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Differentiability With Respect to Parameters of Weak Solutions of Linear Parabolic Equations

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Abstract

We consider the differentiability of weak solutions of linear parabolic equations with respect to parameters and initial data. Under natural assumptions, it is shown that solutions possess as much differentiability with respect to the data as do the terms appearing in the equation. The derivatives are shown to satisfy the appropriate sensitivity equations. The theoretical results are illustrated with an example.

Keywords: Fréchet differentiability, parameters, weak solutions, linear parabolic equations

1 Introduction

In many applications, it is important to determine how solutions to a partial differential equation change with respect to parameters of interest. The change in the solution can be quantified by computing the derivative of the solution with respect to the parameters. This process is known as sensitivity analysis. The derivatives (or sensitivities) can be used to estimate model parameters, estimate solutions of "nearby" problems, quantify model uncertainty, minimize objective functionals, etc. For information on the techniques and applications of sensitivity analysis, see [1, 2, 3, 4, 5].

Since many partial differential equations are naturally understood in weak form, it is important to know when and in what sense solutions of such problems are differentiable with respect to parameters. In particular, theoretical differentiability results can provide insight for choosing appropriate numerical methods to approximate sensitivities. In this note, we

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consider the differentiability with respect to parameters and initial data of solutions of linear parabolic equations of the form

$$\dot{w}(t) + A(t;q)w(t) = f(t;q), \quad w(0) = w_0. \tag{1}$$

The equation is understood to hold in a weak sense. Roughly, it is shown that if $A(t;q)$ and $f(t;q)$ are k times continuously Fréchet differentiable or analytic with respect to the parameter q, then the solution $w(t;q,w_0)$ has the same differentiability with respect to the data q and w_0.

To the author's knowledge, only reference [6] deals with parameter differentiability of weak solutions of partial differential equations. In that work, the authors study a class of parameter dependent linear parabolic problems without forcing where the linear operator generates an analytic semigroup. In the present work, we use a variational integral form of the problem which allows us to treat a larger class of linear parabolic problems with forcing. This work is a first step in using the variational form to treat the differentiability of solutions of evolution equations with respect to the problem data. In future work, differentiability results will be extended to other types of equations.

Traditionally, the parameter differentiability problem has been treated using semigroup methods. We briefly recall other results in Section 2 and give motivation for using a variational formulation in place of semigroup theory. In Section 3, we formulate the main problem and state the assumptions we require for the differentiability theory. Section 4 contains the main result and corollary. The proof of the main result is given in Section 5 and Section 6 illustrates the theory with an example. We close with conclusions and questions for future research.

Note: After this work was complete, the author became aware of results in [7, Section 2.3] treating the weak Gâteaux differentiability of weak solutions of linear parabolic equations and linear undamped and damped hyperbolic equations. Although the method of proof in [7] applies to parabolic as well as hyperbolic equations, the results presented here give more complete results for parabolic equations.

2 Other Parameter Differentiability Results

In this section, we present a brief survey of parameter differentiability results for solutions of abstract differential equations and give motivation for using the variational form of the problem to treat parameter differentiability. As far as the author is aware, there are differentiability results for

1. general nonlinear differential equations holding over a Banach space [8],
2. linear differential equations with the linear operator generating a C_0-semigroup [9, 10, 6], an analytic evolution operator [11], or an integrated semigroup [12, 13],
3. semilinear differential equations with the linear operator generating an analytic C_0-semigroup [14, 15, 16], or an analytic evolution operator [11].

In the first case, one can use a parameter-dependent version of the contraction mapping theorem to show the differentiability of the solution with respect to the initial data and parameters (see [17, 18] for the application to ordinary and functional differential equations). This approach has also been used in [11, 15] to treat the third case when the linear operator is not parameter dependent. Even though these references cover a wide variety of problems, there are still natural cases where the theory may be difficult to apply:

1. If the linear operator is parameter dependent, one must find conditions guaranteeing that the semigroup generated by the linear operator is Fréchet differentiable with respect to the parameter [6, 9, 10, 11, 12, 15, 16].

2. The domain of a linear operator is parameter dependent while the state space is not parameter dependent [12, 13, 19]. (This situation can occur when parameters appear in the boundary conditions; see the example in Section 6.)

