NASA-CR-178,128

NASA Contractor Report 178128

ICASE REPORT NO. 86-38

NASA-CR-178128
19860020951

ICASE

ON COMPACTNESS OF ADMISSIBLE PARAMETER SETS:
CONVERGENCE AND STABILITY IN INVERSE PROBLEMS FOR
DISTRIBUTED PARAMETER SYSTEMS

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Contract Nos. NAS1-17070, NAS1-18107

June 1986

INSTITUTE FOR COMPUTER APPLICATIONS IN SCIENCE AND ENGINEERING
NASA Langley Research Center, Hampton, Virginia 23665

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NF00168

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ABSTRACT

We report on a series of numerical examples and compare several algorithms for estimation of coefficients in differential equation models. Unconstrained, constrained and Tikhonov regularization methods are tested for their behavior with regard to both convergence (of approximation methods for the states and parameters) and stability (continuity of the estimates with respect to perturbations in the data or observed states).

The research for the first author was supported under the National Aeronautics and Space Administration under NASA Contracts No. NAS1-17070 and NAS1-18107 while he was in residence at the Institute for Computer Applications in Science and Engineering (ICASE), NASA Langley Research Center, Hampton, VA 23665.

*Invited lecture, IFIP WG 7.2 Conference on Control Systems Governed by Partial Differential Equations, University of Florida, Gainesville, February 3-6, 1986.

N86-30423#

On Compactness of Admissible Parameter Sets: Convergence and Stability in Inverse Problems for Distributed Parameter Systems

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In this brief note we summarize some of our findings [3] from numerical studies on certain aspects of ill-posedness in inverse or parameter estimation problems involving differential equation constraints. There is a vast literature (which we shall not attempt to discuss here) on a number of questions (e.g., lack of existence and/or uniqueness of solutions, lack of continuous dependence of solutions on data) related to the estimation of parameters even when the constraining systems are algebraic equations or ordinary differential equations. Additional difficulties arise when one is attempting to estimate functional (i.e. time and/or spatially dependent) coefficients in partial differential equation or distributed parameter systems. Here we focus on the role that compactness of the admissible parameter or coefficient set plays in such problems. Due to the limitations of space, our presentation will be sketchy, with all but

the expert reader most likely wishing to consult some of our references for further elaboration.

Consider a general least-squares inverse or parameter estimation problem: Minimize $J(q) = |Cu(q) - z|_Z$ over $q \in Q_{AD}$, $Q_{AD} \subset Q$, subject to the constraints $A(q,u(q)) = F$. Here C is an observation operator from the state space X to an observation or data space Z, Q_{AD} is the admissible subset of parameters in the space Q, and the parameter dependent operator A defines the dynamics that constrain the problem. In the problems of interest to us, $A = F$ represents a partial differential equation (elliptic, parabolic, hyperbolic) with parameter functions q which depend on time and/or spatial coordinates (or even the state u itself in some nonlinear system problems). It is now well-understood (e.g. see [1] for a discussion) that a compactness hypothesis (Q_{AD} compact in some Q topology) for Q_{AD} plays an important <u>theoretical</u> role in both convergence (of approximating solutions) and stability (continuity of the estimated parameters with respect to the data or observations). Here we wish to demonstrate that this compactness also plays an important <u>computational</u> role in such problems. To do this, we illustrate the basic ideas with one dimensional elliptic systems (so we actually have an ordinary differential equation with spatially dependent coefficient). We wish to emphasize, however, that our findings are most certainly relevant to problems with more complex system dynamics (second order parabolic or hyperbolic equations, or higher order equations of elasticity). Indeed we have observed the difficulties and phenomena we discuss here in a number of these technically more challenging problems.

Turning to a class of concrete examples, we consider minimization of

$$J(q) = \int_0^1 |u(q) - \hat{u}|^2 dx \tag{1}$$

over $q \in Q_{AD} \subset Q = C[0,1]$ subject to

$$D(qDu) = f, \quad u(0) = u(1) = 0. \tag{2}$$

Here f is assumed known, $D = \frac{\partial}{\partial x}$, and $\hat{u}$ are given observations for $u = u(q)$ the solution of (2). For computational purposes, we replace this original problem by a sequence of approximating problems where the states u are replaced by Galerkin approximations u^N (for example, here we take

u^N in the N-1 dimensional space of linear splines with grid size 1/N and satisfying the boundary conditions $u^N(0) = u^N(1) = 0$) and the approximate parameters q^M are chosen from an approximating set Q^M for Q_{AD}. That is, our algorithms are used to seek $q^M \in Q^M \subset Q = C[0,1]$ that minimizes

$$J^N(q^M) = \int_0^1 |u^N(q^M) - \hat{u}|^2 dx. \tag{3}$$

A convergence theory (as the dimensions of the approximating spline spaces increase i.e., $N \to \infty$, $M \to \infty$) can be given where one may use either linear or cubic splines for the state approximations and for the parameter approximations (e.g. see [2], [4] for the ideas). An essential feature of these particular convergence proofs is that the admissible parameter set Q_{AD} and its approximations Q^M lie in some compact subset of C[0,1]. This same compactness assumption plays a fundamental role in proving stability (e.g., continuity of the inverse of the mapping from the parameter estimates to the observations or data) as is discussed in [1], for example.

