

Adjoint based parameter recovery

*or: the beauty of
Integration by Parts*

Roger Thelwell

Department of Applied Math
University of Washington

thelwell@amath.washington.edu

Acknowledgments

This work is in collaboration with

- *Paul DuChateau* (Colorado State), and

the *National Science Foundation* is acknowledged for its support (DUE-0324175 and 0221595).

Outline

- Introduction
- Why?
- Adjoint Theory
- Some numerics
- Conclusions

Apology

We'd like to study the Richards Equation:

$$C(h)\partial_t h = \partial_x(K(h)(\partial_x h - 1))$$

where $C(h)$ is soil capacity and $K(h)$ is hydraulic conductivity. But...

Apology

We'd like to study the Richards Equation:

$$C(h)\partial_t h = \partial_x(K(h)(\partial_x h - 1))$$

where $C(h)$ is soil capacity and $K(h)$ is hydraulic conductivity. But...

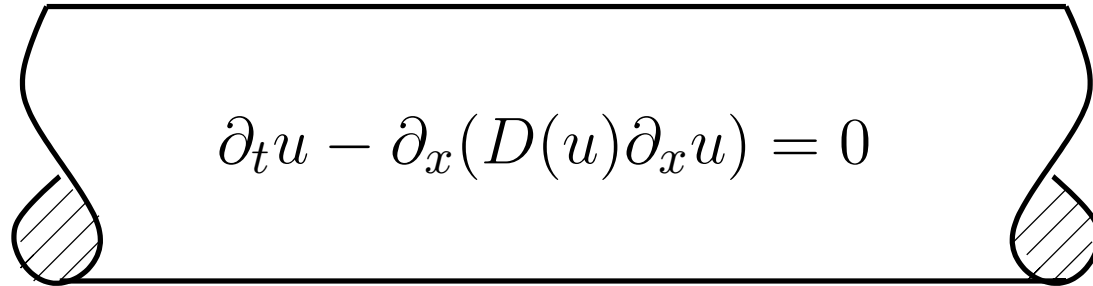
we'll consider the simpler problem

$$\partial_t u = \partial_x(D(u)\partial_x u),$$

which captures many details of the method.

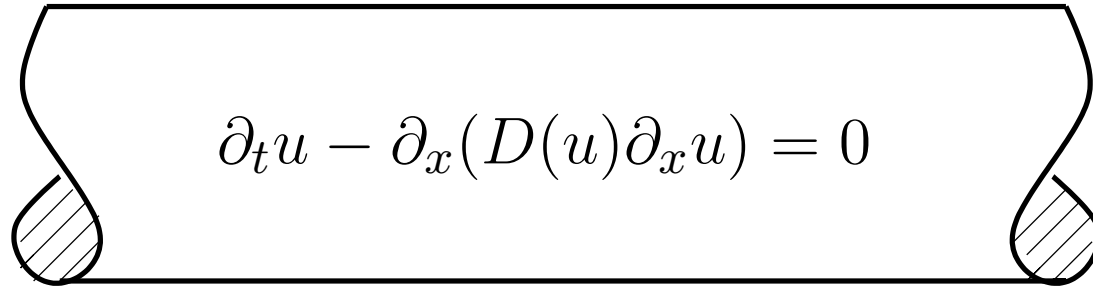
Introduction

The physical set-up

A diagram of a scroll, representing a physical domain. The scroll is a horizontal rectangle with curved ends on the top and bottom. The top and bottom edges are slightly curved inward. The two ends of the scroll are curled up, and the inner surface of these curls is shaded with diagonal lines. In the center of the scroll, the following partial differential equation is written:
$$\partial_t u - \partial_x (D(u) \partial_x u) = 0$$

