Identifying the principal coefficient of parabolic equations with non-divergent form

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Abstract. We deal with an inverse problem of determining a coefficient \( a(x, t) \) of principal part for second order parabolic equations with non-divergent form when the solution is known. Such a problem has important applications in a large fields of applied science. We propose a well-posed approximate algorithm to identify the coefficient. The existence, uniqueness and stability of such solutions \( a(x, t) \) are proved. A necessary condition which is a couple system of a parabolic equation and a parabolic variational inequality is deduced. Our numerical simulations show that the coefficient is recovered very well.

1. Introduction
In this paper we deal with the inverse problem of determining a coefficient of principle part for second order parabolic equations with non-divergent form when the solution is known.

Problems of this type are of some importance in a large fields of applied science. As an example, let us consider the recovering of implied local volatility where one is interesting in to know the structure of the volatility of underlying assets when the option price is given([11], [3] and [6]). In the Black-Scholes framework, Dupire([3], 1995) derived a second order parabolic equation with non-divergence form, which is called Dupire’s equation, that links observed option prices to the local volatility of underlying asset where the solution of the equation is the option pricing, which is a function of strike price and times to maturity. According to the Dupire’s approach the problem of recovering the implied volatility of underlying asset is to solve an inverse problem for determining the coefficient of second derivative term in the Dupire’s equations, if the option pricing is known.

The inverse problem can be stated in the following form.
Suppose \( I \subset R \) is a bounded interval, we consider an initial- boundary value problem of second order parabolic equation in \( Q = I \times (0, T] \) as follows

\[
Lu \equiv u_t - a(x, t)u_{xx} + b(x, t)u_x + c(x, t)u = f(x, t), \quad (x, t) \in Q
\]

(1)

\[
u_x = 0, \quad \text{on } \partial I \times (0, T],
\]

(2)

\[
u(x, 0) = u_0(x), \quad x \in I,
\]

(3)

where \( b(x, t), c(x, t), f(x, t), u_0(x) \) are given smooth functions on \( Q \) and \( I \) respectively.

If the solution \( u(x, t) \) is known as data from measurement in the domain \( \bar{Q} \). Then the problem consists in finding the coefficient \( a(x, t) \) from the given data and the initial-boundary value problem (1)-(3).
Let us start from a simple example where \( a(x, t), b(x, t), c(x, t) \) are only functions of time \( t \), \( f(x, t) = 0 \), and \( I = R \). In this case, we consider the following Cauchy problem

\[
Lu \equiv u_t - a(t)u_{xx} + b(t)u_x + c(t)u = 0, \quad (x, t) \in Q
\]

\[
u(x, 0) = u_0(x), \quad x \in I
\]

where \( b(t), c(t), u_0(x) \) are given smooth functions. We want to determine the coefficient \( a(t) \) if \( u(x_0, t) \) is known for some \( x_0 \in R \). Without loss of generality, we can assume \( x_0 = 0 \) and

\[
u(0, t) = g(t).
\]

Similar problems have received considerable attention in the literature. References of [1] and [2] provide a survey of results.

As we know the Cauchy problem has a solution which can be expressed in a closed form. Thus the condition (6) can be rewritten as follows

\[
F(t, \int_0^1 a(\tau)d\tau) = g(t)
\]

where

\[
F(t, s) = e^{-\int_0^t c(\tau)d\tau} \int_{-\infty}^{\infty} u_0(\eta) e^{-(\eta + \int_0^t b(\tau)d\tau)^2} 2\pi \eta \ d\eta
\]

Suppose

\[
u''_0 \geq 0 (\leq 0), \quad u''_0 \neq 0
\]

then we have

\[
F'_s(t, s) = e^{-\int_0^t c(\tau)d\tau} \int_{-\infty}^{\infty} u''_0(\eta) e^{-(\eta + \int_0^t b(\tau)d\tau)^2} 2\pi \eta \ d\eta > 0 (< 0).
\]

Due to the implicit function theorem, the equation (7) has a unique solution

\[
\int_0^1 a(\tau)d\tau = G(t)
\]

If \( g(t) \in C^1[0, T] \), then we get

\[
a(t) = G'(t) = \frac{g'(t) - F'_s(t, s)}{F'_s(t, s)} \bigg|_{s=G(t)}
\]

There are two problems: first, the initial data \( u_0(x) \) does not convex(or concave) everywhere, in general. In this case, we can not claim that the equation (7) has a unique solution (9); second, the value of \( g(t) \) is given by measurement from discrete data in the practice, the numerical derivative should be used to get \( g'(t) \), thus the algorithm (10) is unstable for determining \( a(t) \). Therefore the key point for our problem is to find a well-posed algorithm to determine the coefficient \( a(t) \) from the extra condition (6).