Perhaps the most direct way to interpret the compactness requirements is in terms of constraints on the parameters. For example, in the computations reported on herein, we imposed compactness in C[0,1] by putting pointwise upper and lower bounds on the parameter function values as well as an upper bound on the absolute values of the slope of the functions. In practice it is common to ignore functional constraints, imposing the pointwise upper and lower bounds to insure that the optimization algorithms perform satisfactorily. The results summarized in this note illustrate the apparent necessity in many examples of including the full compactness constraint in computational algorithms. Examples are given here and in [3] where both stability and convergence properties are as expected whenever a constrained estimation procedure is employed whereas instability and divergence are in evidence when unconstrained techniques are used. It is safe to speculate that similar behavior occurs in problems with parabolic and hyperbolic as well as elliptic systems. In our own work and in that reported in the literature - e.g. see Yoon and Yeh [6], one sometimes encounters severe problems with oscillations in the estimates for q as one pushes the algorithms for increased accuracy in the parameter estimates (i.e. as one lets $M \to \infty$). As the examples in this note and [3] demonstrate, these difficulties can to some extent be alleviated by imposition of compactness constraints.

An alternative but essentially theoretically equivalent approach involves the use of Tikhonov regularization as formulated by Kravaris and Seinfeld in [5]. One restricts the parameter set to $Q_R \subset Q$ with Q_R compactly imbedded in Q and then modifies the original least squares criterion J to minimize $J_\beta = J + \beta|q|_R^2$ where $|\cdot|_R$ is the norm in Q_R and β is a regularization parameter. Thus minimizing sequences for J_β are bounded in Q_R and hence compact in Q; this is, in some sense, roughly equivalent to minimizing J over a restriction of Q which is compact even though the minimization of J_β only produces (hopefully) an approximation to the minimizer for the original criterion J. In the cases considered below, we use $Q_R = H^1$ while $Q = C$ (which corresponds to $\Lambda = C^1$ and $\mathfrak{R} = H^2$ in the notation of [5]).

As we shall see below, each approach has inherent difficulties in choosing related imbedding parameters: in the first, the estimates produced are sensitive to the constraints (the bound L on the derivatives of the parameters in the computations summarized here) while the estimates produced using regularization are quite sensitive to the regularization parameter β.

We carried out a series of numerical tests to compare spline based algorithms (linear spline approximations for both the states and parameters) on a number of examples for three cases: the unconstrained minimization of J; the constrained minimization of J; and unconstrained minimization of a regularized criterion J_β. Details of our packages and the algorithms are given in [3]. Here we only note that for the constrained minimization we used a reduced gradient algorithm with a corresponding gradient algorithm for the unconstrained minimization. For the compactness constraints we used $|Dq^M(x)| \leq L$ and $.5 \leq q^M(x) \leq 10.0$ in all our examples.

Our algorithms were compared on examples for which we knew the true solutions, i.e. we used "true" parameter values q^* to generate data $\hat{u}$ (in some cases with noise) as described in [3]. We summarize our findings and present representative results.

CONVERGENCE

In Figure 1 we compare estimates for several values of approximation indices N, M produced for an example (Example 2 of [3]) with