Introduction

The physical set-up

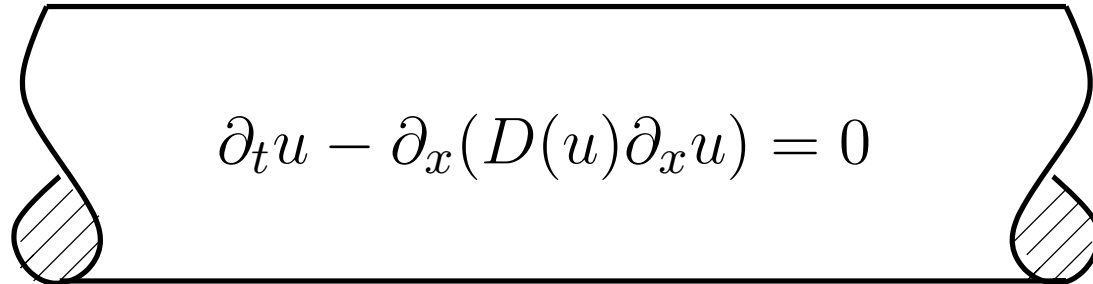


$$u(0, t) = f(t)$$

$$\partial_x u(1, t) = 0$$

Introduction

The physical set-up



$$u(0, t) = f(t)$$

$$\partial_x u(1, t) = 0$$

GOAL:

Given some output measurements of this system, recover $D(u)$.

Introduction

Sufficient conditions ensure existence and uniqueness of solution:

Introduction

Sufficient conditions ensure existence and uniqueness of solution:

- Take $D(u)$ strictly positive, Lipschitz over $(0,1)$, and bounded.
- Take $f(t) \in \mathcal{C}^1$ and $f'(t) > 0$

Introduction

Sufficient conditions ensure existence and uniqueness of solution:

- Take $D(u)$ strictly positive, Lipschitz over $(0,1)$, and bounded.
- Take $f(t) \in \mathcal{C}^1$ and $f'(t) > 0$

Let W represent this class of functions.

Why??

- Why not direct inversion?

Why??

- Why not direct inversion?
- Why not OLS?

Why??

- Why not direct inversion?
- Why not OLS?
- Why the toy problem?

Why??

- Why not direct inversion?
- Why not OLS?
- Why the toy problem?
- Why adjoint methods?

Forward

The (Forward) Problem: Given $D(u)$ and $f(t)$, find u which satisfies:

$$\partial_t u - \partial_x(D(u)\partial_x u) = 0 \quad (x, t) \in U_T$$

$$u(0, t) = f(t) \quad t \in (0, T)$$

$$\partial_x u(1, t) = 0 \quad t \in (0, T)$$

$$u(x, 0) = f(0) \quad x \in (0, 1)$$

Forward

The (Forward) Problem: Given $D(u)$ and $f(t)$, find u which satisfies:

$$\partial_t u - \partial_x(D(u)\partial_x u) = 0 \quad (x, t) \in U_T$$

$$u(0, t) = f(t) \quad t \in (0, T)$$

$$\partial_x u(1, t) = 0 \quad t \in (0, T)$$

$$u(x, 0) = f(0) \quad x \in (0, 1)$$

Why?

Forward

The (Forward) Problem: Given $D(u)$ and $f(t)$, find u which satisfies:

$$\begin{aligned}\partial_t u - \partial_x(D(u)\partial_x u) &= 0 & (x, t) \in U_T \\ u(0, t) &= f(t) & t \in (0, T) \\ \partial_x u(1, t) &= 0 & t \in (0, T) \\ u(x, 0) &= f(0) & x \in (0, 1)\end{aligned}$$

Why?

- Unique weak (forward) solution if D and f from W .
- Model of a simple physical process.
- Measurements of flux at $x = 0$ and state at $x = 1$ possible.

