Inverse Problems

Parameter Identification

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Seminar about Inverse Problems

Previous talks

- Yves van Gennip (21-02-2007)
  Introduction
- Miguel Patricio (07-03-2007)
  Regulisation
- Hans Groot (21-03-2007)
  Regulisation by Galerking Methods
- Marco Veneroni (04-04-2007)
  Inverse eigenvalue problems
- Willem Dijkstra (18-04-2007)
  Image Deblurring

Upcoming talk

- Mark van Kraaij (23-05-2007)
  ??
- Arie Verhoeven (30-05-2007)
  ??
- Martijn Slob (13-06-2007)
  ??
- Marc Noot (20-06-2007)
  ??

Example - Oscillations of a mass-spring system

The oscillations of a mass-spring system can be modeled by

$$m\frac{d^2x}{dt^2} + kx = 0, \quad t > 0, \quad x(0) = x_0, \quad \frac{dx}{dt}(0) = 0,$$

where m is the mass and k is the spring constant. Its solution is

$$x(t) = x_0 \cos(\sqrt{\frac{k}{m}}t).$$

The inverse problem is ill-posed, since observation of the displacement $x(t)$ over an interval of length $2\pi\sqrt{m/k}$ one can uniquely determine the ration k/m, but not k and m separately. Also, the ratio is given by

$$\sqrt{\frac{k}{m}} = \frac{1}{t}\arccos\left(\frac{x(t)}{x_0}\right),$$

which is a nonlinear relation.

The problem

Consider the system

$$\mathcal{A}(q)u = f,$$

where we want to find the parameters q when f is given and u are the state variables.

In the previous example

- $\mathcal{A}(q) = m\frac{d^2}{dt^2} + k$
- $q = m$ or k
- $u = x$
- $f = 0$

The inverse problem

Assume that the observed data can be expressed as

$$d := Cu + \eta,$$

where η is the noise and C is the state-to-observation map, that is,

$$(Cu)_i = u(x_i), \quad i = 1, \ldots, n.$$

The inverse problem is to estimate q given data d.

Regularized least-squares minimization problem

To solve the inverse problem solve the constrained regularized least-squares minimization problem

$$\min \frac{1}{2}\left\|Cu - d\right\|^2 + \alpha J(q) \text{ subject to } A(q)u = f. \quad \dagger$$

Here, $J(q)$ is a regularization functional and α is a positive regularization parameter.

When the forward problem is well-posed, its solution is $u = A(q)^{-1}f$ and † becomes the unconstrained regularized least-squares minimization problem,

$$\min \frac{1}{2}\left\|CA(q)^{-1}f - d\right\|^2 + \alpha J(q).$$

Example

Goal: determine the thermal conductivity of a thin metal rod of unit length.
Given

- The one-dimensional steady-state diffusion equation

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) = f(x), \quad 0 < x < 1.$$

- Dirichlet boundary conditions

$$u(0) = 0, \quad u(1) = 0.$$

- Forcing functions

$$f^1(x) = \delta(x - 1/3) \qquad f^2(x) = \delta(x - 2/3).$$

Example (2)

The data is represented at discrete points, viz.

$$d_i^e = u^e(x_i) + \eta_i^e, \quad i = 1, ..., n-1, \quad e = 1, 2.$$

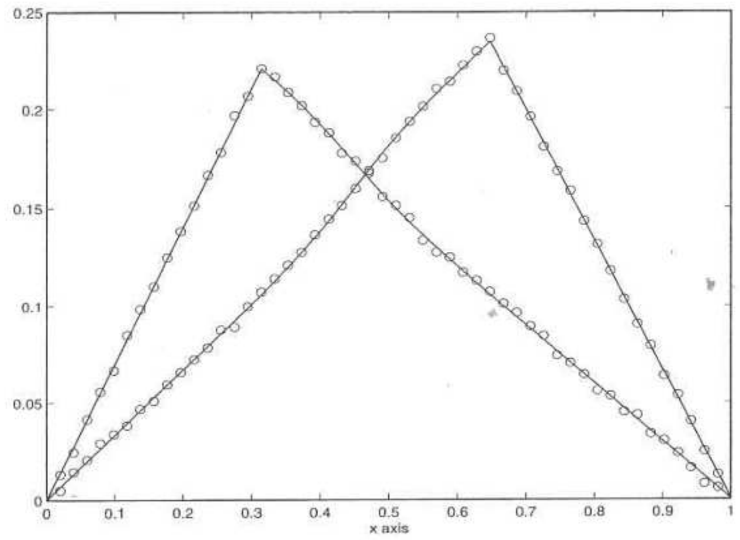


Figure 6.2. *Observed data used for distributed parameter identification in a one-dimensional steady-state diffusion equation. The left curve represents the solution corresponding to a point source at x = 1/3. The right curve represents the solution corresponding to a point source at x = 2/3. Circles represent observed data.*

