An Inverse Coefficient Problem in Adsorption Models

by

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Outline of this talk:

1. The Direct Problem of Adsorption

2. The Inverse Problem of Adsorption

3. Modified Direct Problem

4. Modified Inverse Problem

5. Numerical Algorithms

6. Examples

1. Direct Problem of Adsorption:

$$
\begin{aligned}
(u+a)_t + (c_1(x)u - D_1 u_x)_x &= 0, \\
a_t &= \gamma(\phi(x)u - a),
\end{aligned}
$$

for $0 \le x \le L,\ 0 \le t \le T$ subject to boundary and initial conditions

$$
\begin{aligned}
u(0,t) &= \mu(t),\ 0 \le t \le T \\
u(L,t) + \beta u_x(L,t) &= 0,\ 0 \le t \le T \\
u(x,0) &= 0,\ 0 \le x \le L \\
a(x,0) &= 0,\ 0 \le x \le L
\end{aligned}
$$

- $u(x,t)$, $a(x,t)$ are scaled concentrations of transported and adsorbed substance, resp.

- $c_1(x)$ is transport velocity, D_1 diffusion coefficient and β a positive flux coefficient.

- γ is a rate parameter and $\phi(x)$ a spatially varying adsorption property of the underlying medium.

$$
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$$

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u(x,0) &= 0,\ 0 \le x \le L \\
a(x,0) &= 0,\ 0 \le x \le L
\end{aligned}
$$

2. The Inverse Problem of Adsorption:

Given that $u(x,t)$ is a solution to the direct problem given by and *suitable* exact data, such as

$$g(x) = u(x,T),\ 0 \le x \le L,$$

to determine the coefficient function $\phi(x)$, $x \in [0, L]$.

3. Modified Direct Problem:

We omit the terms $c'(x)$ and u_t to obtain

(DP):

$$\begin{aligned} c_1(x)u_x + a_t &= D_1 u_{xx} && (1) \\ a_t &= \gamma(\phi(x)u - a) && (2) \end{aligned}$$

for $0 \le x \le L,\ 0 \le t \le T$ subject to boundary and initial conditions

$$\begin{aligned} u(0,t) &= \mu(t),\ 0 \le t \le T && (3) \\ u(L,t) + \beta u_x(L,t) &= 0,\ 0 \le t \le T && (4) \\ a(x,0) &= 0,\ 0 \le x \le L. && (5) \end{aligned}$$

The resulting inverse problem is

(IP): given that $u(x,t)$ is a solution to the direct problem given by (1)–(5), and exact data

$$g(x) = u(x,T),\ 0 \le x \le L, \qquad (6)$$

to determine coefficient function $\phi(x), x \in [0,L]$, given in (2).

Parameter Conditions:

1. $\phi \in C[0, L]$ and $\phi(x) > 0$ for $x \in [0, L]$.

2. $c_1(x) \in C[0, L]$.

3. The constants D_1, γ and β are positive.

4. $\mu \in C[0, L]$ and μ is non-negative on $[0, T]$.

5. $\mu \in C^1[0, L]$, $\mu(0) = 0$ and μ' is positive on $(0, T]$.

6. $\mu'(t) - \gamma \int_0^t e^{-\gamma(t-\tau)} \mu'(\tau)\, d\tau \geq 0$, for $0 \leq t \leq T$.

Theorem 1. Assume parameter conditions 1-4. Then direct problem (DP) has a unique non-negative solution $u(x, t)$, $a(x, t)$ with $u_x, u_{xx}, a_t \in C[Q_T]$ where $Q_T = [0, L] \times [0, T]$.