3. The operators appearing in the strong form of the equation are not Fréchet differentiable, but they are differentiable when understood in a weak sense.

4. The problem is easier to formulate in a weak sense rather than in a semigroup framework.

The first two items are often treated in the context of semigroup theory by either restricting how the parameter enters the linear operator or by requiring other auxiliary criteria. In this work, the variational formulation is used to avoid any restrictions on the linear operator. Future work will concentrate on expanding the use of the variational formulation to treat parameter differentiability in many other types of equations for which semigroup theory may not be easily applied.

3 Abstract Framework and Assumptions

We now describe the problem and the assumptions in detail. We want to reformulate the differential equation (1) as a variational integral equation where functions in the solution space and test space are time dependent. Due to the assumptions on A and f given below, we will be able to integrate by parts and cause the initial conditions to appear explicitly in the integral equation. This will allow us to prove the differentiability of the solution with respect to the initial data w_0 and the parameter q.

We begin by describing the standard Hilbert space structure that allows the differential equation to be understood in a weak sense. Let V and H be Hilbert spaces with $(\cdot,\cdot)_H$ and $(\cdot,\cdot)_V$ the inner products on H and V, respectively. Assume these spaces satisfy the following hypothesis:

(H1) The Hilbert spaces H and V and their inner products do not depend on the parameter q, V is separable, and $V \subset H$ where the embedding is continuous and dense.

In applications such as shape optimization, the Hilbert spaces H and V may be parameter dependent. In this case, one may be able to transform the problem so that the spaces do not depend on the parameter q. Otherwise, there are no known differentiability results for problems where the underlying function spaces are parameter dependent. It may be possible to treat parameter dependent inner products using the method presented below, however we do not consider this case here.

To proceed to the weak formulation, identify H with its dual H' so that we have the Gelfand triple $V \subset H \cong H' \subset V'$ where all embeddings are continuous and dense. We denote the value of a functional $f \in V'$ at $v \in V$ by $\langle f, v\rangle$. Let $T > 0$ but finite. Define the Hilbert space $\mathcal{V} = L^2(0, T; V)$ with the inner product

$$(f, g)_{\mathcal{V}} = \int_0^T (f(t), g(t))_V \, dt.$$

The dual space of $\mathcal{V}$ can be identified with $L^2(0, T; V')$ so that for any functional $\ell \in \mathcal{V}'$ there exists $f \in L^2(0, T; V')$ such that for all $v \in \mathcal{V}$,

$$\ell(v) = \int_0^T \langle f(t), v(t)\rangle \, dt \quad \text{and} \quad \|\ell\|_{\mathcal{V}'} = \|f(t)\|_{L^2(0,T;V')} .$$

For $v \in \mathcal{V}'$ and $w \in \mathcal{V}$, we have the Hölder inequality

$$\int_0^T \langle v(t), w(t)\rangle \, dt \le \|v\|_{\mathcal{V}'} \|w\|_{\mathcal{V}} .$$

Let $\mathcal{W} = \{ w \in \mathcal{V} : \dot{w} \in \mathcal{V}'\}$, where the dot denotes the time derivative understood in the distributional sense. With the norm $\|w\|_{\mathcal{W}} = (\|w\|_{\mathcal{V}}^2 + \|\dot{w}\|_{\mathcal{V}'}^2)^{1/2}$, $\mathcal{W}$ is a Hilbert space that is continuously embedded in $C([0, T]; H)$. Therefore, any $w \in \mathcal{W}$ is equal almost everywhere to a function that is continuous in H. This gives an integration by parts: for any $v, w \in \mathcal{W}$,

$$\int_0^T \langle \dot{v}(t), w(t)\rangle \, dt = (v(T), w(T))_H - (v(0), w(0))_H - \int_0^T \langle \dot{w}(t), v(t)\rangle \, dt.$$

The space $\mathcal{W}$ will be the solution space for our differential equation. For details on these spaces, see [20, 21, 22, 23].

The parameter q is required to be in open subset of a Banach space Q:

(H2) The admissible parameter space Q_0 is an open subset of a Banach space Q. The parameter space Q may depend on the time t.

