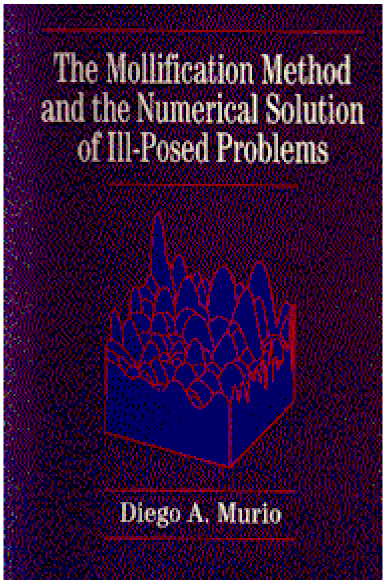
- The Mollification Method is a numerical technique that can be used from smoothing of noisy data and fitting of curves and surfaces to identification of coefficients and functions in ill-posed systems of partial differential equations.

- For a general overview and examples, see the book **"The Mollification Method and the Numerical Solution of Ill-Posed Problems"**, by Diego A. Murio, Wiley-Interscience Publication, New York, 1993.

- For an upgraded version of the basic algorithms see the articles **"Discrete Mollification and Automatic Numerical Differentiation"** (PDF file), by Diego A. Murio, Carlos E. Mejia and Shenghe Zhan, Computers and Mathematics with Applications, Vol. 35, No. 5, pp. 1-16, 1998 and **"Numerical Solution of Generalized IHCP by Discrete Mollification"** (PDF file), by Diego A. Murio and Carlos E. Mejia, Computers and Mathematics with Applications, Vol. 32 , No. 2 , pp. 33-50, 1996.

- You can test the algorithm by interactively differentiating noisy data on the WWW on the fly. Visit the location now and use the **mollification applet**.

- Source code for numerical differentiation of noisy data can be downloaded in **c** or **fortran** or **matlab**. If you prefer, **download** all three together.



John Wiley & Sons

Interscience Division
New York, 1993

ISBN: 0-471-59408-3
254 pages

$69.95

Reviews

CONTENTS

4. Two-Dimensional Inverse Heat Conduction Problem

5. Applications of the Space Marching Solution of the IHCP

6. Applications of Stable Numerical Differentiation Procedures

Appendix A. Mathematical Background

Mathematical Reviews- (AMS) American Mathematical Society

Mathematical Reviews 94m:65003

M. Zuhair Nashed

"The book examines the mollification method and its manifold applications when used as a space marching method for the numerical solution of applied inverse and ill-posed problems. The idea of the method is to find a sequence of mollification operators which map the given inexact data of the ill-posed problem into a family of well-posed problems, and then to determine error estimates and optimal or quasi-optimal mollification parameters. Along the way, the book provides an introduction to a number of essential ideas and techniques for the study of inverse and ill-posed problems. The treatment is strongly computational and partly heuristic. In the subject index, one finds that the mollification method is mentioned on 27 different pages, but none of these give a precise definition of the method; the definition is given in Appendix A on mathematical background. Although the presentation concentrates mostly on problems with origin in mechanical engineering, there are many examples and exercises that demonstrates that the ideas and methods are truly interdisciplinary.

The book consists of six chapters and two appendices. Chapter 1 discusses numerical differentiation as an inverse problem and introduces the mollification method in this context. Chapter 2 is devoted to the numerical solution of Abel's integral equation; four different mollification strategies are developed, including Tikhonov regularization coupled with the adjoint conjugate gradient method, together with numerical implementations and comparisons. Chapter 3 and 4 -the main trust of the book- are devoted to the one-dimensional inverse heat conduction problem (IHCP) and the two-dimensional IHCP, respectively. Several mathematical models and their pertinent numerical algorithms for the approximate determination of the unknown transient temperature and heat flux functions are developed. Chapter 5 contains three different applications for space marching solution of the IHCP: identification of boundary source functions and radiation laws, numerical solution of the inverse Stefan problem, and determination of the initial temperature distribution in a one-dimensional conductor from transient measurements at interior locations. Chapter 6 is devoted to applications of stable numerical differentiation procedures to several inverse identification problems. Appendix B contains an extensive bibliography on the IHCP. References at the end of each chapter are supplemented with comments by the author.