Inverse

The (Inverse) Problem: Given boundary measurements $g(t)$ and $h(t)$, recover $D(u)$ which satisfies:

$$\begin{aligned}\partial_t u - \partial_x(D(u)\partial_x u) &= 0 & (x, t) \in U_T \\ -D(u)\partial_x u(0, t) &= g(t) & t \in (0, T) \\ u(1, t) &= h(t) & t \in (0, T) \\ u(x, 0) &= f(0) & x \in (0, 1)\end{aligned}$$

Inverse

The (Inverse) Problem: Given boundary measurements $g(t)$ and $h(t)$, recover $D(u)$ which satisfies:

$$\begin{aligned}\partial_t u - \partial_x(D(u)\partial_x u) &= 0 & (x, t) \in U_T \\ -D(u)\partial_x u(0, t) &= g(t) & t \in (0, T) \\ u(1, t) &= h(t) & t \in (0, T) \\ u(x, 0) &= f(0) & x \in (0, 1)\end{aligned}$$

Why?

Inverse

The (Inverse) Problem: Given boundary measurements $g(t)$ and $h(t)$, recover $D(u)$ which satisfies:

$$\begin{aligned}\partial_t u - \partial_x(D(u)\partial_x u) &= 0 & (x, t) \in U_T \\ -D(u)\partial_x u(0, t) &= g(t) & t \in (0, T) \\ u(1, t) &= h(t) & t \in (0, T) \\ u(x, 0) &= f(0) & x \in (0, 1)\end{aligned}$$

Why?

- Experimental interest.
- Simple measurements.
- If we can recover a D from W , it should be unique.

Adjoint

Max Min Statement

- for each t , $f(0) < u(x, t) < f(t)$, $0 < x < 1$
- $\partial_x u(x, t) < 0$ a.e. on $(0, 1) \times (0, T)$

Adjoint

Max Min Statement

- for each t , $f(0) < u(x, t) < f(t)$, $0 < x < 1$
- $\partial_x u(x, t) < 0$ a.e. on $(0, 1) \times (0, T)$

An adjoint exercise yields the proof.

Adjoint

Max Min Statement

- for each t , $f(0) < u(x, t) < f(t)$, $0 < x < 1$
- $\partial_x u(x, t) < 0$ a.e. on $(0, 1) \times (0, T)$

An adjoint exercise yields the proof.

Comments:

If we let $B(u) = \int_0^u D(s) ds$, then $D(u)\partial_x u = \partial_x B(u)$.

Also, $B(u) = \int_0^u D(s) ds = (u - 0) D(\tilde{u})$ for some \tilde{u} between u and 0.

Adjoint

Again, let $g(t) := -D(u(0, t))\partial_x u(0, t)$ and $\Phi[D, f] = g(t)$.

We can show that if $D_1(u) > D_2(u)$ then the map Φ is:

- Monotone : $\Phi[D_1, f](t) > \Phi[D_2, f](t)$

These results are easy using an integral identity.

Adjoint

Again, let $g(t) := -D(u(0, t))\partial_x u(0, t)$ and $\Phi[D, f] = g(t)$.

We can show that if $D_1(u) > D_2(u)$ then the map Φ is:

- Monotone : $\Phi[D_1, f](t) > \Phi[D_2, f](t)$
- Continuous: $\|g_1 - g_2\|_{L^2(0, T)} \leq C \|D_1 - D_2\|_{\infty}$

These results are easy using an integral identity.

Adjoint

Again, let $g(t) := -D(u(0, t))\partial_x u(0, t)$ and $\Phi[D, f] = g(t)$.

We can show that if $D_1(u) > D_2(u)$ then the map Φ is:

- Monotone : $\Phi[D_1, f](t) > \Phi[D_2, f](t)$
- Continuous: $\|g_1 - g_2\|_{L^2(0, T)} \leq C \|D_1 - D_2\|_\infty$
- Injective : $\Phi[D_1, f] = \Phi[D_2, f]$ implies $D_1 = D_2$

These results are easy using an integral identity.

