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Properties of a method of fundamental solutions for the parabolic heat equation

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Abstract

We show that a set of fundamental solutions to the parabolic heat equation, with each element in the set corresponding to a point source located on a given surface with the number of source points being dense on this surface, constitute a linearly independent and dense set with respect to the standard inner product of square integrable functions, both on lateral- and time-boundaries. This result leads naturally to a method of numerically approximating solutions to the parabolic heat equation denoted a method of fundamental solutions (MFS). A discussion around convergence of such an approximation is included.

Keywords: fundamental solution, parabolic heat equation
2010 MSC: 65M32, 65M20

1. Introduction

Meshless methods, in particular the method of fundamental solutions, have gained popularity in recent years both for direct and inverse problems, see the surveys [1] and [2]. It is in particular for stationary problems that research activity on meshless methods have been prolific. For time-dependent problems, typically some transformation in time are used to reduce to the stationary case [3, Section 5]. However, reverting such a transformation can cause numerical problems, see [4, p. 25]. In [5], a method of fundamental solutions for the parabolic heat equation was proposed, and in this method there was no transformation in time. Instead, following the stationary case, linear combinations of the fundamental solution of the heat equation were used. This method has then been applied for various other direct and inverse heat problems, see, for example, [6, 7].

A key fact to motivate the MFS in [5] is the linear independence and denseness of linear combinations of fundamental solutions of the heat equation. Proofs thereof in various settings are scattered in those above mentioned works. Therefore, in the present work, we collect the results and shall prove properties of linear independence and denseness for linear combinations of the fundamental solution and derivatives. Moreover, convergence of an MFS approximation will be outlined. This constitute the novelty of the present work together with pinpointing relevant references for the various results needed in the presented proofs.

In the present section, we formulate the main result. In Section 2, we collect some results needed in the proof. The proof itself is given in Section 3. In Section 4, we outline a proof of convergence of the MFS approximation. In the final section, Section 5, some remarks are pointed out.

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We consider the parabolic heat equation

$$\begin{cases} \partial_t u - \Delta u = 0 & \text{in } \Omega \times (0,T), \\ \mathcal{B}u = \psi & \text{on } \Gamma \times (0,T), \\ u(x,0) = \varphi(x) & \text{for } x \in \Omega. \end{cases} \tag{1}$$

Here, Ω is a bounded domain in $\mathbb{R}^n$, $n = 2, 3$, with boundary surface Γ being simple (no self-intersections) closed (the surface has no boundary and is connected) and is at least Lipschitz smooth. The domain Ω_S (S for source) with boundary surface Γ_S, and such that $\overline{\Omega} \subset \Omega_S$, has the similar properties. When $n = 2$, we have two simple closed curves with one contained within the other. Doubly-connected domains and also one-dimensional spatial domains can be adjusted for.

The operator $\mathcal{B}u$ denotes either the Dirichlet condition (when $\mathcal{B} = \mathcal{I}$) or the Neumann condition $\mathcal{B}u = \partial u/\partial \nu$, with ν being the outward unit normal to the boundary.

We shall then formulate the main result to be proved. Let

$$F(x,t;y,\tau) = \frac{H(t-\tau)e^{-\frac{|x-y|^2}{4(t-\tau)}}}{(4\pi(t-\tau))^{\frac{n}{2}}} \tag{2}$$

be the standard fundamental solution to the heat equation (1) representing the temperature at location x and time t resulting from an instantaneous release of a unit point source of thermal energy at location y and time τ, with H the Heaviside function. The fundamental solution has the expected physical properties, for example, it is a positive solution to the heat equation for $t > \tau$, for $x \neq y$ there holds $\lim_{t \to \tau^+} F(x,t;y,\tau) = 0$, the function $F(x,t;x,\tau)$ tends to infinity as $t \to \tau^+$, and $\int_{\mathbb{R}^n} F(x,t;y,\tau)\,dy = 1$ when $t > \tau$; for further properties, see [8] and [9, Chapter 1.4-6].

