf{x}).$$

Corollary 1 indicates that not only for \mathbf{x}_0 but also for *every* point $\mathbf{x} \in D$, the values $f_U^*(\mathbf{x})$ and $f_L^*(\mathbf{x})$ act as upper and lower bounds of $u(\mathbf{x})$. To illustrate the effectiveness of Corollary 1, we draw in Figure 1 three-dimensional surface plots and contour plots of the minimized upper bounding function $f_U^*(x, y)$ and the maximized lower bounding function $f_L^*(x, y)$ for the optimization problems with objective $\min f_U(0, 0)$ and $\max f_L(0, 0)$.

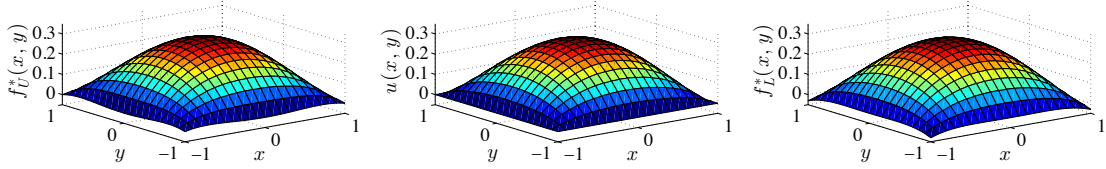


Figure 1. Three-dimensional surface of the minimized upper bounding polynomial function $f_U^*(x, y)$ (left), the analytic solution $u(x, y)$ (middle) and the maximized lower bounding polynomial function $f_L^*(x, y)$ (right) when the objectives are $\min f_U(0, 0)$ and $\max f_L(0, 0)$.

The polynomial degree N (of polynomials f_U and f_L) is indeed arbitrary. With a larger polynomial degree N , the optimized bounds $f_L^*(\mathbf{x}) \leq u(\mathbf{x}) \leq f_U^*(\mathbf{x})$ are expected to be tighter (or at worst, remain the same) as the optimization problem admits a strictly larger feasible region. Moreover, if the problem settings are "smooth", then the optimized bounds converge to the solution $u(\mathbf{x})$. Despite its theoretical interest, however, the convergence results may sometimes not be quite of practical value as the size of semidefinite programming grows so quickly in the polynomial degrees N that even recent high-spec computers may often get stuck.

4 PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

In this section, we extend the framework of Section 2 and 3 to the Dirichlet problem for parabolic partial differential equations. We continue to use the same notations together with basic assumptions imposed in Section 3, such as a bounded spatial domain $D \subset \mathbb{R}^d$, the coefficients $a(\mathbf{x})$ and $b(\mathbf{x})$, the boundary condition $\varphi(t, \mathbf{x})$, the expectation $\mathbb{E}_{t, \mathbf{x}}[\cdot]$ under the probability measure $\mathbb{P}_{t, \mathbf{x}}(\cdot)$ associated to the initial condition $X_t = \mathbf{x}$ of the diffusion process $\{X_t : t \geq 0\}$ defined by (3) and its first exit time τ_D from the bounded domain D defined by (4). The gradient ∇ and the Hessian $\text{Hess}(\cdot)$ are still both taken only with spatial variables.

Consider the function $u : (0, +\infty) \times \bar{D} \rightarrow \mathbb{R}$ solving the the parabolic partial differential equation

$$\frac{\partial}{\partial t} u(t, \mathbf{x}) = \mathcal{A}u(t, \mathbf{x}) + g(t, \mathbf{x}), \quad (t, \mathbf{x}) \in (0, +\infty) \times D,$$

where the operator \mathcal{A} is defined in (1), along with the initial condition

$$u(0, \mathbf{x}) = h(\mathbf{x}), \quad \mathbf{x} \in D,$$

and the boundary condition

$$u(t, \mathbf{x}) = \varphi(t, \mathbf{x}), \quad (t, \mathbf{x}) \in (0, +\infty) \times \partial D.$$

Without loss of physical generality, we assume the initial condition $h(\mathbf{x})$ is bounded over D . Unlike elliptic problems, the domain here contains one additional dimension in time, which is half-unbounded. Hence, it is essential to specify an appropriate initial condition. The problem is evolutionary and computation continues in time for as long as there is interest in the solution. In a similar manner to elliptic problems, the solution $u(t, \mathbf{x})$ has the probabilistic representation (Doob (1955); Dynkin (1965))

$$u(t, \mathbf{x}) = \mathbb{E}_{0, \mathbf{x}} \left[h(X_t) \mathbb{1}(\tau_D > t) + \varphi(t - \tau_D, X_{\tau_D}) \mathbb{1}(\tau_D \leq t) + \int_0^{\tau_D \wedge t} g(t - s, X_s) ds \right], \quad (t, \mathbf{x}) \in (0, +\infty) \times \bar{D},$$

(15)

which is well defined due to boundedness of the functions h , φ and g .