Adjoint

Integral Identity:

Let u, v represent solutions to direct problem with $D = D_1, D_2$, respectively. Subtract, multiply by smooth ϕ and integrate by parts to yield:

$$\begin{aligned} & \iint_{U_T} (u - v)(\phi_t + k\phi_{xx}) - \int_0^1 (u - v)\phi \Big|_{t=0}^{t=T} + \\ & + \int_0^T (D_1(u)u_x - D_2(v)v_x)\phi \Big|_{x=0}^{x=1} + \int_0^T (D_1(u) - D_1(v))(k\phi_x) \Big|_{x=0}^{x=1} \\ & = \iint_{U_T} (D_1(v) - D_2(v))v_x\phi_x \end{aligned}$$

Here $U_T = (0, 1) \times (0, T)$ and $k := D(\tilde{u})$ for some \tilde{u} in the interval (v, u)

Adjoint

The general adjoint problem:

$$\begin{aligned}\partial_t \phi + k \partial_{xx} \phi &= F^*(x, t) & (x, t) \in U_T \\ \phi(x, T) &= p^*(x) & x \in (0, 1) \\ k \phi_x &= g^*(t) & x = 0, t \in (0, T). \\ \phi &= h^*(t) & x = 1, t \in (0, T)\end{aligned}$$

Here $k := D(\tilde{u})$ for some \tilde{u} in the interval (v, u)

Adjoint

The dual data acts like switches. Data appears in a duality pairing with terms of the direct problem.

Taking $F^* = 0, p^* = 0, h^* = 0$, the identity collapses to

$$\int_0^T g^*(g_1 - g_2) = \iint_{U_T} (D_1(v) - D_2(v))v_x \phi_x$$

Adjoint

Letting $\Phi[D, f] = g(t)$, we could cast this formally as:

$$\begin{aligned} (\Phi[D_1, f] - \Phi[D_2, f], \theta)_{L^2} &:= (\delta\Phi[D_1, D_2]\Delta D, \theta)_{L^2} \\ &= \langle \Delta D, {}^t\delta\Phi[D_1, D_2] \theta \rangle_{W \times W^*} \end{aligned}$$

Adjoint

Letting $\Phi[D, f] = g(t)$, we could cast this formally as:

$$\begin{aligned} (\Phi[D_1, f] - \Phi[D_2, f], \theta)_{L^2} &:= (\delta\Phi[D_1, D_2]\Delta D, \theta)_{L^2} \\ &= \langle \Delta D, {}^t\delta\Phi[D_1, D_2] \theta \rangle_{W \times W^*} \end{aligned}$$

The integral identity provides a realization of this expression.

$$\int_0^T g^*(g_1 - g_2) = \iint_{U_T} (D_1(v) - D_2(v))v_x \phi_x$$

Adjoint

Now some quick proofs:

$$\int_0^T g^*(g_1 - g_2) dt = \iint_{U_T} (D_1(v) - D_2(v)) v_x \phi_x dx dt$$

- **Monotone:** Assume $D_1 > D_2$. We know $v_x < 0$. Taking $g^* > 0$ implies $\phi_x < 0$. **So** $g_1(t) > g_2(t)$.

Adjoint

Now some quick proofs:

$$\int_0^T g^*(g_1 - g_2) dt = \iint_{U_T} (D_1(v) - D_2(v)) v_x \phi_x dx dt$$

- **Monotone:** Assume $D_1 > D_2$. We know $v_x < 0$. Taking $g^* > 0$ implies $\phi_x < 0$. So $g_1(t) > g_2(t)$.
- **Continuous:** Take $g^* = (g_1 - g_2) / \|g_1 - g_2\|_{L^2}$.