Over the past twenty years, the subject of ill-posed problems has expanded from a collection of individual techniques to a rich, highly developed branch of applied mathematics. This book is a welcome addition to the literature on computational methods for ill-posed inverse problems. The material is presented in a clear, simple language that makes the subject accessible to engineers and professionals interested in modeling inverse phenomena."

University of Delaware, 1994.

Book Reviews -(SIAM) The Society for Industrial and Applied Mathematics

SIAM Review, September 1994, Volume 36, Number 3

James V. Beck

"The subjects of ill-posed and inverse problems are attracting increased attention from mathematicians, engineers and others. This is indicated by numerous recent national and international conferences occurring, various groups forming, new journals being issued, and books being written.

This book is a fine contribution by Prof. Murio in this area. It is the first book written in English by a mathematician covering ill-posed inverse problems, including the inverse heat conduction problem (IHCP). The IHCP involves the use of transient temperature measurements inside a heat conducting solid to determine the surface temperature or heat flux history.

There are a number of fundamentally different methods of solving ill-posed problems. They include the future temperature, regularization-adjoint-conjugate gradient, hyperbolic, and mollification methods. This book is an exposition of the mollification method, although other methods are discussed and results are compared.

A major attraction of the mollification method is its simplicity in concept. Although the original problem is ill-posed in high frequency components, the use of a Gaussian kernel to smooth the data can make the problem stable. The use of a Gaussian kernel in a convolution form and applied locally with a "burring radius" (whose optimal value is derived in the book) constitutes the main idea of the mollification method. After the data has been operated upon by the mollification method, various procedures are available for solution. In other words, the original problem (which is ill-posed) is replaced by a similar (but now stable) problem. This similar problem is obtained using the mollification method. One of the ways to solve the mollified problem for the finite difference form of the IHCP is the space marching method, which has been independently proposed by M. Raynaud and others.

This book has a number of notable features. First, the method is quite general. It can be used to solve a variety of ill-posed problems. They include differentiation of a measured time history, numerical solution of Abel's integral equation (and other integral equations), one-dimensional inverse heat conduction problem, and two-dimensional inverse heat conduction problem.

Second, the author has given many theorems and proofs that can be used to select smoothing parameters.

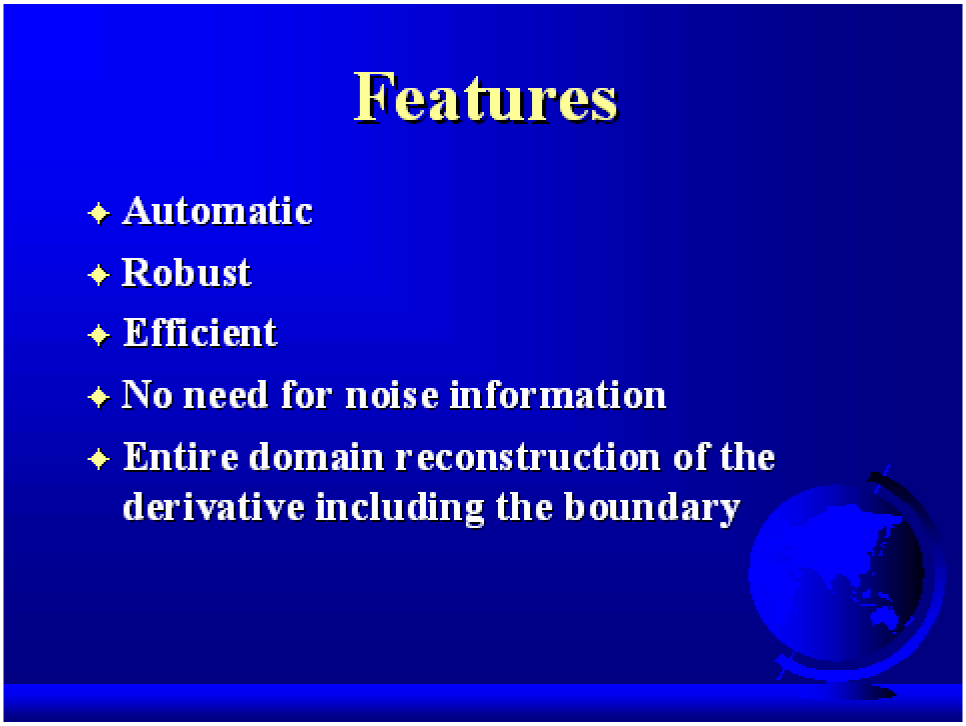
Third, detailed algorithms and equations are given to aid the reader in implementing these techniques. For the IHCP, details are given to allow the extension to nonlinear problems, for both one- and two-dimensional cases.