Discussion of proof:

Integrate (2) and use the initial condition (5) to obtain that for all $(x,t) \in Q_T$,

$$a(x,t) = \gamma\phi(x)\int_0^t e^{-\gamma(t-\tau)}u(x,\tau)\,d\tau. \tag{7}$$

If we substitute (2) and (7) into (1), we obtain the equation

$$c_1(x)u_x + \gamma\phi(x)u - \gamma^2\phi(x)\int_0^t e^{-\gamma(t-\tau)}u(x,\tau)\,d\tau = D_1u_{xx}.$$

Now let $c(x) = c_1(x)/D_1$ and $d = \gamma/D_1$, and this equation becomes

$$-u_{xx} + c(x)u_x + d\phi(x)u - \gamma d\phi(x)\int_0^t e^{-\gamma(t-\tau)}u(x,\tau)\,d\tau = 0. \tag{8}$$

It follows that the direct problem is equivalent to the problem (7), (8), (3) and (4). One can now exploit properties of this integro-differential equation to prove the existence, non-negativity and uniqueness claims of the theorem. □

For later reference, regarding a term in (8):

$$d\phi(x)u - \gamma d\phi(x) \int_0^t e^{-\gamma(t-\tau)} u(x,\tau)\, d\tau = d\phi(x) \int_0^t e^{-\gamma(t-\tau)} u_t(x,\tau)\, d\tau. \tag{9}$$

What do additional parameter conditions yield? Condition 5 yields a maximum principle:

Theorem 2. Assume parameter conditions 1-5. If u, a is a solution to the direct problem, then $u_t \in C[Q_T]$ and for $(x,t) \in Q_T$

$$\mu'(t)k(x) \leq u_t(x,t) \leq \max_{0 \leq t \leq T} \mu'(t),$$

where $k(x)$ is the solution to $-v'' + c(x)v' + d\phi(x)v = 0$ satisfying boundary conditions $k(0) = 1$ and $k(L) + \beta k'(L) = 0$.

Condition 6 yields a comparison principle:

Theorem 3. Assume parameter conditions 1-6. Let $u(x,t;\phi_i), a(x,t;\phi_i)$ be a solution to the direct problem corresponding to ϕ_i, $i = 1, 2$. If $\phi_1(x) \leq \phi_2(x)$ for $x \in [0, L]$, then $u_t(x,t;\phi_1) \geq u_t(x,t;\phi_2)$ for $(x,t) \in Q_T$.

4. Modified Inverse Problem:

(IP) Given that $u(x,t)$ is a solution to the direct problem given by (1)–(5), and exact data

$$g(x) = u(x,T),\ 0 \leq x \leq L, \qquad (10)$$

to determine the coefficient function $\phi(x)$, $x \in [0, L]$, given in (2). We make these assumptions.

Data Conditions:

1. $g(x) \in C^2[0, L]$ and $g(x)$ is a positive function.

2. $g(0) = \mu(T)$ and $g(L) + \beta g'(L) = 0$.

3. $g''(x) - c(x)g'(x) \in C[0, L]$ and is a positive function on $[0, L]$.

We can see an approach to solving this problem by substituting $g(x)$ into (8), then solving this equation for $\phi(x)$ and use (9). Next anticipate a fixed point argument by defining and using the formula for $\phi(x)$ to define a nonlinear operator

$$\phi = A\phi \equiv \frac{g''(x) - c(x)g'(x)}{d\int_0^T e^{-\gamma(T-\tau)} u_t(x,\tau;\phi)\,d\tau}, \tag{11}$$

Certainly $\phi(x)$ is a solution to the equation $A\phi = \phi$, i.e., a fixed point of A. Conversely, if $\widetilde{\phi}$ is a fixed point of A,

$$g''(x)-c(x)g'(x) = d\int_0^T e^{-\gamma(T-\tau)} u_t(x,\tau;\phi)\,d\tau = u_{xx}(x,T;\widetilde{\phi})-c(x)u_x(x,T;\widetilde{\phi}).$$

Since both $g(x)$ and $u(x,T;\widetilde{\phi})$ satisfy the same boundary conditions, $g(x) = u(x,T;\widetilde{\phi})$ so that $\widetilde{\phi}(x)$ is a solution to the inverse problem.