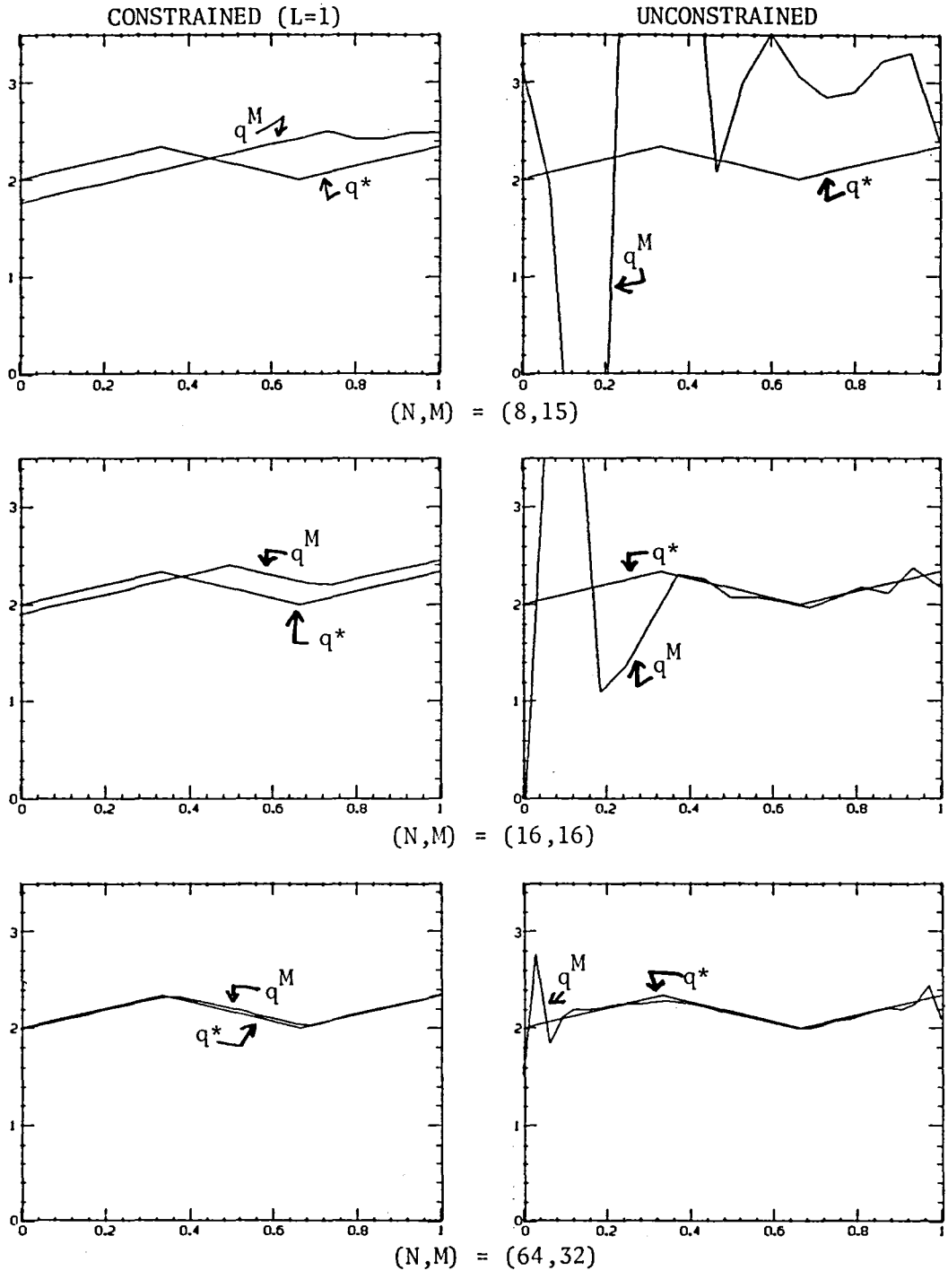
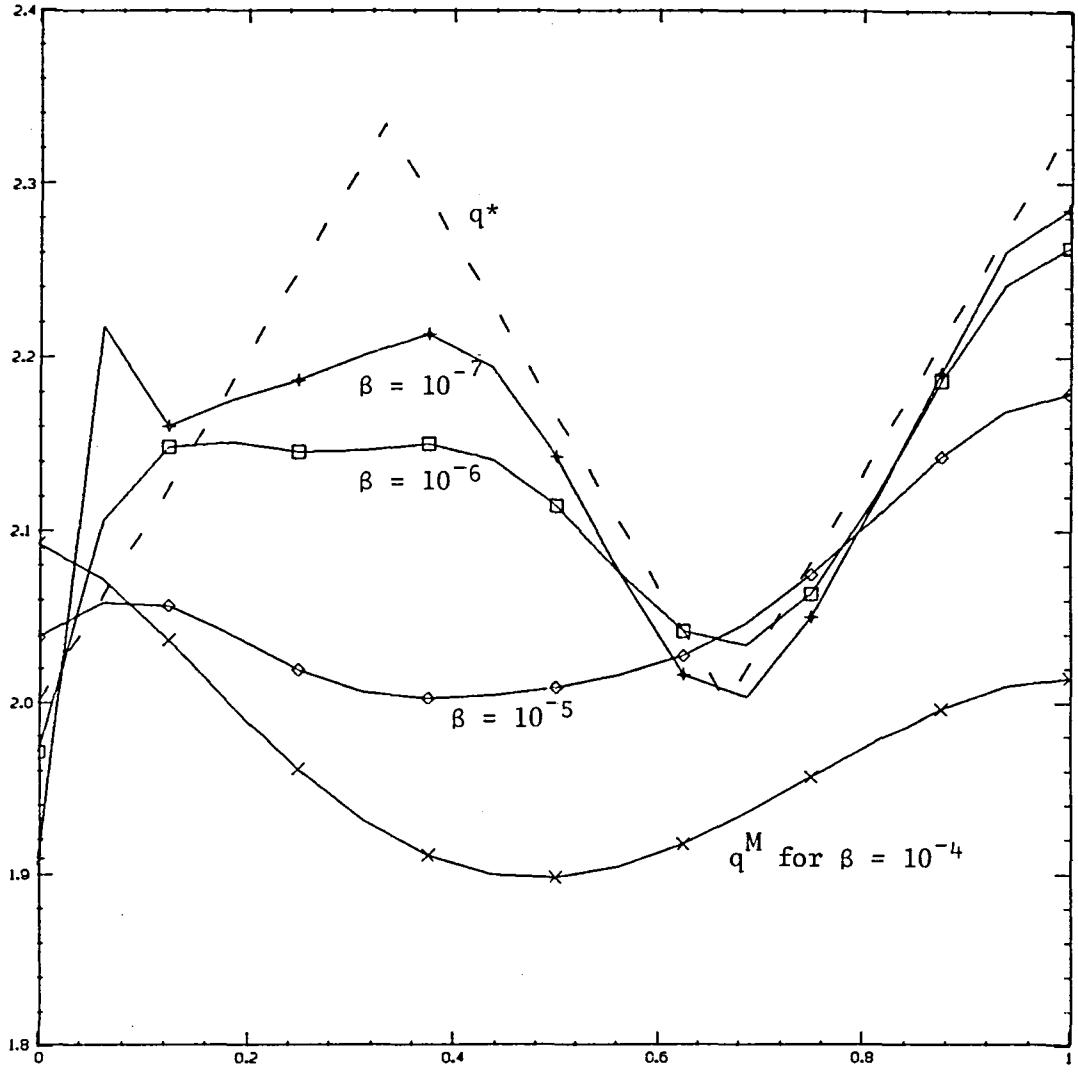