When the coefficients \( a(x, t), b(x, t), c(x, t) \) are only functions of space variable \( x \), in the papers [8] and [7], an optimal control framework is used to determine the coefficient \( a(x) \), if an extra condition is given as follows

\[
u(x, t_0) = g(x), \quad x \in R
\]

for some \( t_0 > 0 \). And the existence of \( a(x) \) is proved, the necessary condition and a well-posed algorithm are obtained to find the coefficient \( a(x) \) from (11).
Now let us come back to the general case. For the initial-boundary value problem (1)-(3), if the extra condition is given by the following form
\[ u(x, t) = g(x, t), \quad (x, t) \in \bar{Q}, \]  
(12)
we want to determine the coefficient \( a(x, t) \) in the domain \( \bar{Q} \), from the given data (12) and the initial-boundary value problem (1)-(3).

As we said before, the problem is improperly posed, for the similar reason that though \( a(x, t) \) can be found directly from the equation (1) and got a formula
\[ a(x, t) = \frac{u_{t} + b(x, t)u_{x} + c(x, t)u - f(x, t)}{u_{xx}}, \]  
(13)
but we have to assume \( u_{xx} \neq 0 \) everywhere, and to evolve numerical derivatives of \( u(x, t) \) with respect to \( x \) and \( t \), especially the second derivative with respect to \( x \) for using the formula (13). A small perturbation in \( u \) itself may result in a big change in its derivative, thus the result is unstable.

We still like to use the optimal control framework to solve this inverse problem just as we did in [8] and [7]. The difference here is that the unknown coefficient \( a(x, t) \) not only depends on the space variable \( x \), but also depends on the time \( t \), so it is an evolutional type inverse problem. We solve it by using semi-discrete scheme first, i.e. we find \( a(x, t_{n}) \) step by step, where \( t_{n} = nh \) and \( h = \frac{T}{N}, \ n = 0, 1, \ldots, N \). In fact, if \( a(x, t_{0}), \ldots, a(x, t_{n-1}) \) has been defined, then we find \( a(x, t_{n}) \) such that
\[ J_{n}(a(\cdot, t_{n})) = \inf_{a \in A} J_{n}(a) \]
where \( A \) is an appropriately admissible set and \( J_{n}(a) \) is a cost functional(see (20) below). One of key points of our contribution is to give a concrete form of \( J_{n}(a) \). Thus for any \( h \) we obtain an approximate function \( a^{h}(x, t) \) defined as follows
\[ a^{h}(x, t) = \begin{cases} a(x, t_{n}) & t = t_{n} \\ \text{linear} & t_{n-1} \leq t \leq t_{n} \end{cases} \]

Certain estimates of \( a^{h}(x, t) \) are established which are uniformly bounded, independently of mesh parameter \( h \). Then we will be able to take the limit for the approximate sequence \( a^{h}(x, t) \) as \( h \to 0 \).

And a necessary condition, which is a couple system of parabolic equation and a parabolic variational inequality with initial and boundary values, is deduced for determining the solution \( \{u(x, t), a(x, t)\} \). The uniqueness and stability of the problem are proved, it shows that the procedure of recovering the unknown coefficient \( a(x, t) \) is well-posed.

The present paper is organized as follows. In section 2 an optimal control method is introduced to obtain the semi-discrete approximate solution \( a^{h}(x, t) \). In section 3 the limit \( a(x, t) \) of \( a^{h}(x, t) \) is derived and a necessary condition is deduced. And the uniqueness and stability results are proved. In section 4, we present our numerical experiments to justify the accuracy of our method.