It follows from Theorem 2 that for a positive $\phi(x)$,

$$A\phi = \frac{g''(x) - c(x)g'(x)}{d\int_0^T e^{-\gamma(T-\tau)} u_t(x,\tau;\phi)\, d\tau} \geq \frac{g''(x) - c(x)g'(x)}{d\int_0^T e^{-\gamma(T-\tau)} \mu_M \, d\tau} \equiv h(x) \tag{12}$$

where $\mu_M = \max_{0 \leq t \leq T} \mu'(t)$. We define

$$E = \{\phi(x) \in C[0, L] \,|\, \phi(x) \geq h(x),\ x \in [0, L]\}.$$

Then $E \subset P$, the set of positive functions in $C[0, L]$. Throughout the following, we use the uniform norms $\|\cdot\|$ in $C[0, L]$ and $C[Q_T]$. The operator A is said to be *monotone* if, for functions $\phi(x)$ and $\Psi(x)$ in the domain of A with $\phi(x) \leq \Psi(x)$ for $x \in [0, L]$, we have $A\phi(x) \leq A\Psi(x)$ for $x \in [0, L]$. Operator A is *compact* if it is continuous and maps bounded sets into precompact sets. A well known theorem asserts that if the operator A is monotone and compact, and operator A maps the non-empty order interval $[u_0, u^0] = \{u \,|\, u_0 \leq u \leq u^0\}$ into itself, then the sequences of iterates $\{A^n u_0\}$ or $\{A^n u^0\}$ converge to fixed points of A.

With this terminology we can show

Theorem 4. The operator $A : P \to E$ given by (11) is a continuous and monotone operator which maps bounded sets into equicontinuous sets.

Theorem 4 is used to show the key theorem for the existence of solutions to (IP).

Theorem 5. If parameter conditions 2-6 and data conditions 1-3 are satisfied, then a necessary and sufficient condition for the inverse problem (IP) to have a solution is that there exist a positive function $\phi_0(x) \in C[0, L]$ for which $A\phi_0(x) \leq \phi_0(x)$, $0 \leq x \leq L$.

Discussion of proof:

If (IP) has a solution $\phi(x)$, we have already that $A\phi = \phi$, so take $\phi_0 = \phi$.

Conversely, suppose that positive continuous function $\phi_0(x)$ satisfies the inequality $A\phi_0(x) \leq \phi_0(x)$. By (12) we have that for any positive $\phi(x)$ and $x \in [0, L]$, $h(x) \leq A\phi(x)$. Consequently, the monotonicity of A implies that A maps the order interval

$$I = \{\phi(x) \in C[0, L] \,|\, h(x) \leq \phi(x) \leq \phi_0(x),\, 0 \leq x \leq L\}$$

into itself. By Theorem 4 the operator $A : I \to I$ is a monotone compact operator. It follows that the sequence of iterates $\phi_0, A\phi_0, A^2\phi_0, \ldots$ converges to a fixed point ϕ of A, which as we have seen in the introduction of this section, must satisfy $u(x, T; \phi) = g(x)$, $0 \leq x \leq L$.

A computationally useful fact:

Corollary 1. If the inverse problem (IP) has a solution, then the sequence of iterates h, Ah, A^2h, $\ldots$ converges to a solution of (IP).

Remark. One can construct functions $\phi_n(x)$ such that $u_n(x, T) = u(x, T; \phi_n)$ converge to $u_0(x, t) = u(x, t; \phi_0)$ uniformly on $[0, L]$, yet $\|\phi_n - \phi_0\| = n$ tends to ∞ with n. Thus the inverse problem (IP) is not stable.

5. Numerical Algorithms:

BVP algorithm: for the system defined on Q_T

$$-u_{xx}+p(x)u_x+q(x)u-\gamma q(x)\int_0^t e^{-\gamma(t-\tau)}u(x,\tau)\,d\tau = F(x,t) \tag{13}$$

$$u(0,t) = \mu(t),\ 0 \le t \le T \tag{14}$$

$$u(L,t)+\beta u_x(L,t) = 0,\ 0 \le t \le T \tag{15}$$

define

$$U(x,t) = \int_0^t e^{-\gamma(t-\tau)}u(x,\tau)\,d\tau. \tag{16}$$

Let $\Delta x = L/M$ and $\Delta t = T/N$ be step sizes in x and t to be used in the discretization of this problem, where M and N are positive integers. We view (13) and (16) as an evolutionary system in the unknowns u and U. The evolutionary aspect of U is made clearer by the observation that

$$\begin{aligned} U(x,t) &= \int_0^{t-\Delta t} e^{-\gamma(t-\tau)}u(x,\tau)d\tau + \int_{t-\Delta t}^t e^{-\gamma(t-\tau)}u(x,\tau)d\tau \qquad (17) \\ &= e^{-\gamma\Delta t}U(x,t-\Delta t) + \int_{t-\Delta t}^t e^{-\gamma(t-\tau)}u(x,\tau)\,d\tau. \end{aligned}$$