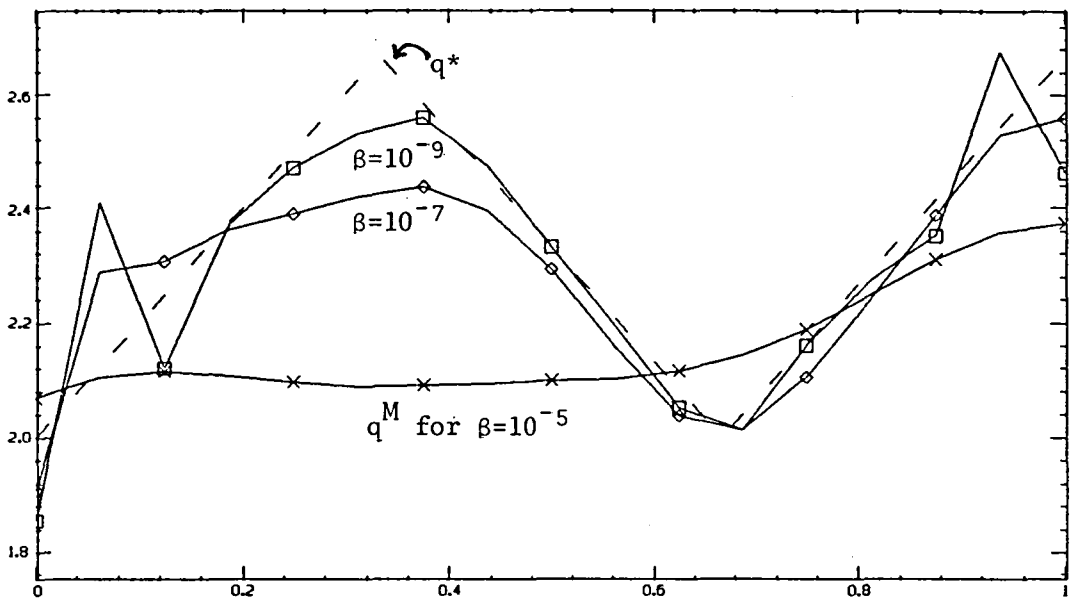