Let $\{y_k, \tau_\ell\}_{k,\ell=1,2,\ldots}$ be a dense set of points on the outer lateral (cylindrical) surface $\Gamma_S \times (0,T)$; notation means that $\{y_k\}_{k=1,2,\ldots}$ is dense on Γ_S and $\{\tau_\ell\}_{\ell=1,2,\ldots}$ is dense in $(0,T)$. By a dense set in L^2, we mean that the span of the set is dense. We can then state the main result:

Theorem 1.1. *The set of functions $\{F(x,t;y_k,\tau_\ell)\}_{k,\ell=1,2,\ldots}$ is linearly independent and dense in $L^2(\Gamma \times (0,T))$. The same hold for the set consisting of the normal derivatives, $\{\partial_{\nu(x)} F(x,t;y_k,\tau_\ell)\}_{k,\ell=1,2,\ldots}$. Moreover, restriction in time generates a set $\{F(x,t_0;y_k,\tau_\ell)\}_{k,\ell=1,2,\ldots}$, which is linearly independent and dense in $L^2(\Omega)$ for any $0 < t_0 \leq T$.*

In the next section, we formulate some results needed in the proof. Note that it is for ease of presentation that we chose points on $\Gamma_S \times (0,T)$ as above, that is a dense set in space and a dense set in time. A more general dense set with the points on Γ_S changing with time is also possible.

2. Some results on the parabolic heat equation

The space $L^2(0,T;X)$, where X is a Hilbert space, consists of those measurable functions $u(\cdot,t) : (0,T) \to X$, with $\int_0^T \|u(\cdot,t)\|_X^2\,dt < \infty$. The space $H^k(\Omega)$, $k > 0$, is the standard Sobolev space of functions having weak and square integrable derivatives up to order k, with trace space $H^{k-1/2}(\Gamma)$.

We first recall a well-posedness result for (1):

Proposition 2.1. *Let $\varphi \in L^2(\Omega)$ and let the element ψ be sufficiently regular. Then there exists a unique weak solution $u \in L^2(0,T;H^1(\Omega))$ to (1) with $u_t \in L^2(0,T;L^2(\Omega))$, and this solution depends continuously on the data.*

This is a standard result and a proof can, for example, be found in [10, Chapter 4, Section 15], where also precise spaces for ψ are presented.

Let u be the weak solution to (1), and let v be a (weak) solution of the adjoint equation, that is $\partial_t v + \Delta v = 0$ in $\Omega \times (0,T)$. Then the following Green's formula holds,

$$\int_\Omega u(x,T)v(x,T)\,dx - \int_\Omega u(x,0)v(x,0)\,dx = \int_0^T\int_\Gamma v(x,t)\frac{\partial u(x,t)}{\partial \nu}\,dx\,dt - \int_0^T\int_\Gamma u(x,t)\frac{\partial v(x,t)}{\partial \nu}\,dx\,dt, \tag{3}$$

and this follows from [11, Proposition 2.24].

The fundamental solution $F(x,t;y,\tau)$ is defined in all of $\mathbb{R}^n$ for $t > \tau$ and satisfies the heat equation, we shall therefore also need a well-posedness result for the heat equation in $\mathbb{R}^n$:

Proposition 2.2. *Consider the Cauchy problem*

$$\begin{cases} \partial_t u - \Delta u = 0 & \text{in } \mathbb{R}^n \times (0,T), \\ u(x,0) = \xi(x) & \text{for } x \in \mathbb{R}^n. \end{cases} \tag{4}$$

Provided the data ξ does not grow faster than $e^{c|x|^2}$, for some positive constant c, there is a unique solution to (4) *among solutions satisfying the similar exponential growth bound.*

A proof of this standard result is given in, for example, [9, Chapter 1.7–9]; without a growth condition uniqueness can be violated, see [9, pp. 30–31] with further details in [12, pp. 211–213].

Finally, we need a result on the lateral (and in general ill-posed) Cauchy problem.

Proposition 2.3. *Let u be a sufficiently smooth solution of the heat equation in $\Omega \times (0,T)$, which is such that both u and its normal derivative vanish on a portion Γ_c of the boundary of Ω for an interval in time, that is*

$$u = \frac{\partial u}{\partial \nu} = 0 \quad \text{on} \quad \Gamma_c \times (0,T).$$

Then u is identically zero in $\overline{\Omega} \times [0,T]$.

A proof of this is given in [13, Section 3]. A general account on uniqueness from such Cauchy data with precise function spaces and estimates is given in [14, Chapter 3.3].

3. Proof of Theorem 1.1

We shall then make proof of Theorem 1.1.