Set $t_n = n\Delta t$, $n = 1, 2, \ldots N$ and $x_k = k\Delta x$, $k = 1, 2, \ldots M$. Define $p_k = p(k\Delta x)$, $q_k = q(k\Delta x)$, $\mu_n = \mu(n\Delta t)$, $F_{k,n} = F(k\Delta x, n\Delta t)$, $u_{k,n} \approx u(x_k, t_n) = u(k\Delta x, n\Delta t)$ and $U_{k,n} \approx U(x_k, t_n) = U(k\Delta x, n\Delta t)$ Use centered first and second differences to discretize (13) and a trapezoidal method to discretize (17). We obtain

$$-\left(1 + p_k \frac{\Delta x}{2}\right) u_{k-1,n} + \left\{2 + (\Delta x)^2 q_k \left(1 - \frac{\gamma \Delta t}{2}\right)\right\} u_{k,n} - \left(1 - p_k \frac{\Delta x}{2}\right) u_{k+1,n} =$$

$$(\Delta x)^2 \left\{F_{k,n} + \gamma e^{-\gamma \Delta t} q_k \left(U_{k,n-1} + \frac{\Delta t}{2} u_{k,n-1}\right)\right\}. \tag{18}$$

$$U_{k,n} = e^{-\gamma \Delta t} U_{k,n-1} + \frac{\Delta t}{2} e^{-\gamma \Delta t} \left(u_{k,n-1} + u_{k,n}\right). \tag{19}$$

These equations account for the interior nodes (x_k, t_n), $k = 1, \ldots, M$ and $n = 1, 2, \ldots N$. Use boundary conditions to eliminate terms $u_{0,n}$ and $u_{M+1,n}$. Problem (13)-(15) is now solved by single step marching method, which is explicit in time and implicit in space: given U, u at $(n-1)$-th time level, solve the linear system (18) for values of u at the n-th level, then use (19) to solve explicitly for U at the n-th level.

Remark. Impose the stability restrictions $\Delta t < 2/\gamma$ and $\Delta x < 2/\|p\|$, and the BVP algorithm converges to the solution with truncation errors in even powers of the step sizes, so that it is second order in step sizes. Therefore, the algorithm can be computed at step and half step sizes, followed by a single step of Richardson extrapolation to yield a fourth order method.

Discretization of operator A: Recall that $A\phi = \frac{g''(x)-c(x)g'(x)}{d\int_0^T e^{-\gamma(T-\tau)}u_t(x,\tau;\phi)\,d\tau}$. Assume exact data. First, discretize the data function g and argument function ϕ via $g_k = g(k\Delta x)$, $k = 0, 1, \ldots M+1$, and $\phi_k = \phi(k\Delta x)$, $k = 1, 2, \ldots, M$. We can differentiate equation (13) to obtain that $v(x,t) = u_t(x,t)$ also satisfies such an equation, together with boundary conditions $v(0,t) = \mu'(t)$ and $v(L,t) + \beta v_x(L,t) = 0$, so that the function $V(x,t) =) \int_0^t e^{-\gamma(t-\tau)}u_t(x,\tau)\,d\tau$ can be approximated by the output of the BVP algorithm, applied to $v(x,t)$, resulting in approximate node values $V_{k,N}$.