We assume the differential equation (1) is parabolic at a fixed $q_0 \in Q_0$ in the sense that the linear operator $A(t; q_0)$ satisfies the following hypothesis:

(H3) Let q_0 be fixed in Q_0. For any $t \in [0, T]$ and $u, v \in V$, set $a(t, u, v) = \langle A(t; q_0)u, v\rangle$. Then for all $u, v \in V$,

(H3a) the function $t \mapsto a(t, u, v)$ is measurable, (H3b) there exists $M > 0$ such that $a(t,u,v) \leq M \|u\|_V \|v\|_V$ for all $t \in [0,T]$,

(H3c) there exists $\alpha > 0$ and $\lambda \geq 0$ such that $\text{Re } a(t,v,v) + \lambda \|v\|_H^2 \geq \alpha \|v\|_V^2$ for all $t \in [0,T]$.

If the forcing $f(\cdot\,;q_0)$ is in $\mathcal{V}'$, it is well known that the linear initial problem (1) has a unique solution $\phi(\cdot\,;q_0,\xi) \in \mathcal{V}$ for any initial condition $\xi \in H$ [20, 21, 22, 24].

In order to reformulate the differential equation (1) as a variational integral equation, the linear operator $A(\cdot\,;q)$ and the forcing $f(\cdot\,;q)$ must map $\mathcal{V}$ to $\mathcal{V}'$ for $q \in Q_0$.

(H4) For each $q \in Q_0$, $A(\cdot\,;q)$ is a bounded linear map from $\mathcal{V}$ into $\mathcal{V}'$, and the forcing $f(\cdot\,;q)$ is in $\mathcal{V}'$.

Since $A(\cdot\,;q)$ is only a bounded map from $\mathcal{V}$ to $\mathcal{V}'$, we do not know if there is a unique solution of the linear problem (1) for any $q \in Q_0$; however, suppose $w(\cdot\,;q,w_0) \in \mathcal{V}$ is a solution for $q \in Q_0$ and $w_0 \in H$. It follows that $\dot{w} \in \mathcal{V}'$ since $\dot{w}(t) = -A(t;q)w(t) + f(t;q) \in \mathcal{V}'$ and therefore $w \in \mathcal{W}$. Define the test function space $\Phi = \{\, \varphi \in \mathcal{W} : \varphi(T) = 0\}$ with the $\mathcal{W}$ norm. Since the differential equation (1) holds in $\mathcal{V}'$, for any $\varphi \in \Phi \subset \mathcal{W}$ we have, after a legitimate integration by parts,

$$-(w_0, \varphi(0))_H + \int_0^T -\langle \dot{\varphi}(t), w(t) \rangle + \langle A(t;q)w(t), \varphi(t) \rangle - \langle f(t;q), \varphi(t) \rangle \, dt = 0. \tag{2}$$

Therefore, any solution $w \in \mathcal{V}$ of (1) must satisfy the variational integral equation (2). It can also be shown that these formulations are equivalent (see Sections III.2 and III.4 in [21]).

We will use the implicit function theorem on this variational integral equation to show that solutions of the differential equation are differentiable with respect to the data. For $(q, w_0, w) \in Q_0 \times H \times \mathcal{V}$ and for $\varphi \in \Phi$, define

$$[F(q,w_0,w)]\varphi = -(w_0, \varphi(0))_H + \int_0^T -\langle \dot{\varphi}(t), w(t) \rangle + \langle A(t;q)w(t), \varphi(t) \rangle - \langle f(t;q), \varphi(t) \rangle \, dt. \tag{3}$$

To apply the implicit function theorem, we must be able to differentiate through the integral with respect to w and q. This will be fulfilled if the linear operator A and the forcing f have certain differentiable properties with respect to $q \in Q_0$. Let $\mathcal{L}(\mathcal{V}, \mathcal{V}')$ denote the Banach space of all bounded linear operators from $\mathcal{V}$ to $\mathcal{V}'$ with the operator norm.

(H5) The mappings $A(\cdot\,;q) : Q_0 \subset Q \to \mathcal{L}(\mathcal{V}, \mathcal{V}')$ and $f(\cdot\,;q) : Q_0 \subset Q \to \mathcal{V}'$ are k times continuously Fréchet differentiable or analytic.