FIGURE 1

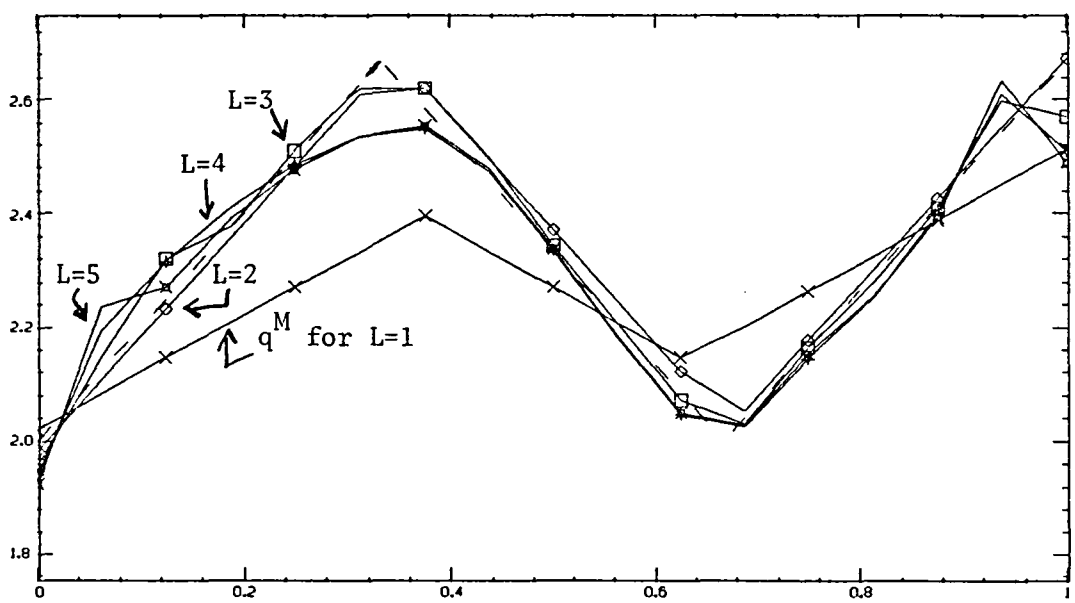


TIKHONOV ESTIMATES
AS β VARIES

FIGURE 2



TIKHONOV ESTIMATES AS β VARIES



CONSTRAINED ESTIMATES AS L VARIES

(N,M) = (64,16)

FIGURE 3

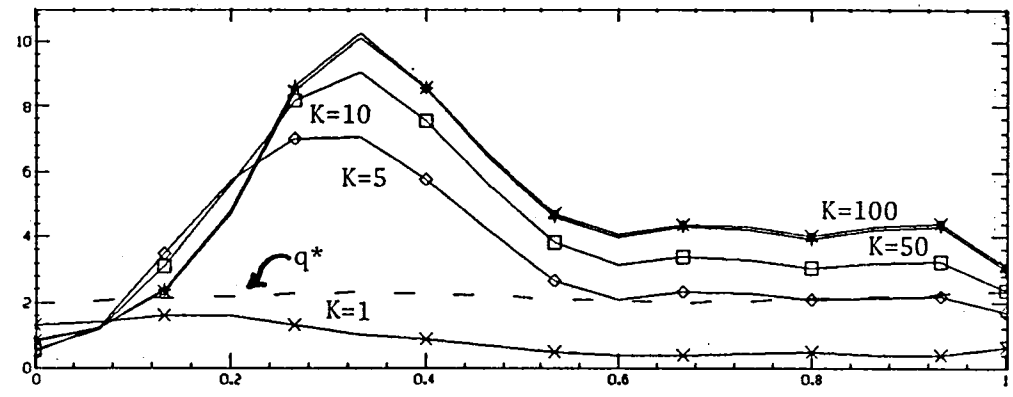
$$q^*(x) = \begin{cases} 2 + x & 0 \leq x \leq 1/3 \\ 8/3 - x & 1/3 \leq x \leq 2/3 \\ 4/3 + x & 2/3 \leq x \leq 1, \end{cases} \tag{4}$$

$$u(x) = \sqrt{x}(1 - \sqrt{x}), \tag{5}$$

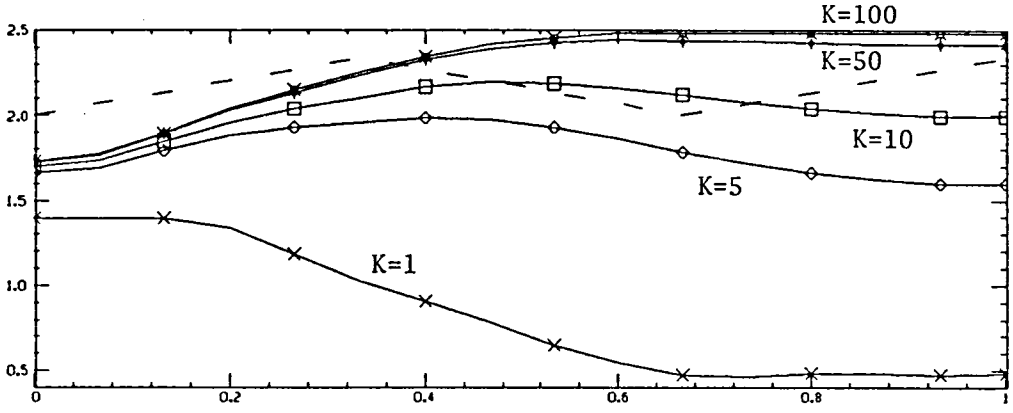
in the system (2). We chose $L = 1$ (the exact maximum of $|Dq^*(x)|$) for the constrained algorithms. For low values of N (often a desirable situation in practice) compared to M, the unconstrained estimates are totally useless. For larger values of N, the unconstrained estimates are improved with only small oscillations appearing at each end. In all cases, convergence took much longer for the unconstrained package. For this same example we depict in Figure 2 the estimates obtained using Tikhonov regularization with $N = 64$, $M = 16$ and several values of the regularization parameter β. Results for a slightly different example (Example 3 of [3]) with the same u but $q^*(x)$ piecewise linear as in (4) except with slopes ∓ 2 are depicted in Figure 3. Here we illustrate, for $N = 64$, $M = 16$, the typical performance of Tikhonov regularization as β changes and that of the constrained minimization as L varies. As one might expect, the estimates begin to resemble unconstrained estimates as $\beta \to 0$ and $L \to \infty$.