Adjoint

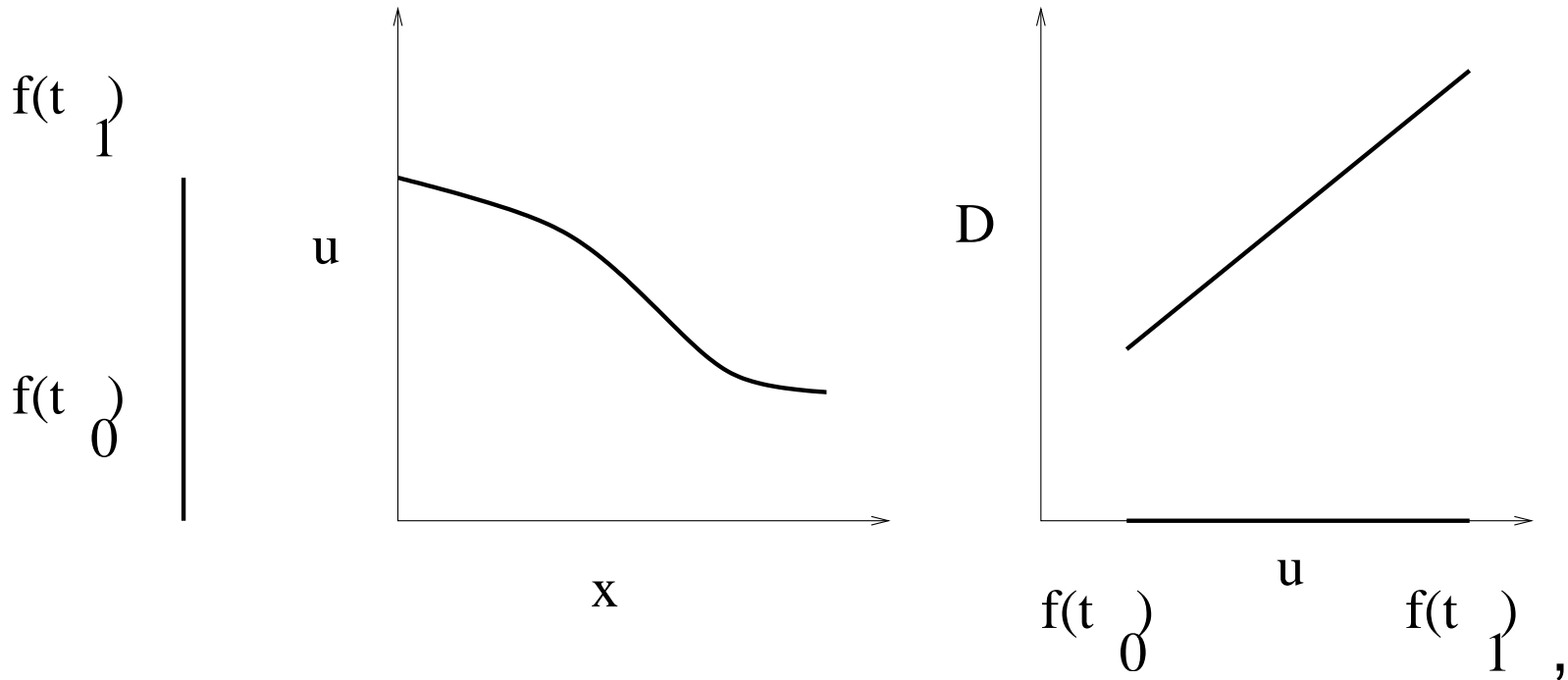
Now some quick proofs:

$$\int_0^T g^*(g_1 - g_2) dt = \iint_{U_T} (D_1(v) - D_2(v)) v_x \phi_x dx dt$$

- **Monotone:** Assume $D_1 > D_2$. We know $v_x < 0$. Taking $g^* > 0$ implies $\phi_x < 0$. So $g_1(t) > g_2(t)$.
- **Continuous:** Take $g^* = (g_1 - g_2) / \|g_1 - g_2\|_{L^2}$.
- **Injective:** Assume $D_1 - D_2 \not\equiv 0$. This implies that $g_1 - g_2 \not\equiv 0$.