This hypothesis will guarantee that F is k times continuously Fréchet differentiable or analytic as a mapping of $(q, w_0, w) \in Q_0 \times H \times \mathcal{V} \subset Q \times H \times \mathcal{V}$ into Φ' (see Lemma 5.1). Since $F(q_0, \xi, \phi) = 0$, the requirements of the implicit function theorem will be fulfilled if $D_w F(q_0, \xi, \phi)$ is a bijection as a mapping from $\mathcal{V}$ to Φ'. Differentiating through the integral shows that this condition holds if the following linearized problem is uniquely solvable: for any $\ell \in \Phi'$, find $s \in \mathcal{V}$ such that

$$\int_0^T -\langle \dot{\varphi}(t), s(t) \rangle + \langle A(t;q_0)s(t), \varphi(t) \rangle \, dt = \ell(\varphi(\cdot))$$

holds for all $\varphi \in \Phi$. Hypothesis **(H3)** is sufficient to guarantee that this problem has a unique solution for any $\ell \in \Phi'$ (see Theorem 5.1). Therefore, the above hypotheses will ensure that the solution of the differential equation (1) is differentiable with respect to the data w_0 and q.

4 The Main Result

We can now state the main result which is a consequence of the implicit function theorem applied to the function F defined in (3) (see [15, Section 1.2.6]). The details of the proof are given in the next section. This theorem also guarantees the existence of a solution of the differential equation for data in a small neighborhood of the given problem data.

Theorem 4.1 *Suppose $0 < T < \infty$ and let $\phi(\cdot\,; q_0, \xi) \in \mathcal{V} = L^2(0, T; V)$ be the unique solution of the linear differential equation (1) for initial data $\xi \in H$ and parameter $q_0 \in Q_0 \subset Q$. If hypotheses **(H1)-(H5)** hold, then there exist $r_0, r > 0$ such that for every $(q, w_0) \in Q_0 \times H$ satisfying*

$$\|q - q_0\|_Q + \|w_0 - \xi\|_H \leq r_0, \tag{4}$$

there exists a unique solution $w = w(\cdot\,; q, w_0) \in \mathcal{V}$ to (1) such that

$$\|w(\cdot\,; q, w_0) - \phi(\cdot\,; q_0, \xi)\|_{\mathcal{V}} \leq r.$$

This solution is k times Fréchet differentiable or analytic in (q, w_0).

This result covers the possibility that the linear problem does not remain parabolic as the parameter varies. Before we give a proof, we present a useful corollary.

The solution $w(\cdot\,; q, w_0)$ satisfies $F(q, w_0, w) = 0$ and we can differentiate through the integral in (3) to obtain sensitivity integral equations for the derivatives. The arguments in Section 3 can be used to show that these sensitivity integral equations are also equivalent to differential equations. These equations can be used to approximate the sensitivities.

Corollary 4.1 *Let $(q, w_0) \in Q_0 \times H \subset Q \times H$ be in the small neighborhood of (q_0, ξ) as in equation (4) in the above theorem. Denote the Fréchet derivatives of the solution $w(\cdot\,; q, w_0)$ of (1) evaluated at (q, w_0) by*

$$S_1(t) = D_q w(t; q, w_0) \quad \textit{and} \quad S_2(t) = D_{w_0} w(t; q, w_0).$$

Then for any $(p, \zeta) \in Q_0 \times H$, the sensitivities $s_1(t) = S_1(t)p$ and $s_2(t) = S_2(t)\zeta$ satisfy the linear initial value problems

$$\dot{s}_1(t) + A(t; q)s_1(t) = -[D_q A(t; q)\, p]\, w(t; q, w_0) + D_q f(t; q)\, p, \qquad s_1(0) = 0,$$
$$\dot{s}_2(t) + A(t; q)s_2(t) = 0, \qquad s_2(0) = \zeta.$$

These sensitivity equations can be obtained by formally differentiating through the differential equation (1), using the chain rule, and interchanging the order of differentiation. Higher order sensitivity equations can be derived in a similar manner.

5 Proof of the Main Result

This section contains the proof of the main theorem. We use the function spaces introduced in Section 3 and the function F defined in equation (3). As before, we assume the final time T is finite. In order to apply the implicit function theorem, the function F must be continuously differentiable as a mapping from $Q_0 \times H \times \mathcal{V}$ into Φ' and $D_w F(q_0, \xi, \phi)$ must be a bijection as a mapping from $\mathcal{V}$ to Φ'. The differentiability properties of F are established in the following Lemma.