Given an argument $\Phi = (\phi_1, \ldots, \phi_M)$, the discretized operator is given by

$$(A_M \Phi)_k = \frac{(1 + c_k \frac{\Delta x}{2}) g_{k-1} - 2g_k + (1 - c_k \frac{\Delta x}{2}) g_{k+1}}{dV_{k,N} (\Delta x)^2} \tag{20}$$

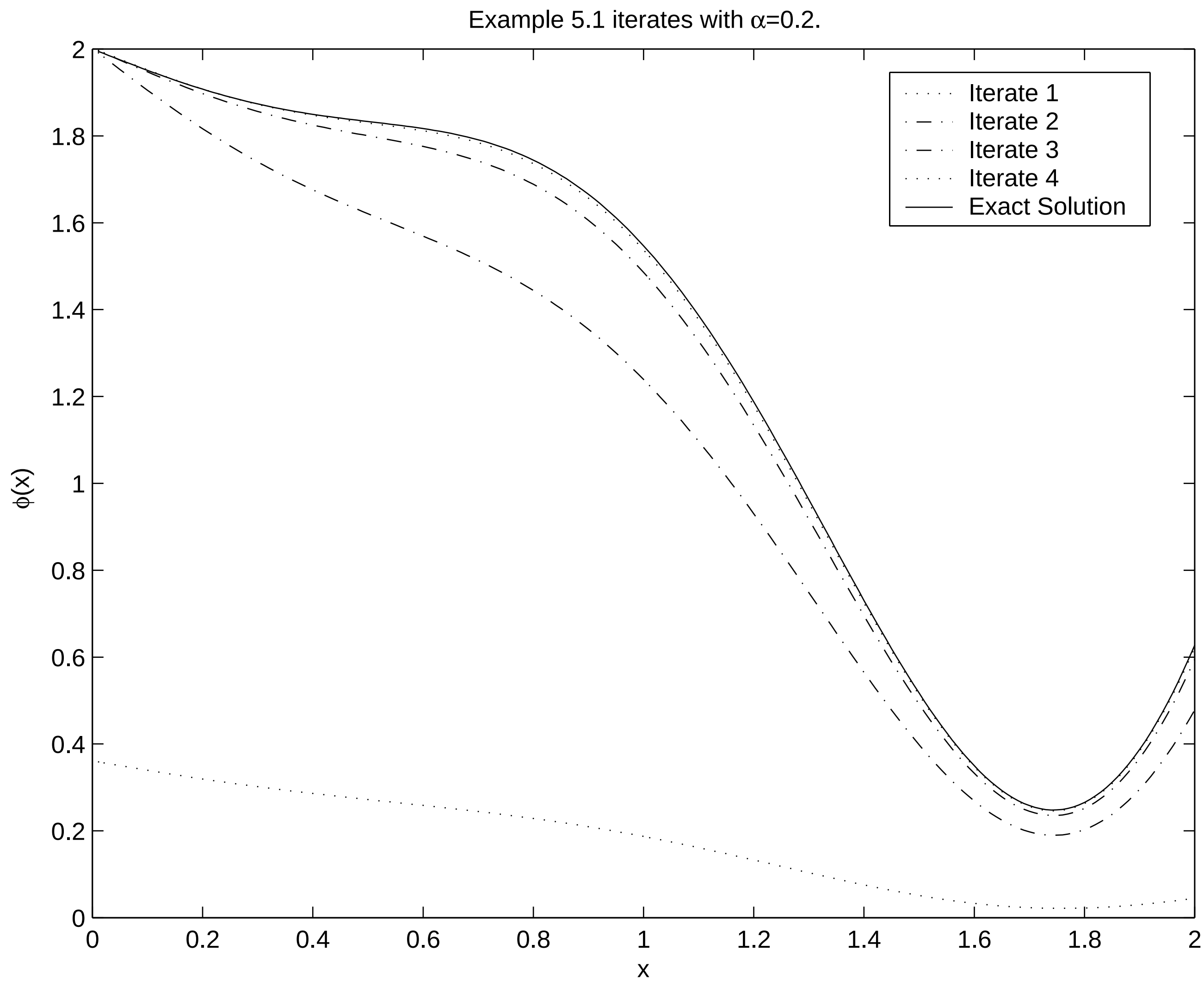
which is valid for $k = 1, 2, \ldots M$. This requires a value for g_{M+1}, g_0, which are determined by the boundary conditions.