STABILITY

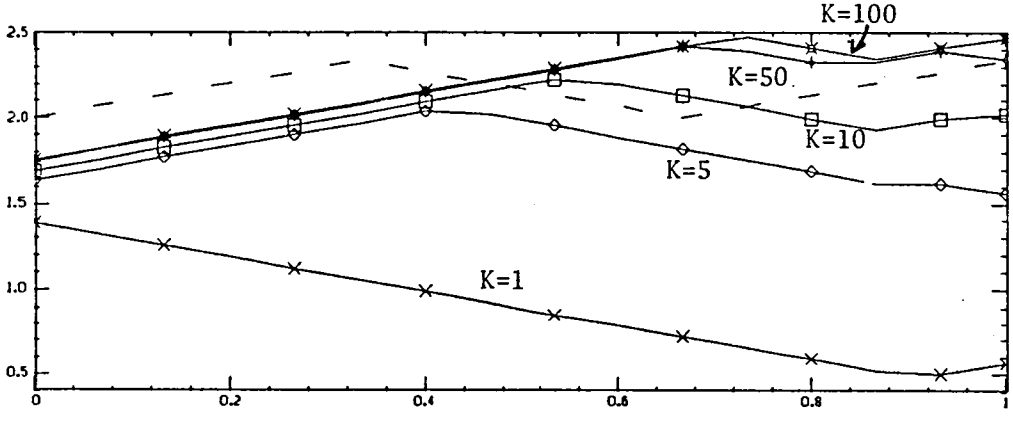
To investigate stability with respect to noise in the data, we took the true u, q^* and f associated with (4), (5) above but perturbed u to produce data $\hat{u} = u_p$ for the least squares criterion J^N of (3). We used perturbations of the form $u_p(x) = u(x) + p(x)/K$ where $p(x)$ is a perturbing function and K can be varied to control the size of the perturbation. As $K \to \infty$, we have $u_p(x) \to u(x)$ for bounded perturbations p. In our numerical experiments we used two different perturbation functions: $p_1(x) = x(1 - x)$, $p_2(x) = 1$. Note that p_1 (like u) satisfies the homogeneous boundary conditions while p_2 does not. The unconstrained, constrained and Tikhonov estimates for several values of K with perturbation function p_1 in the data and $N = 8$, $M = 15$ are given in Figure 4. The depicted behavior is typical: For all values of N the behavior of the constrained and Tikhonov methods are similar, with the estimates improving steadily as $u_p(x) \to u(x)$, i.e. as the noise in the observations tends to zero. In Figure 5, we present results obtained using the perturbation p_2 with the unconstrained, constrained and Tikhonov estimation procedures for several