Lemma 5.1 *If hypotheses **(H1)**-**(H2)** and **(H4)**-**(H5)** hold, the function F defined in (3) is k times continuously Fréchet differentiable or analytic as a mapping from $(q, w_0, w) \in Q_0 \times H \times \mathcal{V} \subset Q \times H \times \mathcal{V}$ into Φ'.*

Proof: The function F is clearly linear in $\varphi \in \Phi$. We show it is bounded for a fixed $(q, w_0, w) \in Q_0 \times H \times \mathcal{V}$. Using the Hölder inequality, we have

$$[F(q, w_0, w)]\varphi \le \|w_0\|_H \|\varphi(0)\|_H + \|w\|_{\mathcal{V}} \|\dot{\varphi}\|_{\mathcal{V}'} + \|A(\cdot\,; q)w(\cdot)\|_{\mathcal{V}'} \|\varphi\|_{\mathcal{V}} + \|f(\cdot; q)\|_{\mathcal{V}'}\|\varphi\|_{\mathcal{V}}.$$

Since V is embedded continuously into H, there exists a positive constant c such that $\|u\|_H \le c\|u\|_V$ for any $u \in V$. This combined with the Hölder inequality for the (real valued) Lebesgue integral gives

$$\|\varphi(0)\|_H \le \int_0^T 1 \cdot \|\varphi(t)\|_H \, dt \le cT^{1/2} \left(\int_0^T \|\varphi(t)\|_V^2 \, dt \right)^{1/2} = cT^{1/2} \|\varphi\|_{\mathcal{V}}$$

This implies

$$[F(q, w_0, w)]\varphi \le (cT^{1/2} \|w_0\|_H + \|w\|_{\mathcal{V}} + \|A(\cdot\,; q)\|_{\mathcal{L}(\mathcal{V},\mathcal{V}')} \|w\|_{\mathcal{V}} + \|f(\cdot; q)\|_{\mathcal{V}'})(\|\varphi\|_{\mathcal{V}} + \|\dot{\varphi}\|_{\mathcal{V}'}).$$

For any $a, b \ge 0$, $a + b \le \sqrt{2}(a^2 + b^2)^{1/2}$; thus for $a = \|\varphi\|_{\mathcal{V}}$ and $b = \|\dot{\varphi}\|_{\mathcal{V}'}$, we obtain

$$[F(q, w_0, f, w)]v \le C(q, w_0, w)(\|\varphi\|_{\mathcal{V}}^2 + \|\dot{\varphi}\|_{\mathcal{V}'}^2)^{1/2} = C(q, w_0, w) \|\varphi\|_{\Phi} .$$

This shows that F is bounded and linear as a function of $\varphi \in \Phi$ and therefore maps $Q_0 \times H \times \mathcal{V} \subset Q \times H \times \mathcal{V}$ into Φ'.

To show the desired differentiability properties of F, we examine each term separately. First, the term

$$-(w_0, \varphi(0))_H + \int_0^T - \langle \dot{\varphi}(t), w(t) \rangle \, dt$$

is clearly analytic as a function of $w_0 \in H$ and $w \in \mathcal{V}$. For the last term, define $g : \mathcal{V} \times Q_0 \subset \mathcal{V} \times Q \to \Phi'$ by

$$[g(w, q)]\varphi = \int_0^T \langle A(t; q)w(t), \varphi(t) \rangle - \langle f(t; q), \varphi(t) \rangle \, dt.$$

Since $A(\cdot\,;q)w(\cdot)$ is analytic in $w(\cdot)$, it is clear that g is also analytic in $w \in \mathcal{V}$. If A and f are k times continuously Fréchet differentiable as functions of q, then they can be expanded in a Taylor series in q. The converse Taylor theorem for continuously Fréchet differentiable functions (see Theorem 7.4, page 197, of [25]) shows that g is also k times continuously Fréchet differentiable as functions of q. In particular, one can pass the derivative through the integral to give

$$\begin{aligned}
[D_q^{(j)} g(w,q)p^j]\varphi &= \int_0^T \left\langle [D_q^{(j)} A(t;q)p^j]w(t), \varphi(t)\right\rangle - \left\langle D_q^{(j)} f(t;q)p^j, \varphi(t)\right\rangle \, dt, \\
[D_w g(w,q)]s &= \int_0^T \langle A(t;q)s(t), \varphi(t)\rangle \, dt,
\end{aligned}$$

where p^j stands for the j-vector $(p, \ldots, p)$. All higher derivatives with respect to w are zero. If A and f are analytic in q, the Hölder inequality can be used to obtain uniform estimates on the operator norm of the derivatives of g. This shows that g is analytic in q (see [26, Theorem 12.6]). □

To show $D_w F(q_0, \xi, \phi)$ is a bijection as a mapping from $\mathcal{V}$ to Φ', we use the following result found in [20, Theorem 3.4.2].