2. Related semi-discrete optimal control problem
Let \( I \subset R \) be an open bounded interval, \( T \) be a positive constant and \( Q = I \times (0, T) \). Assume that \( b(x, t), c(x, t), f(x, t), u_{0}(x) \) are given functions which satisfy
\[ b, c, f, u_{0} \in C^{\alpha, \frac{\alpha}{2}}(\bar{Q}), \quad b_{x}, b_{t} \in L^{\infty}(Q), \quad u_{0} \in C^{2, \alpha}(I) \]  
(14)
for some $\alpha > 0$. Consider the following initial- boundary value problem of second order parabolic equation

\begin{align*}
Lu &\equiv u_t - \tilde{a}(x,t)u_{xx} + b(x,t)u_x + c(x,t)u = f(x,t), \quad (x,t) \in Q \\
u_x &= 0, \quad \text{on } \partial I \times (0,T], \quad (16) \\
u(x,0) &= u_0(x), \quad x \in I. \quad (17)
\end{align*}

Suppose that $u_0(x)$ is consistent with the homogenous boundary condition $u_x = 0$. The well known theory for parabolic equations guarantees that, for any given positive coefficient $\tilde{a} \in C^{0,\frac{1}{2}}(\bar{Q})$, there is a unique solution, $u(x,t) \in C^{2+\alpha,1+\frac{\alpha}{2}}(\bar{Q})$, to the problem (15)-(17).

Suppose that $g \in C^{0,\frac{1}{2}}(\bar{Q})$ is a given observed function and there exists a constant $C$ such that

$$
\|g\|_{C^{0,\frac{1}{2}}(\bar{Q})} \leq C, \quad \max_{0 \leq t \leq 1} \|g(\cdot, t)\|_{H^1(I)} \leq C. \quad (18)
$$

The inverse problem we will discuss can be stated as follows

**Problem P** Find a positive coefficient $a \in C^{0,\frac{1}{2}}(\bar{Q})$ such that the solution of (15)-(17) with $\tilde{a} = a$ closes to the given observed function $g(x,t)$.

To reconstruct the unknown coefficient, we will introduce the following time semi-discrete cost functional and time semi-discrete optimal control problem. Let $0 = t_0 < t_1 < \cdots < t_N = T$ be a partition of interval $[0,T]$ with $t_n = nh$ and $h = \frac{T}{N}$. Let

$$
A = \{a \in H^1(I) \mid a \leq a(x) \leq \bar{a}\} \quad (19)
$$

be the admissible set, where $a$ and $\bar{a}$ are given positive constants.

Beginning with a given function $a_0(x) \in A$ with

$$
a_0(x) \in W^{1,\infty}(I),
$$

we inductively construct two sequences of cost functional $J_n$ and function $a_n \in A, n = 1, \cdots, N$, as follows. For each $n$, if $a_0, a_1, \cdots, a_{n-1} \in A$ are given, we introduce the cost functional

$$
J_n(a) = \frac{1}{2} \|a - a_{n-1}\|_{L^2(I)}^2 + \frac{1}{2} \|\nabla a\|_{L^2(I)}^2 + \frac{1}{2\bar{a}} \|u(\cdot, t_n; a) - g(\cdot, t_n)\|_{L^2(I)}^2 \quad (20)
$$

for $a \in A$, where $u(x,t;a)$ is the solution of (15)-(17) in $[0,t_n]$ corresponding to coefficient

$$
\tilde{a} = \begin{cases}
\frac{t-t_{n-1}}{h}a(x) + \frac{t_n-t}{h}a_{n-1}(x) & t_{n-1} \leq t \leq t_n \\
\frac{t-t_{k-1}}{h}a_k(x) + \frac{t_n-t_k}{h}a_{k-1}(x) & t_{k-1} \leq t \leq t_k, 1 \leq k \leq n-1
\end{cases} \quad (21)
$$

and $\sigma > 0$ is a regularization parameter.

We now introduce the following optimal control problem

**Problem $P_n$** Assume that $a_0, a_1, \cdots, a_{n-1} \in A$ are known. Find an $a_n \in A$ such that

$$
J_n(a_n) = \inf_{a \in A} J_n(a)
$$

Such an $a_n$, if it exists, is called an optimal control of semi-discrete optimal control problem $P_n$.

It is easily seen that $J_n(a)$ is a non-negative lower semi-continuous functional and the admissible set $A$ is a convex bounded set in Hölder space, $C^{0,\frac{1}{2}}(I)$. Based on the state analysis, we can establish the existence for the above optimal control problem.

**Theorem 2.1** Problem $P_n$ admits an optimal control, $a_n \in A$.
The proof of this theorem is available in [8].

From this theorem, the functions $a_0, a_1, \cdots, a_N \in A$ are well defined when $a_0 \in A$ is given. Let, for $(x, t) \in \bar{Q}$,

$$a^h(x, t) = \frac{t - t_{n-1}}{h} a_n(x) + \frac{t_n - t}{h} a_{n-1}(x), \quad t_{n-1} \leq t \leq t_n, \quad n = 1, \cdots, N.$$  

It is easy to see that $a^h \in C^{1,1}$ from its definition. $a^h(x, t)$ is called the discrete reconstruction of unknown coefficient. Then recovering the unknown coefficient is reduced to finding the sequence of optimal control and investigating the behavior of the sequence of optimal control and the discrete reconstruction $a^h(x, t)$ as $h \to 0$.