Theorem 2. Fix $T > 0$. Suppose that there exist functions f_U in $C^{1,2}((0, T) \times D; \mathbb{R}) \cap C([0, T] \times \bar{D}; \mathbb{R})$ such that

$$\begin{aligned} f_U(T, \mathbf{x}) &\geq h(\mathbf{x}), \quad \mathbf{x} \in D, \\ f_U(t, \mathbf{x}) &\geq \varphi(T - t, \mathbf{x}), \quad (t, \mathbf{x}) \in [0, T) \times \partial D, \\ \frac{\partial}{\partial t} f_U(t, \mathbf{x}) + \mathcal{A} f_U(t, \mathbf{x}) + g(T - t, \mathbf{x}) &\leq 0, \quad (t, \mathbf{x}) \in (0, T) \times D, \end{aligned}$$

and f_L in $C^{1,2}((0, T) \times D; \mathbb{R}) \cap C([0, T] \times \bar{D}; \mathbb{R})$ such that

$$\begin{aligned} f_L(T, \mathbf{x}) &\leq h(\mathbf{x}), \quad \mathbf{x} \in D, \\ f_L(t, \mathbf{x}) &\leq \varphi(T - t, \mathbf{x}), \quad (t, \mathbf{x}) \in [0, T) \times \partial D, \\ \frac{\partial}{\partial t} f_L(t, \mathbf{x}) + \mathcal{A} f_L(t, \mathbf{x}) + g(T - t, \mathbf{x}) &\geq 0, \quad (t, \mathbf{x}) \in (0, T) \times D. \end{aligned}$$

Then, it holds that for every $\mathbf{x} \in \bar{D}$,

$$f_L(0, \mathbf{x}) \leq u(T, \mathbf{x}) \leq f_U(0, \mathbf{x}).$$

If moreover $g(t, \mathbf{x})$ and $\varphi(t, \mathbf{x})$ are independent of t , it holds that for every $(t, \mathbf{x}) \in [0, T] \times \bar{D}$,

$$f_L(t, \mathbf{x}) \leq u(T - t, \mathbf{x}) \leq f_U(t, \mathbf{x}).$$

To demonstrate the effectiveness of Theorem 2, we focus on a one-dimensional simple setting with domain $D = (x_L, x_U)$, no advection $a(x) \equiv 0$, a homogeneous diffusion $b(x) \equiv \sigma > 0$, and the triangular initial condition

$$h(x) = \begin{cases} x - x_L, & \text{if } x \in (x_L, (x_U + x_L)/2], \\ x_U - x, & \text{if } x \in ((x_U + x_L)/2, x_U), \end{cases}$$

which is continuous itself and is connected, without discontinuities, to the homogeneous boundary condition $\varphi(x_L) = \varphi(x_U) = 0$. In this case, the underlying diffusion process in the probabilistic representation (15) is simply a Brownian motion starting from $x \in D$, that is, $X_t = x + \sigma W_t$, where $\{W_t : t \geq 0\}$ is the standard Brownian motion in \mathbb{R} . In this simple problem setting, the solution is available in closed form

$$u(t, x) = \frac{4(x_U - x_L)}{\pi^2} \sum_{\substack{k=1 \\ k \text{ odd}}}^{+\infty} \frac{1}{k^2} \sin\left(k\pi \frac{x - x_L}{x_U - x_L}\right) e^{-\left(\frac{k\sigma\pi}{x_U - x_L}\right)^2 \frac{t}{2}}, \quad (t, x) \in [0, +\infty) \times \bar{D}. \quad (16)$$

With the unit spatial domain $(x_L, x_U) = (0, 1)$, the unit diffusion coefficient $\sigma = 1$ and the polynomial degree 14, the semidefinite programming formulation yields the results presented in Figure 2. After a certain time (or before around $t = 0.7$, as the time runs backwards), the upper and lower bounds $f_U^*(t, x)$ and $f_L^*(t, x)$ give an impressively good picture about the solution $u(T - t, x)$ over the spatial domain.

5 CONCLUDING REMARKS

We have described a deterministic optimization approach to finding hard upper and lower bounds of the solution of the Dirichlet problem for elliptic and parabolic partial differential equations through the probabilistic representation of the solution. Our methodology uses the class of polynomial functions in order to formulate the optimization problem in the semidefinite programming framework. Although implementation of our method requires a small amount of initial work, the method is still easy to adopt. We have demonstrated that a single implementation of the optimization problem yields a upper (or lower) bounding polynomial function over the entire domain, both in time and space. In the case of smooth conditions, one upper and the other lower bounding polynomial functions tend to be so close to each other that the true solution can often be identified well over the entire domain.

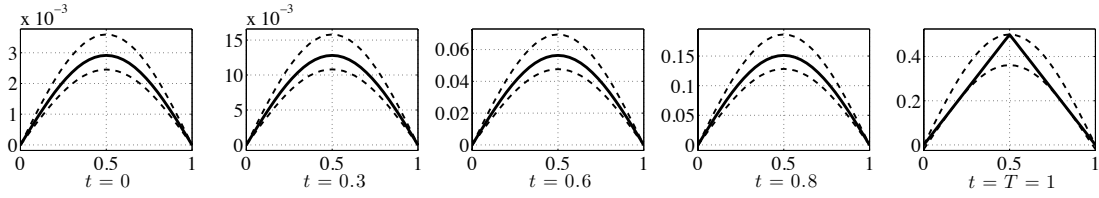


Figure 2. The optimal upper and lower bounding polynomial functions $f_U^*(t, x)$ and $f_L^*(t, x)$, along with the solution $u(T - t, x)$ (bold), for the time-dependent Dirichlet problem with the solution (16) at $t = \{0, 0.3, 0.6, 0.8, 1\}$.

There are various future research directions to address along this line. For example, employing piecewise polynomial functions on the partitioned domain adds some flexibility to the formulation and is expected to provide significant improvement in the quality of bounds when partitioning is wisely chosen. The proposed method may be applied to more intricate problems, such as the Neumann problem, Stokes equations, etc. Moreover, Theorem 1 and 2 can be interpreted in an opposite direction, that is, to amend a smooth function to a hard bound in such a way that the function does not violate the constraints. Those topics will be investigated in subsequent papers Kawai (2013a,b,c,d).

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