Theorem 5.1 (Lions) *Suppose $A(t;q_0)$ satisfies hypothesis* ***(H3)*** *with $\lambda = 0$ in (H3c) and denote its adjoint by $A^*(t;q_0)$. For any $\ell \in \Phi'$, there exists a unique $s \in \mathcal{V}$ such that the variational integral equation*

$$\int_0^T \langle -\dot{\varphi}(t) + A^*(t;q_0)\varphi(t), s(t)\rangle \, dt = \ell(\varphi(\cdot)) \tag{5}$$

holds for all $\varphi \in \Phi$.

It is interesting to note that this variational integral equation can be viewed as a linear differential equation with initial data in H and very general forcing (see Sections 3.4 - 3.6 in [20]). This result allows us to prove the main theorem.

Proof of Theorem 4.1: First, consider the case where the linear operator $A(t;q_0)$ satisfies hypothesis **(H3)** with $\lambda = 0$ in (H3c). Let $\phi \in \mathcal{V}$ be the unique solution to the linear initial value problem (1) for $q = q_0$ and $w_0 = \xi$. Due to Lemma 5.1, $F : Q_0 \times H \times \mathcal{V} \subset Q \times H \times \mathcal{V} \to \Phi'$ is k times continuously Fréchet differentiable or analytic in (q, w_0, w). Differentiating through the integral shows that $D_w F(q_0, \xi, \phi)$ is a bijection as a mapping from $\mathcal{V}$ to Φ' if there is a unique solution to the following problem: for any $\ell \in \Phi'$, find $s \in \mathcal{V}$ such that

$$\int_0^T -\langle \dot{\varphi}(t), s(t)\rangle + \langle A(t;q_0)s(t), \varphi(t)\rangle \, dt = \ell(\varphi(\cdot))$$

for all $\varphi \in \Phi$. This problem is equivalent to the variational integral equation (5). Theorem 5.1 shows that this problem has a unique solution. Since $F(q_0, \xi, \phi) = 0$, all of the assumptions of the implicit function theorem (see [15, Section 1.2.6]) are satisfied which proves the theorem for the case $\lambda = 0$.

If $\lambda \neq 0$ in (H3c), we use the familiar exponential shift to obtain a transformed problem satisfying all of the hypotheses of the theorem with $\lambda = 0$. Make the change of variables $z(t) = e^{-\lambda t} w(t)$ so that $z(t)$ satisfies

$$\dot{z}(t) + (A(t;q) + \lambda I)z(t) = e^{-\lambda t} f(t;q), \quad z(0) = w_0.$$

Hypotheses **(H1)-(H5)** hold for this transformed problem with the linear operator $\tilde{A}(t;q) = A(t;q) + \lambda I$ satisfying hypothesis **(H3)** with $\lambda = 0$ in (H3c). The theorem is true for this case; inverting the change of variables shows that the theorem holds for the original problem where $\lambda \neq 0$. □

6 An Example

In this section, we briefly present an example that highlights the types of problems covered by the theory presented here. For more examples that fit into the framework presented above, see [20, 21, 22].

Consider the heat equation for a composite rod with a source term given by

$$w_t(t,x) = (\kappa(x) w_x(t,x))_x + f(t,x),$$

where the subscripts denote partial derivatives and the functions $\kappa(x)$ and $f(t,x)$ are given by

$$\kappa(x) = \begin{cases} \kappa_1, & 0 \leq x < a \\ \kappa_2, & a < x \leq 1 \end{cases}, \quad f(t,x) = \begin{cases} g(t), & c \leq x \leq d \\ 0, & \text{otherwise} \end{cases}.$$

Here, κ_1 and κ_2 are positive constants, a, c and d are all in $(0,1)$, and the function g is in $L^2(0,T)$ for some $T > 0$. Assume the temperature is fixed at the left end of the rod and a flux condition is imposed at the right end:

$$w(t,0) = 0, \quad \kappa_2 w_x(t,1) + \alpha w(t,1) = 0,$$

where $\alpha > 0$. The initial heat distribution is given by $w(0,x) = w_0(x)$.