Linear independence on $\Gamma \times (0,T)$. Assume that linear independence does not hold. Then, after a possible renumbering of the points $\{y_k, \tau_\ell\}_{k,\ell=1,2,\ldots}$,

$$\sum_{k=1}^{M} \sum_{\ell=1}^{N} c_{k,\ell} F(x,t;y_k,\tau_\ell) = 0 \quad \text{on} \quad \Gamma \times (0,T), \tag{5}$$

for some integers $M, N > 0$ with at least one of the coefficients $c_{k,\ell}$ being non-zero, say c_{k_0,ℓ_0}. The function

$$u_{M,N}(x,t) = \sum_{k=1}^{M} \sum_{\ell=1}^{N} c_{k,\ell} F(x,t;y_k,\tau_\ell) \tag{6}$$

satisfies the heat equation in $\Omega \times (0,T)$, is zero on $\Gamma \times (0,T)$ and $u_{M,N}(x,0) = 0$. Thus, by Proposition 2.1, $u_{M,N}$ is identically zero in $\overline{\Omega} \times [0,T]$. In particular, $u_{M,N}$ and its normal derivative vanish on $\Gamma \times (0,T)$. Using Proposition 2.3, $u_{M,N}(x,t)$ is therefore also identically zero for x in the region between the two boundary surfaces Γ and Γ_S, for $t \in [0,T]$.

Let then (x,t) in $(\Omega_S \setminus \overline{\Omega}) \times (0,T]$ approach (y_{k_0}, τ_{ℓ_0}), a point with $c_{k_0,\ell_0} \neq 0$ in (5), such that the ratio

$$r = \frac{|x - y_{k_0}|^2}{4(t - \tau_{\ell_0})} \tag{7}$$

remains bounded. This leads to a contradiction to having $u_{M,N}(x,t) = 0$ in $(\Omega_S \setminus \overline{\Omega}) \times [0,T]$, since the term $c_{k_0,\ell_0} F(x,t;y_{k_0},\tau_{\ell_0})$ in (5) can be as large as we please by choosing (x,t) sufficiently close to (y_{k_0}, τ_{ℓ_0}) obeying (7), while the other terms remain bounded. From this contradiction, we conclude that $\{F(x,t;y_k,\tau_\ell)\}_{k,\ell=1,2,\ldots}$ is a linearly independent set.

For the normal derivative of the fundamental solution (2), we have by direct calculation

$$\frac{\partial F(x,t;y,\tau)}{\partial \nu_x} = -\frac{[(x-y) \cdot \nu_x]}{2(t-\tau)} F(x,t;y,\tau). \tag{8}$$

The heat equation supplied with a zero initial condition and a zero normal derivative on the boundary has also a unique solution according to Proposition 2.1 (choosing $\mathcal{B}u$ in (1) as the normal derivative). Therefore, we can again conclude that (6) is identically zero in $\Omega_S \times [0, T]$. Thus, approaching a suitably chosen point on the boundary $\Gamma_S \times (0, T)$ keeping the ratio (7) bounded, the reader can check that the same arguments as given above render a contradiction (since (8) will grow indefinitely), which in turn establishes linear independence of the corresponding set of normal derivatives of fundamental solutions.

Denseness on $\Gamma \times (0, T)$. Assume that there exists an element $f \in L^2(\Omega)$ with

$$\int_0^T \int_\Gamma f(x,t)F(x,t;y_k,\tau_\ell)\,dx\,dt = 0 \tag{9}$$

for every $k \geq 1, \ell \geq 1$. Consider a single-layer representation

$$v(y,\tau) = \int_\tau^T \int_\Gamma f(x,t)F(x,t;y,\tau)\,dx\,dt.$$

Then v is a solution to the adjoint equation $\partial_t v + \Delta v = 0$ in the exterior and interior of Γ, and is smooth in those two regions. Since $\{y_k, \tau_\ell\}_{k,\ell=1,2,\ldots}$ is a dense set of $\Gamma_S \times (0, T)$ and v in (9) vanish on this set by the choice of f, we conclude, since v is smooth in the exterior of Γ, that v is identically zero on Γ_S for $0 < \tau < T$. We note that v is a decaying solution of the adjoint heat equation in the exterior of Γ_S, with zero Dirichlet boundary condition for $t \in (0, T)$, hence v is zero in that exterior region. Appealing to Proposition 2.3, we have that v is zero in all of the exterior of Ω for $0 < \tau < T$. Using this and the continuity of the single-layer potential across Γ, imply that v is zero on Γ. Hence, due to the uniqueness of the Dirichlet problem in Ω, v is zero also in Ω. Therefore, using jump properties of the derivative of the single-layer potential across $\Gamma \times (0, T)$, it follows that $f = 0$. Thus, $\{F(x,t;y_k,\tau_\ell)\}_{k,\ell=1,2,\ldots}$ is dense in $L^2(\Gamma \times (0, T))$.