Now we derive the necessary condition for the optimal control problem $P_n$. The proof of the following theorem is in [12].

**Theorem 2.2** Assume that $a_0 \in A$ are given. Let $a_n \in A$ be an optimal control of Problem $P_n$, $n = 1, \cdots, N$, and $u^h(x, t)$ be the solution of (15)-(17) in $[0, T]$ corresponding to coefficient $\tilde{a} = a^h(x, t)$. Then we have, for any $w \in A$

$$\int_I \left[ \frac{a_n - a_{n-1}}{h} (w - a_n) + \nabla a_n \cdot \nabla (w - a_n) + f_n(w - a_n) \right] dx \geq 0,$$

where

$$f_n(x) = \frac{1}{\sigma h} \int_{t_{n-1}}^{t_n} \frac{t - t_{n-1}}{h} \phi^h(x, t) u^h_{xx}(x, t) dt,$$

$$\phi^h(x, t) = \int_I G^h(y, t; x, t) (u^h(y, t_n) - g(y, t_n)) dy$$

and $G^h(y, \tau; x, t)$ is the Green function for operator

$$L^h = \frac{\partial}{\partial t} - a^h \frac{\partial^2}{\partial x^2} + b \frac{\partial}{\partial x} + c$$

in $Q$ with the homogeneous Neumann boundary condition.

3. Limiting equation, uniqueness and stability

We will derive uniform estimates for the sequence of discrete optimal controls $a_0, a_1, \cdots, a_N$ and the discrete reconstruction, $a^h(x, t)$, of unknown coefficient as $h \to 0$.

In [12], we obtain the following estimate.

**Theorem 3.1** There exists a constant $C$ such that

$$\|a^h\|_{C^{1,1}_{\frac{1}{2}}(\bar{Q})} \leq C.$$  

**Remark** The constants in theorem 3.1 is independent of $\|u_0\|_{C^{2+\alpha,1+\frac{\alpha}{2}}(I)}$, they depend only on $\|u_0\|_{H^1(I)}$.

We will discuss the limiting behavior of the discrete reconstruction, $a^h(x, t)$, of unknown coefficient as $h \to 0$. Let

$$\tilde{A} = \{ a(x, t) \mid a \leq a(x, t) \leq \tilde{a}, \quad a \in H^1(Q) \cap L^\infty([0, T], H^1(I)) \}.$$  

From the estimate in theorem 3.1 we have the following convergence results

**Theorem 3.2** There exist a subsequence of $a^h(x, t)$ and a function $a \in \tilde{A}$, such that

$$a^h \to a \text{ weakly in } H^1(Q), \quad a^h \to a \text{ in } C(\bar{Q})$$
\[ \bar{a}^h \to a \text{ in } L^2(Q), \quad \nabla \bar{a}^h \to \nabla a \text{ weakly in } L^2(Q), \]

where \( \bar{a}^h \) is defined for \((x,t) \in \tilde{Q} \)

\[ \bar{a}^h(x,t) = a_n(x), \quad t_{n-1} \leq t \leq t_n. \]  

(27)

Function \( a(x,t) = \lim_{h \to 0} a^h(x,t) \) is the recovering of the unknown coefficient. We call it the limiting optimal control of our problem. Now we derive the necessary condition for \( a(x,t) \).

**Theorem 3.3** Let \( a(x,t) \) be the limiting optimal control and \( u \) be the solution of the following problem

\[ Lu \equiv u_t - a(x,t)u_{xx} + b(x,t)u_x + c(x,t)u = f(x,t), \quad \text{in } Q \]  

(28)

\[ u_x = 0, \quad \text{on } \partial I \times (0,T] \]  

(29)

\[ u(x,0) = u_0(x), \quad x \in I \]  

(30)

Then, for any \( w \in \tilde{A} \), we have

\[ \int_{Q} \left[ a_t(w-a) + \nabla a \cdot \nabla (w-a) + \frac{1}{2\sigma}(u-g)u_{xx}(w-a) \right] dxdt \geq 0 \]  

(31)

\[ a(x,0) = a_0(x), \quad x \in I \]  

(32)

To prove the uniqueness and stability of the limiting optimal control \( a(x,t) \), we establish the following estimate.