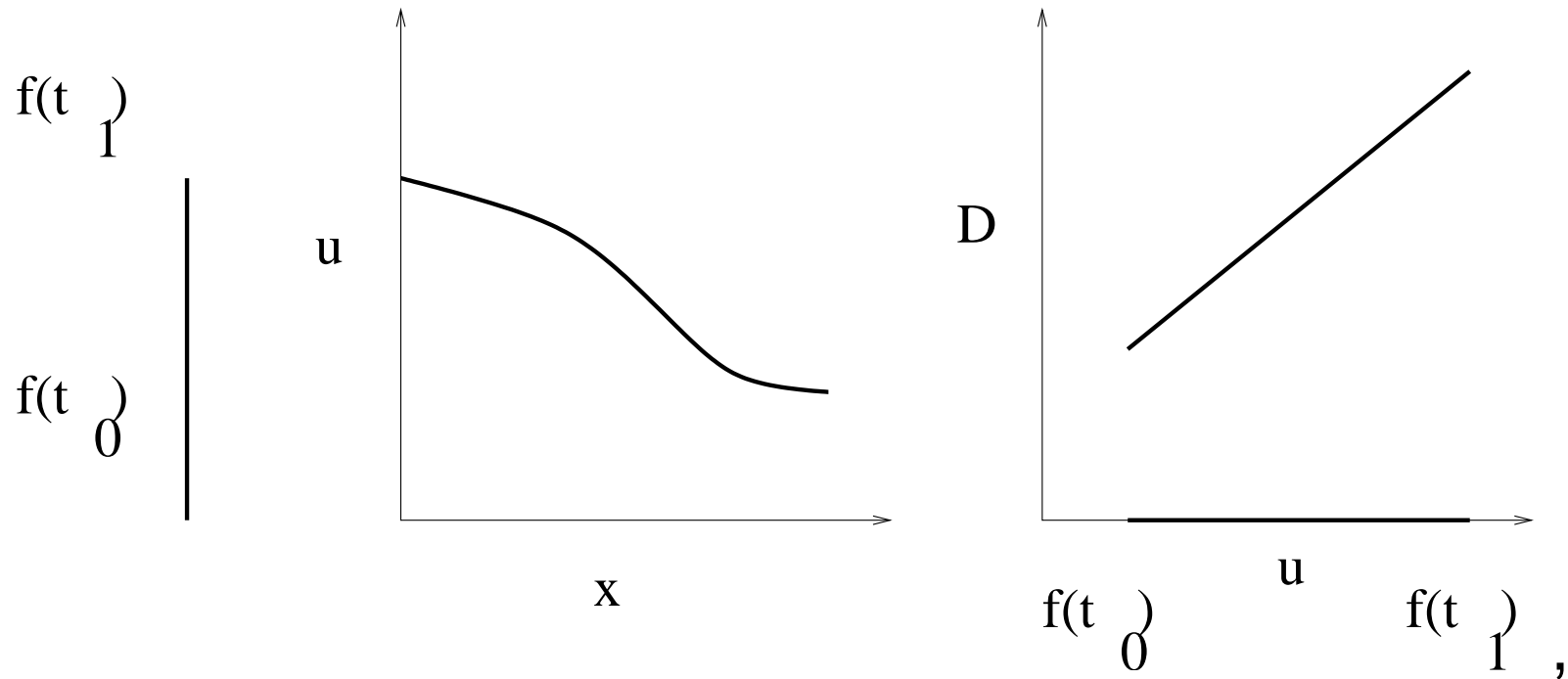
Numerics

Since



Numerics

Since



and so $[t_0, t_1] \implies [u_0, u_1]$. If

$$\hat{D}(u) = \sum_{k=0}^N d_k \Lambda_k,$$

Numerics

The integral ID,

$$\int_0^T g^*(g_1 - g_2) = \iint_{U_T} (D_1(u) - D_2(u))u_x \phi_x,$$

becomes

Numerics

The integral ID,

$$\int_0^T g^*(g_1 - g_2) = \iint_{U_T} (D_1(u) - D_2(u))u_x \phi_x,$$

becomes

$$\int_0^T g^*(g_1 - g_2)dt = (d_1 - \delta_1) \iint_{U_t} \Lambda u_x \phi_x dx dt$$