UNCONSTRAINED ESTIMATES



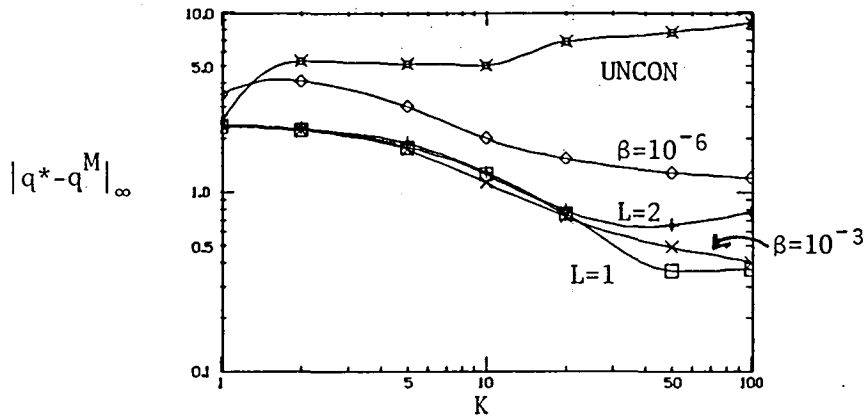
TIKHONOV ESTIMATES



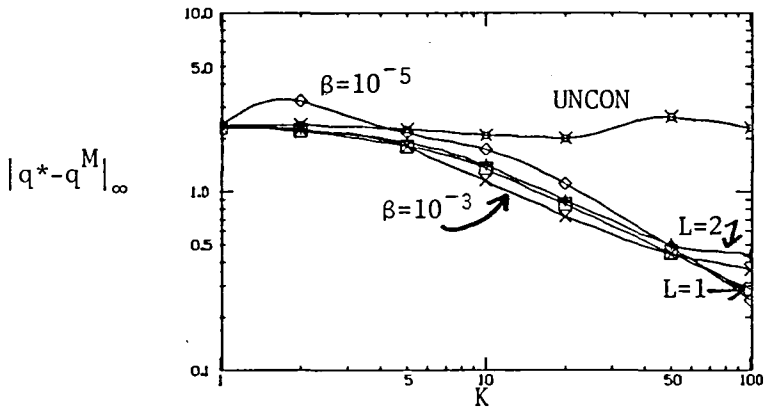
CONSTRAINED ESTIMATES

(N,M) = (8,15), PERTURBATION p_1

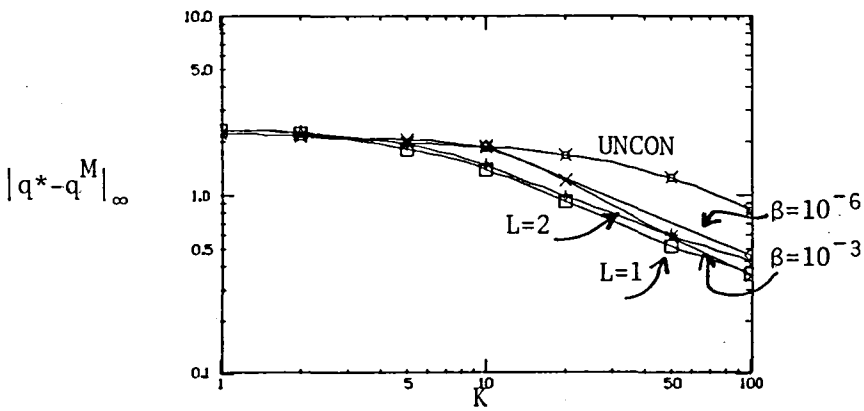
FIGURE 4



(N,M) = (8,15)



(N,M) = (16,16)



(N,M) = (64,16)
UNCONSTRAINED, CONSTRAINED, TIKHONOV, PERTURBATION p_2

FIGURE 5

values of (N,M) : (8,15), (16,16) and (64,16). The L^{∞} norm of the error (from the true values q^*) in the final estimates is graphed versus the values of K.

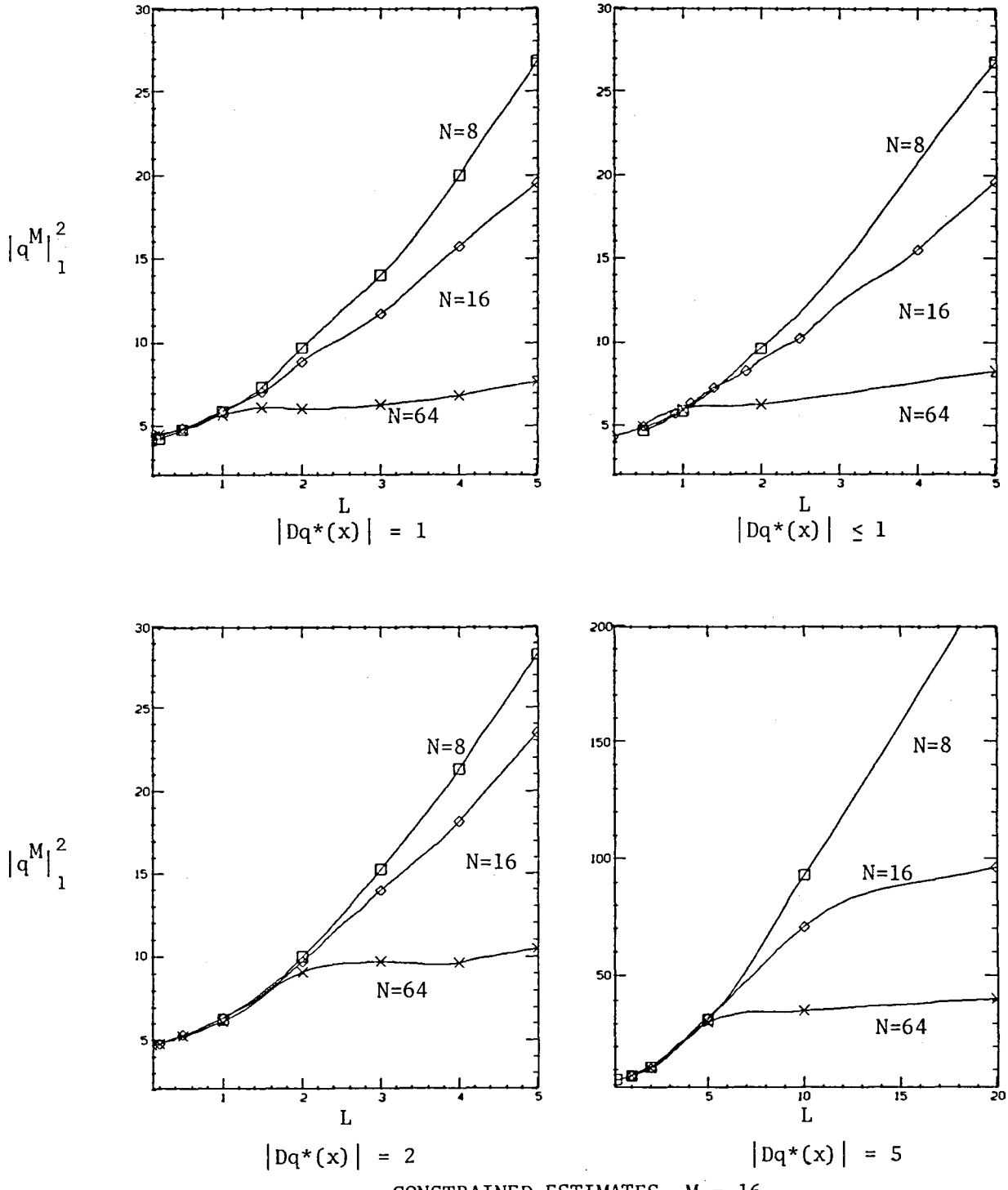
SUMMARY REMARKS

The results here and in [3] demonstrate severe problems in some instances with using an unconstrained algorithm to estimate the parameter q in examples such as (1), (2). When modified, either by regularizing the problem using Tikhonov regularization or by constraining the estimate set as in this note, the algorithm does give good estimates.