We remark that the properties used for the single-layer potential are classical for a smooth surface (or curve) and a continuous density, see, for example, [9, Chapter 5.1-4]. In the case of, for example, a square integrable density and Lipschitz domain, the continuity of the single-layer operator and the jump properties of the derivative still hold, see [11, Theorem 3.4].

To show the similar result for the normal derivative of fundamental solutions, the above goes through the same by replacing the single-layer operator with the double-layer, as can be verified by the reader.

Linear independence on $\Omega \times \{t_0\}$. Assume that the given set is not dense. Then, again after a possible re-numbering of the points $\{y_k, \tau_\ell\}_{k,\ell=1,2,\ldots}$, we have

$$u_{M,N}(x,t) = \sum_{k=1}^{M}\sum_{\ell=1}^{N} c_{k,\ell}F(x,t_0;y_k,\tau_\ell) = 0 \quad \text{for} \quad x \in \Omega, \tag{10}$$

for some integers $M, N > 0$ with at least one of the coefficients $c_{k,\ell}$ being non-zero, and $t_0 \in (0, T)$. Since $F(x,t_0;y_k,\tau_\ell)$ is identically zero for $\tau_k \geq t_0$, we can assume that each τ_k in (10) is less than t_0. Then $F(x,t_0;y_k,\tau_\ell)$ is real analytic in the spatial variable in all of $\mathbb{R}^n$ (see [12, p. 219]); therefore the relation (10) can be extended and is valid for $x \in \mathbb{R}^n$. Clearly, $u_{M,N}$ satisfies an exponential bound in the spatial variable x. Hence, from Proposition 2.2, it follows that $u_{M,N}$ is identically zero in $\mathbb{R}^n$ for $[t_0, T]$. In particular, it is zero on $\Gamma \times (t_0, T)$, and from the first part of the proof we know that restrictions to the boundary of fundamental solutions constitute a linearly independent set. Thus, we conclude that all the coefficients in (10) are identically zero, and linear independence of the given set for a fixed instance in time is thereby established.

Denseness on $\Omega \times \{t_0\}$. Assume that there exists an element $g \in L^2(\Omega)$ such that

$$\int_\Omega g(x)F(x,t_0,y_k,\tau_\ell)\,dx = 0, \tag{11}$$

for every $k, \ell \geq 1$. Let v be a solution to the adjoint equation $\partial_t v + \Delta v = 0$ in $\Omega \times (0, t_0)$, supplied with $v = 0$ on $\Gamma \times (0, t_0)$ and a final condition $v(x, t_0) = g$. Using (3) together with (11) noting that $F(x, 0, y_k, \tau_\ell) = 0$, we obtain

$$\int_0^{t_0} \int_\Gamma F(x,t,y_k,\tau_\ell)\frac{\partial v(x,t)}{\partial \nu_x}\,dx\,dt = 0. \tag{12}$$

Since, as shown above, $\{F(x, t; y_k, \tau_\ell)\}_{k,\ell=1,2,\ldots}$ is dense in $L^2(\Gamma \times (0, T))$, choosing $T = t_0$, we conclude from (12) that the normal derivative of v vanishes on $\Gamma \times (0, t_0)$. Then v is an element with vanishing lateral Cauchy data, and by Proposition 2.3, v is identically zero for $0 \le t \le t_0$. Hence, $g = 0$, and the given set is dense for $t = t_0$. □

The first part of the proof, that is linear independence and denseness on the lateral surface for function values, follows the ideas of [15], the results for derivatives and for a fixed t_0 were not discussed in that work.

4. A Method of Fundamental Solutions for the heat equation (1) and convergence thereof

We outline a method of fundamental solutions for approximating a solution to (1) with a Dirichlet boundary condition ($\mathcal{B} = \mathcal{I}$). To accommodate for the initial condition in (1), let now $\{y_k, \tau_\ell\}_{k,\ell=1,2,\ldots}$ be a dense set of points on the outer lateral (cylindrical) surface $\Gamma_S \times (-t_0, T)$, where $t_0 > 0$. These points are referred to as source points. Let the index set I correspond to those ℓ with $\tau_\ell < 0$ and I' corresponds to the remaining ones, that is those ℓ with $\tau_\ell \ge 0$.