or

Numerics

The integral ID,

$$\int_0^T g^*(g_1 - g_2) = \iint_{U_T} (D_1(u) - D_2(u))u_x \phi_x,$$

becomes

$$\int_0^T g^*(g_1 - g_2)dt = (d_1 - \delta_1) \iint_{U_t} \Lambda u_x \phi_x dx dt$$

or

$$(d_1 - \delta_1) = \frac{\int_0^T g^*(g_1 - g_2)dt}{\iint_{U_t} \Lambda u_x \phi_x dx dt}$$

Numerics

The four step program:

- Given $f(t)$, collect $g_1(t)$ data from a physical lab experiment.

Numerics

The four step program:

- Given $f(t)$, collect $g_1(t)$ data from a physical lab experiment.
- Given $f(t)$, generate $u(x, t)$ and $g_2(t)$ with current \hat{D}

Numerics

The four step program:

- Given $f(t)$, collect $g_1(t)$ data from a physical lab experiment.
- Given $f(t)$, generate $u(x, t)$ and $g_2(t)$ with current \hat{D}
- Given $g^*(t)$ and k , solve adjoint problem to generate $\phi(x, t)$

Numerics

The four step program:

- Given $f(t)$, collect $g_1(t)$ data from a physical lab experiment.
- Given $f(t)$, generate $u(x, t)$ and $g_2(t)$ with current \hat{D}
- Given $g^*(t)$ and k , solve adjoint problem to generate $\phi(x, t)$
- Apply integral ID to compute update for D .