Example - The analytical solution

Standard Galerkin finite element method

$$u(x) = \sum_{i=1}^{n-1} u_i \phi_i(x).$$

The basis functions ϕ_i are piecewise linear functions such that

$$\phi_i(x_j) = \delta_{ij}.$$

The coefficient vector $\mathbf{u} = [u_1, ..., u_{n-1}]^T$ solves the linear system

$$\mathbf{Au} = \mathbf{f},$$

with

- $A_{ij} = \int_0^1 \kappa(x) \frac{d\phi_j}{dx} \frac{d\phi_i}{dx} dx,$
- $f_i = \int_0^1 f(x) \phi_i(x) dx.$

Example - The analytical solution (2)

By applying the midpoint quadrature, we have

$$\mathbf{A}(\boldsymbol{\kappa}) = \frac{1}{h}\begin{bmatrix} \kappa_1+\kappa_2 & -\kappa_2 & 0 & 0 & \cdots & 0 \\ -\kappa_2 & \kappa_2+\kappa_3 & -\kappa_3 & 0 & \cdots & 0 \\ 0 & -\kappa_3 & \kappa_3+\kappa_4 & -\kappa_4 & \cdots & 0 \\ 0 & 0 & -\kappa_4 & \kappa_4+\kappa_5 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \kappa_{n-1}+\kappa_n \end{bmatrix}.$$

with $\kappa_i = \kappa(x_i^{\text{mid}})$ and $x_i^{\text{mid}} = (x_{i-1}+x_i)/2$ for $i = 1, ..., n-1$. $\mathbf{A}$ can be rewritten as

$$\mathbf{A}(\boldsymbol{\kappa}) = \frac{1}{h}\mathbf{B}^T \text{diag}(\boldsymbol{\kappa})\mathbf{B}.$$

Then the solution is

$$\mathbf{u}^e = \mathbf{A}(\boldsymbol{\kappa})^{-1}\mathbf{f}^e, \quad e = 1, 2.$$

Example - The regularization term

Estimate κ given the data vector $\mathbf{d}^e$

$$T(\kappa) = \frac{1}{2}\sum_{e=1}^{2}\left\|\underbrace{\mathbf{A}(\kappa)^{-1}\mathbf{f}^e}_{\mathbf{F}(\kappa)} - \mathbf{d}^e\right\|^2 + \alpha J_{reg}(\kappa).$$

The regularization term is taken to be a discretization of the H^1 regularization functional (penalizing non-smooth solutions), viz.

$$J_{reg}(\kappa) = \frac{1}{2}\sum_{i=1}^{n-1}(\kappa_{i+1} - \kappa_i)^2 h = \frac{1}{2}\boldsymbol{\kappa}^T\mathbf{L}\boldsymbol{\kappa},$$

where

$$\mathbf{L} = \frac{1}{h}\begin{bmatrix} 1 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Example - Gradient

The gradient of the regularization term $\alpha J_{reg}(\kappa)$ is $\mathbf{g}_{reg} = \alpha \mathbf{L}\boldsymbol{\kappa}$.
To compute the gradients of the least squares fit-to-data terms, the costate method is used.
Define

$$\frac{d\mathbf{A}}{d\,\kappa}\mathbf{e}_i := \frac{d}{d\,\tau}\mathbf{A}(\kappa + \tau\mathbf{e}_i)|_{\tau=0}$$

Then

$$(\mathbf{g}^e_{\mathrm{LS}})_i = \langle \left(\frac{d\mathbf{A}}{d\,\kappa}\mathbf{e}_i\right)\mathbf{u}^e, \mathbf{z}^e\rangle_{n-1} = \frac{1}{h}\langle \mathbf{B}^T\mathrm{diag}(\mathbf{e}_i)\mathbf{B}\mathbf{u}^e, \mathbf{z}^e\rangle_{n-1}$$
$$= \frac{1}{h}\langle \mathrm{diag}(\mathbf{e}_i)\mathbf{B}\mathbf{u}^e, \mathbf{B}\mathbf{z}^e\rangle_n = \frac{1}{h}(\mathbf{B}\mathbf{u}^e)_i(\mathbf{B}\mathbf{z}^e)_i, \quad i = 1, ..., n,$$

where $\mathbf{u}^e$ and $\mathbf{z}^e$ are the solutions to the discrete state and costate equations, $\mathbf{A}(\boldsymbol{\kappa})\mathbf{u}^e = \mathbf{f}^e$ and $\mathbf{A}^T(\boldsymbol{\kappa})\mathbf{z}^e = \mathbf{A}(\kappa)^{-1}\mathbf{f}^e - \mathbf{d}^e$.

Example - Gradient and Hessian

The gradient of $T(\kappa)$ is

$$\mathbf{g} = \mathbf{g}^1_{\mathrm{LS}} + \mathbf{g}^2_{\mathrm{LS}} + \mathbf{g}_{\mathrm{reg}}.$$

For Newton-like optimization we also need the Hessian, which can be obtained by finite differences or the costate method applied to $\mathbf{g}$. For Gauss-Newton, the Hessian of the least squares functional can be expressed as

$$\mathbf{H}(\kappa) = \underbrace{\left(\frac{d\mathbf{F}}{d\kappa}\right)^* \frac{d\mathbf{F}}{d\kappa}}_{\mathbf{H}^{\mathrm{GN}}} + \frac{d^2\mathbf{F}}{d\kappa^2}(\mathbf{A}(\kappa)^{-1}\mathbf{f} - \mathbf{d}).$$

Thus an estimation of the Hessian is used.