Algorithm for (IP): Use Corollary 1 to devise a simple method, which we term the IP algorithm, for computing the solution to the inverse problem; let the initial guess Φ_0 be the discretization of $h(x)$ as defined in (12). Then use fixed point iteration of (20) until convergence.

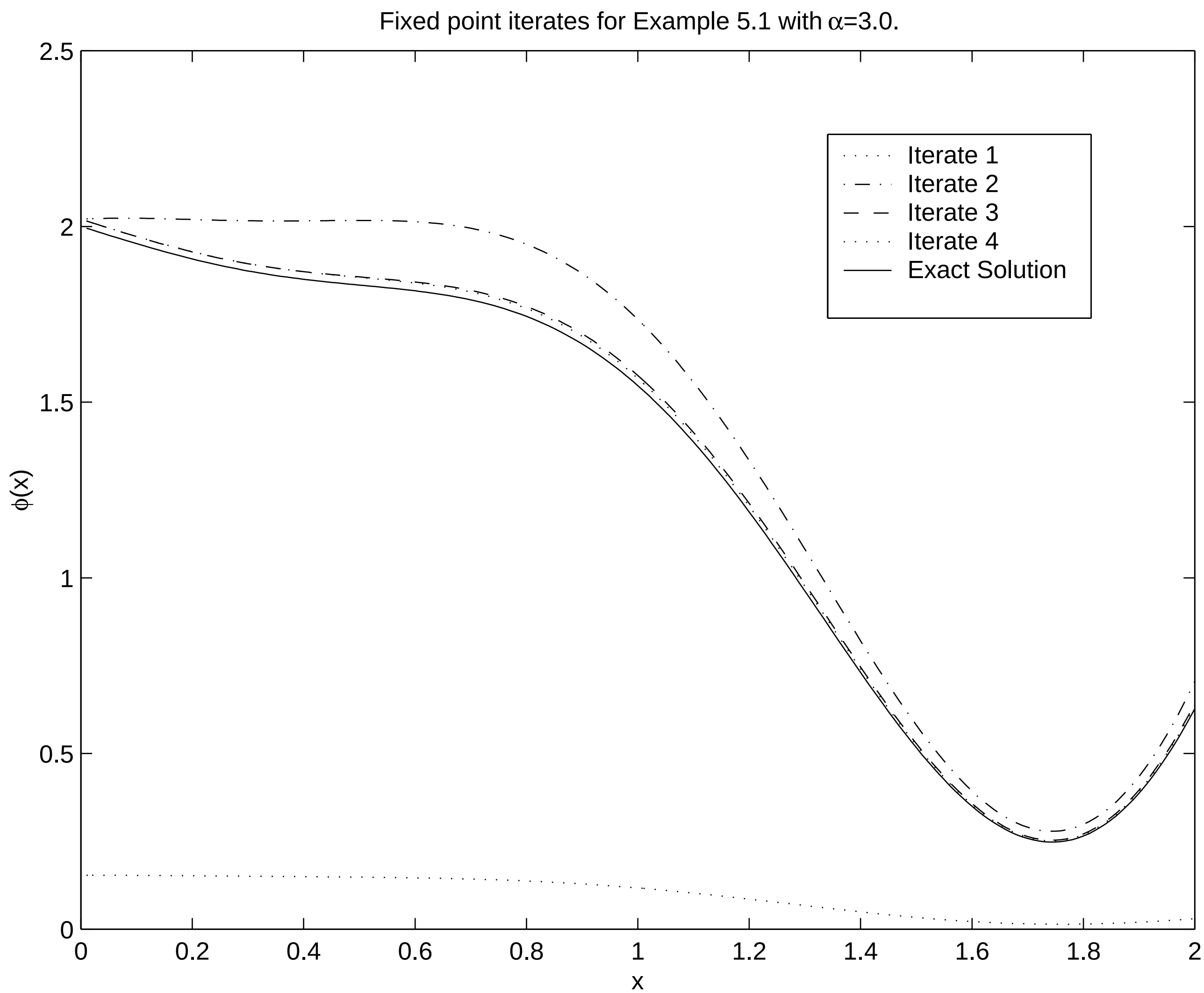
6. Examples:

1. Let $L = 2$, $T = 2$, $\gamma = \beta = 1$, $c(x) = 1 + \cos(3x)/3$, $\phi(x) = 2 - x/2 + x^2 \sin(3x)/3$ and $\mu(t) = (1 - e^{-\alpha t})/\alpha$, where $\alpha > 0$. Parameter conditions 2-5 are satisfied. Parameter condition 6 is satisfied if $\alpha_0 < 0.2031$. We set $\alpha = 0.2$ and $\Delta x = \Delta t = 0.01$. Use the extrapolated BVP algorithm to obtain the data function $g(x)$ to a higher order of accuracy than the expected accuracy of solution to the inverse problem. Then use IP algorithm in tandem with unextrapolated BVP to compute the solution to this inverse problem.

Here the initial guess for $\phi(x)$ is the function $\phi_0(x) = h(x)$ of (12). We see an approximately linear rate of convergence until about the fifth iteration, where the discretization error causes fixed point iteration to stall.



At the fourth iteration, the norm of the error is $\|g - \phi_4\| \doteq 0.0021$. The monotone behavior of the operator A is evident. When we halved both Δx and Δt, the final error was decreased by a factor of about four, confirming that the BVP algorithm is second order accurate.



Parameter condition 6, $\mu'(t) - \gamma \int_0^t e^{-\gamma(t-\tau)} \mu'(\tau)\, d\tau \geq 0$, for $0 \leq t \leq T$, fails for $\alpha = 3$. We see from the picture that this condition is really needed for the monotone property of A.

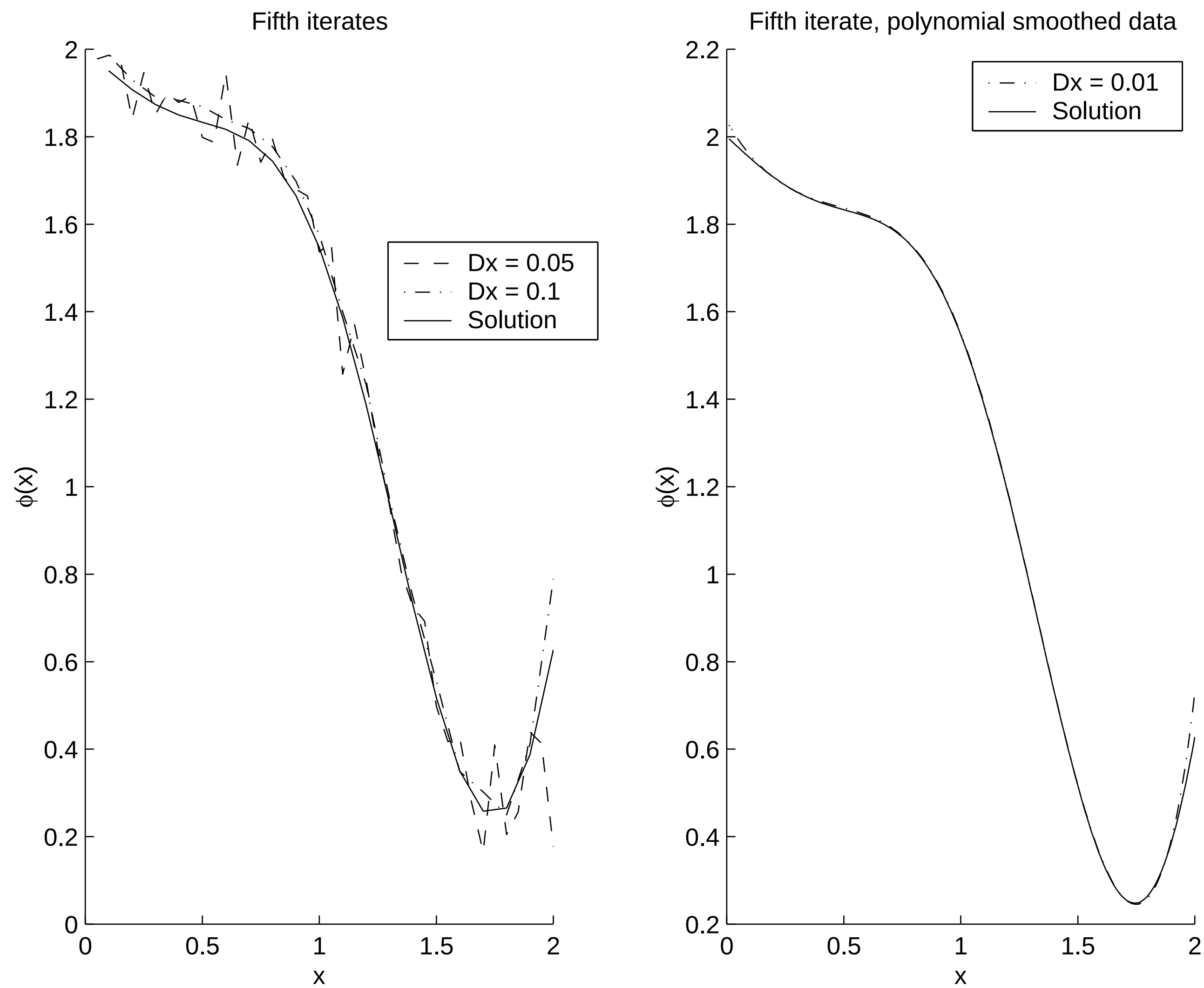
2. Effect of noise. These effects are strong. Since operator A is compact, one needs a regularization strategy. Discretization of the definition (11) of A by way of (20) is itself a regularization strategy with regularization parameter Δx. Since the operator A is nonlinear, an exact analysis of the error is difficult; however, one expects that the principal source of difficulty is in the discretization of the numerator in (11). A simple Taylor series analysis shows that if the noise level is bounded by δ, then the discretization error is bounded by a function of the form