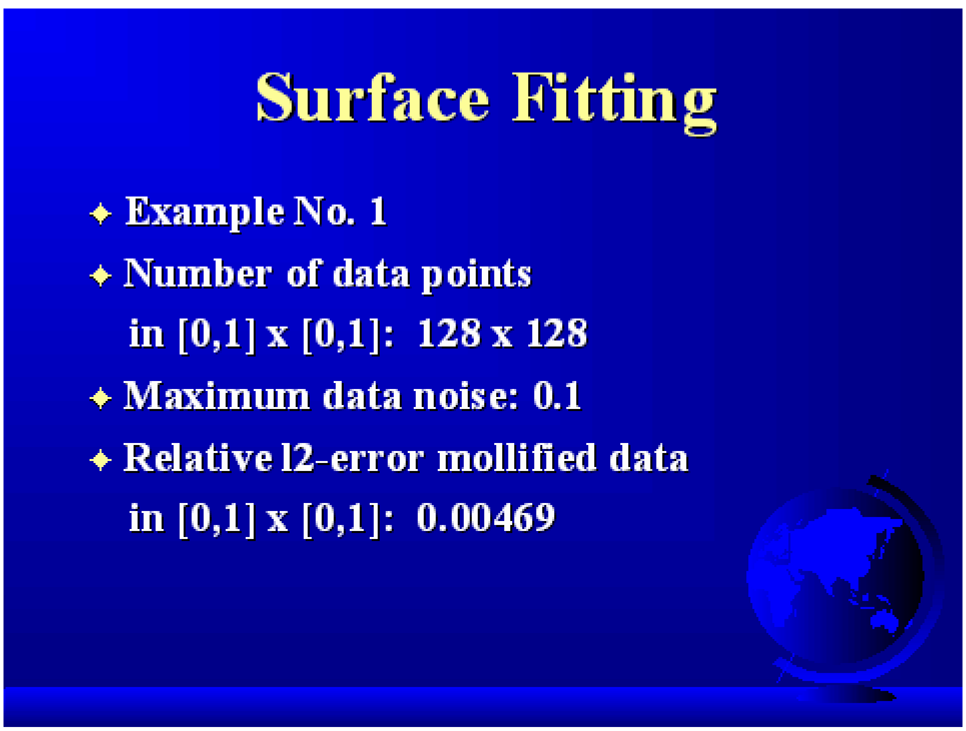
Fourth, many examples are given, covering not only the mollification method but others also. The effects of zero measurement errors and of a couple of larger errors are shown.