Example - Results

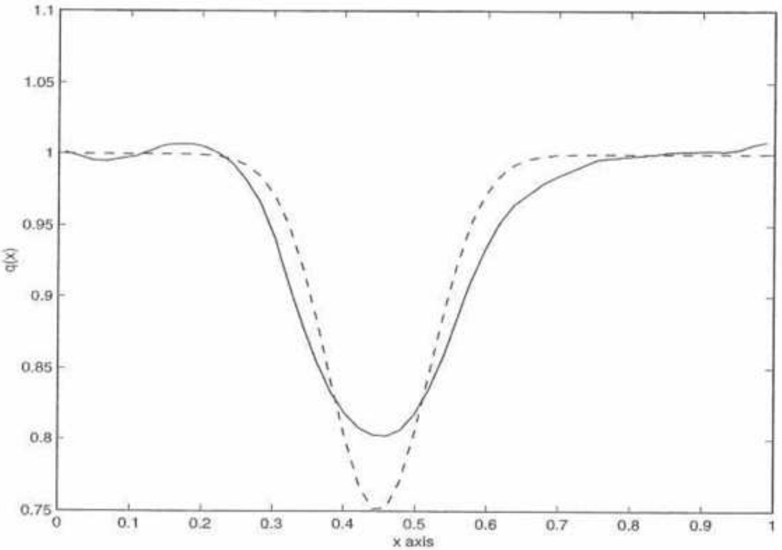


Figure 6.1. *True and estimated distributed parameters in a one-dimensional steady-state diffusion equation. The dashed line denotes the true diffusion coefficient; the solid line denotes the estimated diffusion coefficient obtained using a regularized least squares approach.*

What is α?

Example - Results (2)

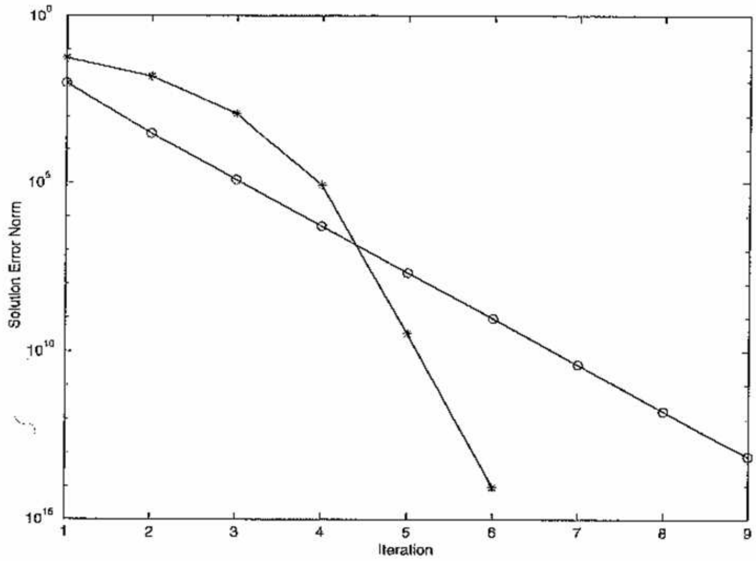


Figure 6.3. *Numerical performance of unconstrained optimization methods for parameter identification using penalized least squares. Asterisks denote the norm of the iterative solution error for Newton's method, and circles represent the iterative solution error for the Gauss–Newton method.*

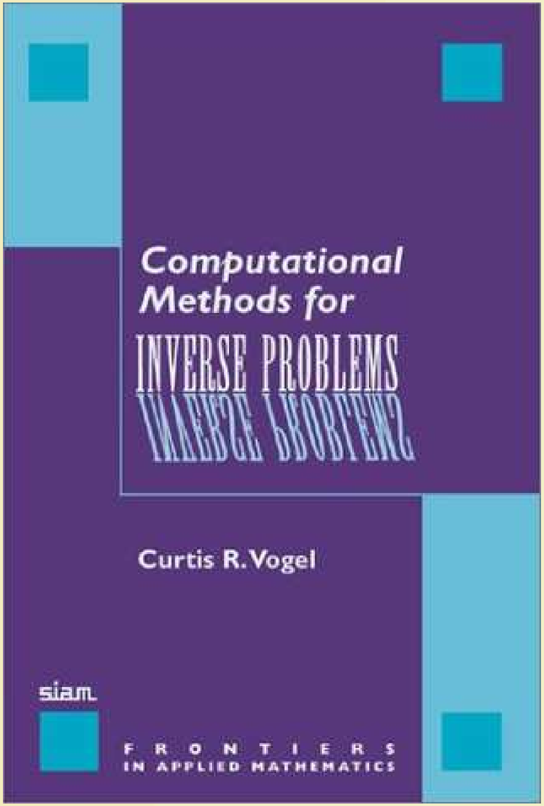
Conclusions

When

- a mathematical model is available and
- measurements are available,

regularization terms are required to obtain a smooth solution.

Literature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Questions ?