$$\frac{\delta}{(\Delta x)^2} + \frac{c_1 \delta}{\Delta x} + c_2 (\Delta x)^2$$

for suitable constants c_1, c_2 depending on $c(x)$ and the second and third derivatives of u_t and $c(x)$. This expression is minimized (to leading order in Δx) at $\Delta x = (c_2 \delta)^{1/4}$, which provides a regularization strategy. Alternately, one could use Tikhonov regularization on the operator equation $\varphi = A\phi$. This would alter the form of our calculations significantly. Or one could use some sort of smoothing or filtration of the data in the discretization we employ in (20).

A simple approach is to do a least squares fit of the data points to a polynomial of some degree.

Use the same parameters as in Example 1, calculate the data “exactly” using a higher accuracy calculation, and then add noise. The noise is random and uniformly distributed on the interval $[-\delta/2, \delta/2]$. We took $\delta = 0.0001$. In view of the discussion preceding this example, one expects the optimum regularization parameter to be $\Delta x \approx 0.1$. Since we are lacking *a priori* derivative information, trial and error will suggest an optimal value. Computations for $\Delta x = 0.05$ and $\Delta x = 0.1$ are illustrated, along with the exact solution. To compare, we smoothed the data by doing a least squares fit of a tenth degree polynomial to it, then applied IP algorithm with $\Delta x = 0.01$. The plotted result clearly indicates that polynomial smoothing is a superior regularization for (IP).



($\Delta x = 0.01$ was too bad to be put in the first graph.)

Current Research:

We are continuing research on the general Direct and Inverse Problems. Our analysis of (DP) and (IP) have important connections to the general problems.

To see why, we note that much of our analysis carries through if a source term $f(x,t)$ is placed on the right hand side of (1). Introduce a time derivative for u in (DP) to obtain

$$\begin{aligned} -D_1 u_{xx} + c_1(x) u_x + a_t &= -u_t \\ a_t &= \gamma(\phi(x)u - a) \end{aligned}$$

The corresponding operator for the inverse problem is

$$\phi = A\phi \equiv \frac{g''(x) - c(x)g'(x) - u_t(x,T;\phi)}{d\int_0^T e^{-\gamma(T-\tau)} u_t(x,\tau;\phi)\, d\tau}$$

These forms naturally suggest "Kacănov" type iteration schemes for deriving solution to the direct problem and fixed point iteration for the inverse problem.