**Theorem 3.4** Suppose that \( a_0(x), \bar{a}_0(x), g(x,t), \bar{g}(x,t) \) are given functions, \( a_0, \bar{a}_0 \in A \cap W^{1,\infty}(Q) \) and \( g, \bar{g} \) satisfy conditions (18). Let \( a(x,t), \bar{a}(x,t) \) be the limiting optimal controls corresponding to \( (g,a_0), (\bar{g},\bar{a}_0) \) respectively. Then there exists a constant \( C \) such that

\[ \|a - \bar{a}\|_{L^\infty(0,T],L^2(I))} + \|\nabla(a - \bar{a})\|_{L^2(Q)} \leq C\left(\|g - \bar{g}\|_{L^2(Q)} + \|a_0 - \bar{a}_0\|_{L^2(I)}\right) \]  

(33)

**Remark** Here constant \( C \) is depending on regularization parameter \( \sigma \). Hence the stability and closeness of the limiting optimal control depend on regularization parameter \( \sigma \).

**Corollary 3.5** Based on the uniqueness of the solution \( a(x,t) \), by theorem 3.2, we claim that the whole sequence \( \{a^h(x,t)\} \) defined by a linear interpolation of minimizers \( a_n(x) \) of optimal control problems \( P_h(n = 0, 1, \ldots, N) \) converges to the recovered coefficient \( a(x,t) \) uniformly on domain \( \tilde{Q} \).

As a conclusion of our contribution, let us summarize the main results as follows

**Main Theorem** Under assumptions (14), (18), \( u_0(x)|_{\partial I} = 0 \) and

\[ \underline{a} \leq a_0(x) \leq \bar{a}, \quad a_0(x) \in W^{1,\infty}(I), \]

the inverse problem \( P \) has a solution \( a(x,t) \) which satisfies

(1) \( \underline{a} \leq a(x,t) \leq \bar{a} \) and

\[ a(x,t) \in C^{\frac{1}{2},\frac{1}{4}}(\tilde{Q}) \cap H^1(Q) \cap L^\infty(0,T;H^1(I)). \]

(2) \( \{a(x,t), u(x,t)\} \) is the unique solution of the couple system of a parabolic equation (28) and a parabolic variational inequality (31) with initial and boundary values (29), (30) and (32).

(3) There exists a sequence \( \{a^h(x,t)\} \) which is defined by a linear interpolation of minimizers \( a_n(x) \) of optimal control problems \( P_h(n = 0, 1, \ldots, N) \), such that

\[ a^h \to a \text{ in } C(\tilde{Q}), \quad a^h \to a \text{ weakly in } H^1(Q). \]

(4) The procedure of recovering \( a(x,t) \) from a given function \( g(x,t) \) is stable in the sense of (33).
4. Numerical simulations

For the simplicity we discuss our problem with \( b(x, t) = 0, c(x, t) = 0 \). Let \( I = [0, 1] \), \( T = 1 \) and \( f(x, t) = \frac{10x^2 - 12x + 2}{(t+1)^2}[0.2 - (x^2 - x)^2]e^{\frac{1}{t+1}} \). Given the observation \( g(x, t) = [0.2 - (x^2 - x)^2]e^{\frac{1}{t+1}} \), we would then determine the exact coefficient \( \pi(x, t) = \frac{0.2 - (x^2 - x)^2}{t+1} \) from (13).

With \( a_0(x) = \pi(x, 0) \) and \( u_0(x) = g(x, 0) \), we can solve the fully nonlinear couple system (28)-(32) numerically to obtain the recovering coefficient \( a(x, t) \). The algorithm for solving PDEs is omitted. By comparing the computed coefficient \( a(x, t) \) with true coefficient \( \pi(x, t) \), we are able to justify the accuracy of our method.

In our numerical experiments, the basic parameters are: \( \sigma = 0.0001, a = 0.01, \pi = 0.5 \). Figure shows the results of the numerical experiments when \( t = 0.1, 0.2, 0.5 \) and \( t = 1 \) respectively. In figure, the solid line are the true coefficient \( \pi(x, t) \), and the dots are the computed coefficient \( a(x, t) \).

**Figure 1.** The coefficient as \( t = 0.1 \).

**Figure 2.** The coefficient as \( t = 0.2 \).

**Figure 3.** The coefficient as \( t = 0.5 \).

**Figure 4.** The coefficient as \( t = 1 \).
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