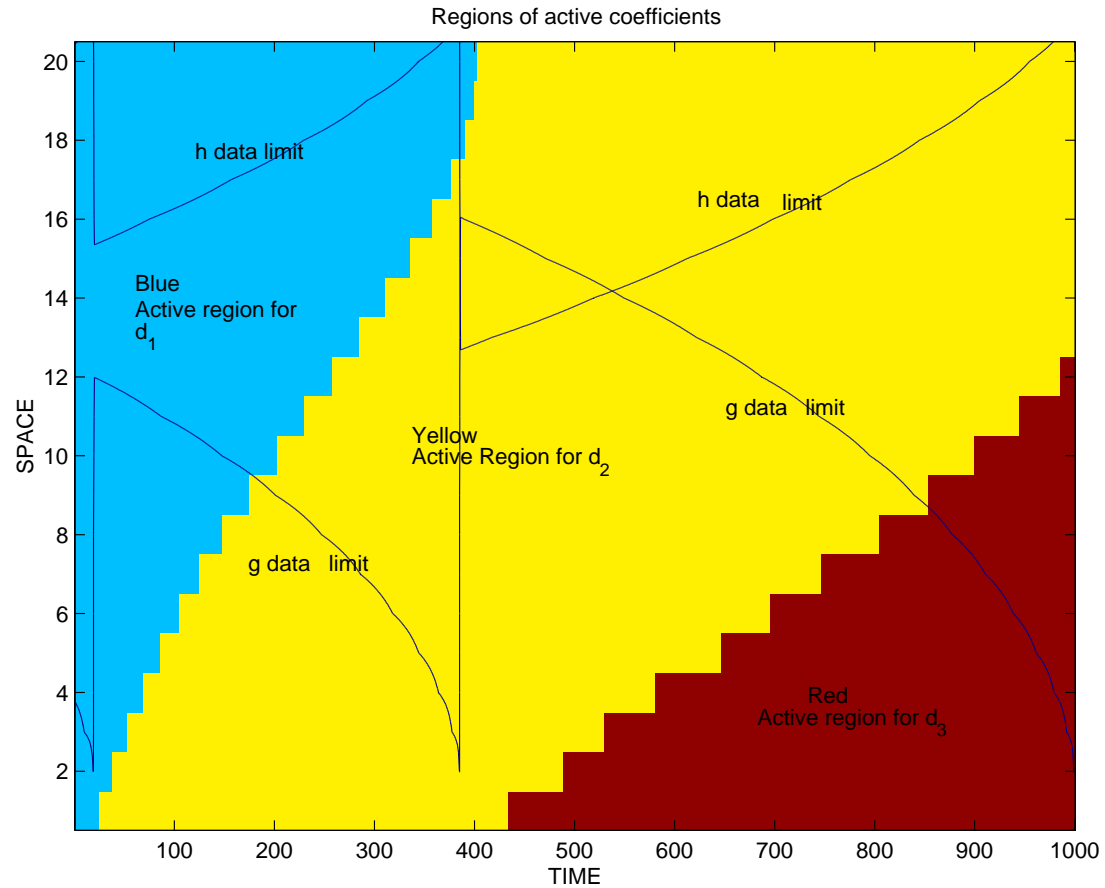
Numerics

The four step program:

- Given $f(t)$, collect $g_1(t)$ data from a physical lab experiment.
- Given $f(t)$, generate $u(x, t)$ and $g_2(t)$ with current \hat{D}
- Given $g^*(t)$ and k , solve adjoint problem to generate $\phi(x, t)$
- Apply integral ID to compute update for D .
- Repeat

Numerics

Regions of coefficient activity



Numerics

Apply identity to region where only d_1 is active.

$$b_1 = \int_0^{t_1} g^* \Delta g = (d_1 - \delta_1) \iint_{R_{11}} \Lambda_1(u) u_x \phi_x = A_{11} \Delta d_1$$

where $R_{11} = \{(x, t) \in U_{t_1} : u_0 < u(x, t) < u_1\}$

Numerics

Apply identity to the U_{t_2} time strip. Only d_1 and d_2 are active.

$$\begin{aligned} b_2 &:= \int_{t_1}^{t_2} g^* \Delta g = (d_2 - \delta_2) \iint_{R_{22}} \Lambda_2(u) u_x \phi_x + \\ &\quad + (d_1 - \delta_1) \iint_{R_{21}} \Lambda_1(u) u_x \phi_x \\ &= A_{22} \Delta d_2 + A_{21} \Delta d_1 \end{aligned}$$

with

$$\begin{aligned} R_{21} &= \{(x, t) \in U_{t_2} : u_0 < u < u_1\} \\ R_{22} &= \{(x, t) \in U_{t_2} : u_1 < u < u_2\} \end{aligned}$$

Numerics

By the Q_{t_N} strip, a diagonal system forms.

$$\begin{bmatrix} A_{11} & 0 & \cdots & 0 \\ A_{21} & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ A_{N1} & \cdots & \cdots & A_{NN} \end{bmatrix} \begin{bmatrix} \Delta d_1 \\ \Delta d_2 \\ \vdots \\ \Delta d_N \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{bmatrix}$$

where $A_{ij} = \iint_{R_{ij}} \Lambda_j(u) u_x \phi_x$ and $b_i = \int_{t_{i-1}}^{t_i} g^* \Delta g$

Numerics

Now for some demos:

- Is some data better?
- Noise?
- ????

Conclusions

- tool for analysis

Conclusions

- tool for analysis
- natural setting

Conclusions

- tool for analysis
- natural setting
- simple toolbox

Conclusions

- tool for analysis
- natural setting
- simple toolbox
- proofs are easy

Conclusions

- tool for analysis
- natural setting
- simple toolbox
- proofs are easy
- process is transparent

Conclusions

- tool for analysis
- natural setting
- simple toolbox
- proofs are easy
- process is transparent
- recovery tool?

Conclusions

- tool for analysis
- natural setting
- simple toolbox
- proofs are easy
- process is transparent
- recovery tool?
- Thanks!!