Consider the set $\{F(x, t; y_k, \tau_\ell)\}_{k=1,2,\ldots;\ell\in I}$. From Theorem 1.1, it is a linearly independent and dense set in $L^2(\Omega)$ for $t = 0$. Hence, we can apply the Gram-Schmidt procedure to generate a total orthonormal set $\{\Phi_m\}_{m=1,2,\ldots}$ in $L^2(\Omega)$ (total refers to that the span of the set is dense); an overview including numerical aspects and history of the Gram-Schmidt orthogonalization is given in [16]. From the construction each Φ_m is generated from fundamental solutions of the heat equation, thus each Φ_m has a natural extension in time to a solution of the heat equation for $0 < t < T$.

We can then, since $\{\Phi_m\}_{m=1,2,\ldots}$ is a total orthonormal set, choose an integer $M = M(\varepsilon) > 0$ and coefficients $\{c_m\}$, with

$$\Big\|\varphi - \sum_{m=1}^{M} c_m \Phi_m\Big\|_{L^2(\Omega)} \le \varepsilon, \tag{13}$$

for a given $\varepsilon > 0$, where $\varphi \in L^2(\Omega)$.

Similarly, the functions $\{F(x, t; y_k, \tau_\ell)\}_{k=1,2,\ldots;\ell\in I'}$ is linearly independent and dense in $L^2(\Gamma \times (0, T))$. We can use the Gram-Schmidt procedure to generate a total orthonormal set $\{\Psi_n\}_{n=1,2,\ldots}$ in $L^2(\Gamma\times(0, T))$. Each Ψ_n can be extended to a solution to the heat equation in $\Omega \times (0, T)$. We can choose an integer $N = N(\varepsilon)$ and coefficients $\{d_n\}$, with

$$\Big\|\psi - \sum_{m=1}^{M} c_m \Phi_m - \sum_{n=1}^{N} d_n \Psi_n\Big\|_{L^2(\Gamma\times(0,T))} \le \varepsilon, \tag{14}$$

for a given $\varepsilon > 0$, where $\psi \in L^2(\Omega)$.

Let

$$u_{M,N}(x, t) = \sum_{m=1}^{M} c_m \Phi_m(x, t) + \sum_{n=1}^{N} d_n \Psi_n(x, t). \tag{15}$$

Then, using the linearity of the heat equation, $u - u_{M,N}$ is a solution to (1) with initial data $\varphi - \sum_{m=1}^{M} c_m \Phi_m$ and boundary data $(\psi - u_{M,N}|_{\Gamma\times(0,T)})$. Estimating the solution $u - u_{M,N}$ in terms of the data,

$$\|u - u_{M,N}\|_{L^2(\Omega\times(0,T))} \le C\Big(\Big\|\varphi - \sum_{m=1}^{M} c_m \Phi_m\Big\|_{L^2(\Omega)} + \Big\|\psi - \sum_{m=1}^{M} c_m \Phi_m - \sum_{n=1}^{N} d_n \Psi_n\Big\|_{L^2(\Gamma\times(0,T))}\Big)$$

and this can be made arbitrarily small by choosing M and N sufficiently large according to (13) and (14).

Thus, one can approximate the solution to the heat equation (1) arbitrarily well in L^2 by linear combinations from the set $\{F(x, t; y_k, \tau_\ell)\}_{k,\ell=1,2,\ldots}$.

Since also the normal derivative of the set of fundamental solutions is dense on the boundary according to Proposition Theorem 1.1, the similar error estimate between the solution and approximation can be shown in the case of a Neumann boundary condition in (1).

In practise, data is often at least continuous making pointwise evaluation meaningful. Then typically a set of collocation points are chosen on $(\Gamma \cup \Omega) \times (0, T)$, and the coefficients in an approximation

$$u_{appr}(x, t) = \sum_{k=1}^{M} \sum_{\ell=1}^{N} c_{k,\ell} F(x, t; y_k, \tau_\ell), \tag{16}$$

are found by imposing that this expansion matches the given data in (1) at the collocation points. Matching first the initial condition generates coefficients in (16) corresponding to the index set I above. Details and examples of the generation of source and collocation points are given, for example, in [7, Section 3].

5. Some remarks

We point out the following:

(i) The techniques presented can be applied also when Δ in (1) is replaced by a general second order linear elliptic operator $L(x, t)$; there is then usually no explicit expression for the fundamental solution. A similar MFS for other time-dependent problems such as the unsteady Stokes system can be derived.

(ii) There are well-posedness results for (1) in L^p-spaces, see [17], and one can thus investigate linear independence and denseness of fundamental solutions in such spaces.

(iii) Parabolic equations can be studied in abstract form in Banach spaces. There are fundamental solutions, see [18], thus one can propose an MFS in that setting as well.

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