Due to the discontinuity in $\kappa(x)$, this problem is naturally understood in weak form. Define the Hilbert spaces $H = L^2(0,1)$ with the standard inner product and $V = \{v \in H^1 : v(0) = 0\}$ with the inner product $(u,v)_V = \int u_x v_x \, dx$. The weak form of the problem is to find $w \in L^2(0,T;V)$ such that

$$\dot{w}(t) + Aw(t) = f(t), \quad w(0) = w_0,$$

where $w_0 \in H$, A is a linear operator mapping V to V' given by

$$\langle Au, v \rangle = \int_0^1 \kappa(x) u_x(x) v_x(x) \, dx + \alpha u(1) v(1),$$

and $f \in L^2(0,T;H) \subset L^2(0,T;V')$ is defined by $\langle f, v \rangle = (f,v)_H = \int_0^1 f(t,x) v(x) = g(t) \int_c^d v(x)$.

It can be checked that A satisfies hypothesis **(H3)** and therefore we only need to check that A and f are continuously Fréchet differentiable or analytic with respect to a parameter to apply the main theorem. It is clear that A is analytic with respect to κ_1, κ_2, and α, and f is also analytic with respect to $g \in L^2(0,T)$; therefore the solution is also analytic with respect to these parameters.

For the strong form of this problem, one would consider the strong form of the operator $A : D(A) \to H$ given by

$$[Aw](x) = (\kappa(x) w_x(x))_x,$$

where

$$D(A) = \{w \in H^1 \ : \ \kappa w_x \in H^1, \ \ w(0) = 0, \ \ \kappa_2 w_x(1) + \alpha w(1) = 0\}.$$

Since the domain of A depends on the parameters κ_1, κ_2 and α, it is complicated to use semi-group theory to prove the differentiability of the solution with respect to these parameters [12, 13, 19]. A weak formulation of the problem avoids this difficulty.

For the parameter d, the Fréchet derivative $D_d f(d) \in L^2(0,T;V')$ is given by $D_d f(d) = g(\cdot)\delta_d$, where δ_d is the delta function centered at $x = d$. It can be checked that $D_d f(d)$ is continuous in d and so the solution w must be continuously differentiable with respect to d. However, f does not have a second Fréchet derivative with respect to d since elements of V do not have continuous first derivatives. Also, the linear operator A only appears to be differentiable with respect to a in a very weak sense [27]. The theory presented here does not cover this case.

For all of these cases, one can use the differential sensitivity equations given in Corollary 4.1 to approximate the sensitivities. Note that a weak formulation of this problem is essential to treat the differentiability of the solution with respect to d since f is only continuously differentiable with respect to d as a function in $L^2(0,T;V')$. Although this example is somewhat artificial, it is quite possible that solutions of more realistic problems may only be differentiable with respect to certain parameters in a weak sense.

7 Conclusion

In this work, we gave natural conditions guaranteeing that weak solutions of linear parabolic problems are differentiable with respect to parameters and initial data. The derivatives of the solution were also shown to be solutions of (weak) sensitivity equations. These results are important for determining appropriate numerical methods for approximating sensitivities in various applications. Therefore, it would be useful to extend the theory presented here to other types of problems.

We note that it is not difficult to extend the theory presented here to cover nonlinear problems of the form

$$\dot{w}(t) + G(t, w(t); q) = f(t; q), \quad w(0) = w_0,$$

where the linearization of the operator G about a solution satisfies hypothesis **(H3)** and G maps $w \in L^2(0,T;V)$ into $L^2(0,T;V')$. However, this last condition is rarely satisfied in problems of interest; usually the nonlinearity only maps into $L^2(0,T;V')$ if the function $w \in L^2(0,T;V)$ also lies in some auxiliary space (for examples, see [24]). In this case, Theorem 5.1 does not apply and the method of proof presented above breaks down. A future work will report on a different technique using a variational form to treat the differentiability with respect to parameters of weak solutions of various nonlinear equations.

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