Unlike the unconstrained algorithm, both the Tikhonov and constrained algorithms are stable with respect to increasing M while holding N fixed. However as N is increased the estimates from the Tikhonov algorithm do not improve as much as do those of the constrained algorithm. The Tikhonov estimates are biased by the regularization of the cost functional, and never show all the detail of q when q has significant variation.

Both the constrained and Tikhonov estimation algorithms are stable with respect to systematic errors in the observation data, while, except when N is large, the unconstrained algorithm fails to give good results on even the exact data.

For both the Tikhonov and constrained algorithms there are parameters which affect the algorithm's performance. For the constrained algorithm suitable constraints must be found while for the Tikhonov algorithm suitable values of β must be found. The constrained algorithm has the advantage that the constraints used here, i.e. limits on the slope of q, have an obvious meaning, and so may well be (at least approximately) known in advance. In the Tikhonov algorithm β has no obvious meaning. It must be chosen by looking at the change in the estimate behavior as β changes and perhaps using some a priori knowledge about the shape of q to choose values of β that give an estimate that is neither too flat, nor too oscillatory. For the constrained algorithms, the estimates are sensitive to the slope constraint parameter L. We have begun investigations into how one might use this sensitivity in some type of adaptive manner in algorithms to choose a "best" value of L (and hence a good parameter estimate). In Figure 6 we depict some of our initial findings. In this figure



CONSTRAINED ESTIMATES, M = 16

FIGURE 6

we graph the square of the H^1 norm of the final estimate versus the constraint L for several different examples and various values of N (with M fixed at 16). All but the second of the examples involve true parameters q^* of the form (4), differing only in the slope of the piecewise linear functions. In the first example $Dq^*(x) = \mp 1$, while in the last two $Dq^*(x) = \mp 2$ and $Dq^*(x) = \mp 5$ respectively. The second is made up of piecewise linear and parabolic segments satisfying $|Dq^*(x)| \leq 1$. Note that it is not necessary to know the true values q^* in order to obtain the graphs in this figure. Furthermore, we observe a striking separation in the values of the H^1 norm of the estimate for q^M at the value of L corresponding to the desired value of L to be used with each example. We are continuing our investigations into how these and other features of some of our results might be used to develop "adaptive" constrained parameter estimation algorithms.

ACKNOWLEDGMENTS

This research was supported in part by the National Science Foundation under NSF Grant MCS-8504316, the Air Force Office of Scientific Research under Contract AFOSR-84-0398, and the National Aeronautics and Space Administration under NASA Grant NAG-1-517. Part of this research was carried out while the first author was a visiting scientist at the Institute for Computer Applications in Science and Engineering (ICASE), NASA Langley Research Center, Hampton, VA, which is operated under NASA Contracts NAS1-17070 and NAS1-18107.

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Standard Bibliographic Page

1. Report No. NASA CR-178128 ICASE Report No. 86-38	2. Government Accession No.	3. Recipient's Catalog No.
4. Title and Subtitle On Compactness of Admissible Parameter Sets: Convergence and Stability in Inverse Problems For Distributed Parameter Systems		5. Report Date June 1986
		6. Performing Organization Code
7. Author(s) H. T. Banks, D. W. Iles		8. Performing Organization Report No. 86-38
9. Performing Organization Name and Address Institute for Computer Applications in Science and Engineering Mail Stop 132C, NASA Langley Research Center Hampton, VA 23665-5225		10. Work Unit No.
		11. Contract or Grant No. NAS1-17070, NAS1-18107
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D.C. 20546		13. Type of Report and Period Covered Contractor Report
		14. Sponsoring Agency Code 505-31-83-01

15. Supplementary Notes

Langley Technical Monitor:
J. C. South

Final Report

Submitted to Proc. IFIP Conf. on Control Systems Governed by Partial Differential Equations.

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17. Key Words (Suggested by Authors(s)) parameter estimation, convergence and stability, numerical methods	18. Distribution Statement 64 - Numerical Analysis 66 - Systems Analysis Unclassified - unlimited

19. Security Classif.(of this report) Unclassified	20. Security Classif.(of this page) Unclassified	21. No. of Pages 16	22. Price A02

For sale by the National Technical Information Service, Springfield, Virginia 22161

NASA-Langley, 1986

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