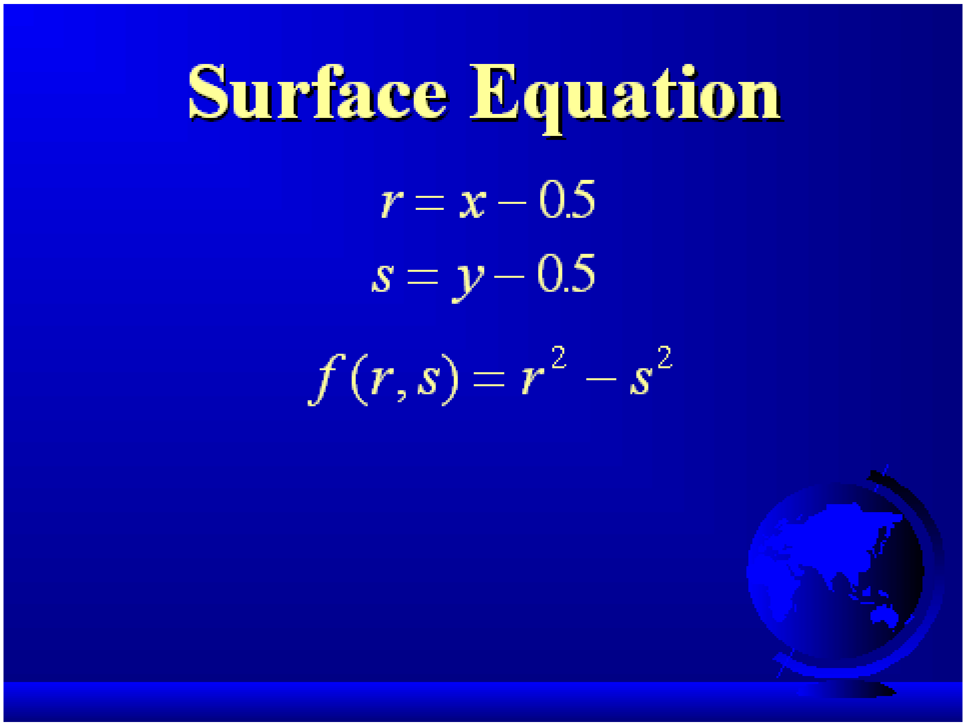
In order to contrast the mollification method with others, a few comments are given. This method is uniquely simple in concept and can be used with virtually all other methods. (When using with other methods, the optimal choice of parameters may no longer be clear, however.) Another positive aspect of the method is that be used for a variety of problems. Some negative aspects (from my perspective but maybe not that of mathematicians) is that there is little usage of statistics, that multiple sensors cannot be used in one-dimensional problems, and that many sensors which are equally=spaced along a single line are needed for two-dimensional problems.

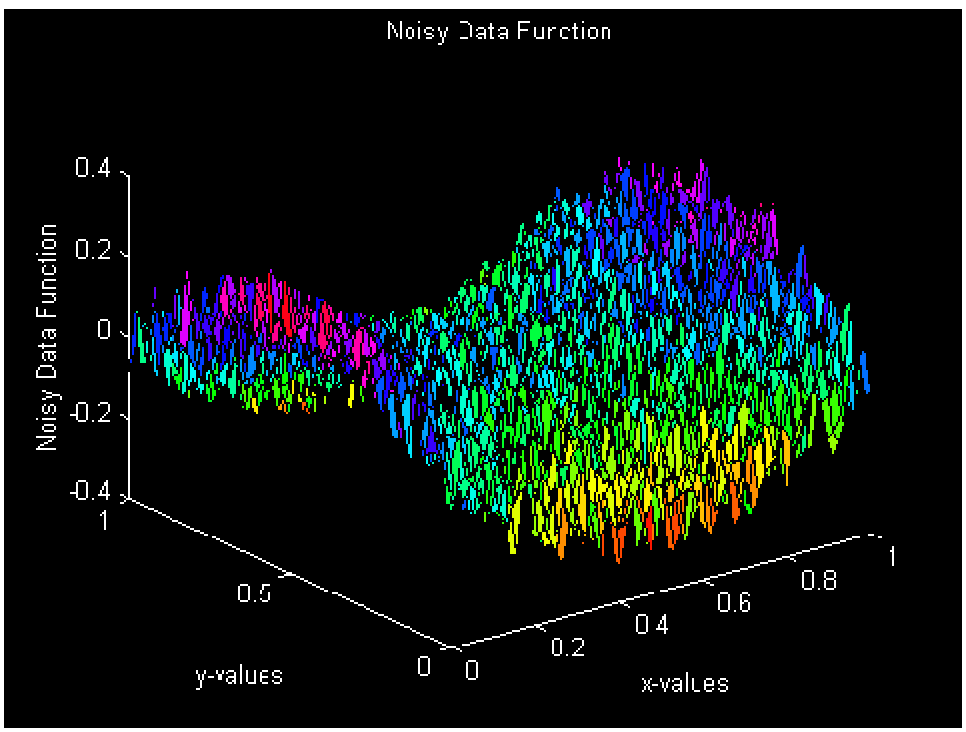
There is no question regarding the importance of this book for applied mathematicians working in inverse problems and for engineers, physicists, geologists, and others who need to recover functions from data. This book should be on the bookshelf of all practitioners of the solution of inverse problems."

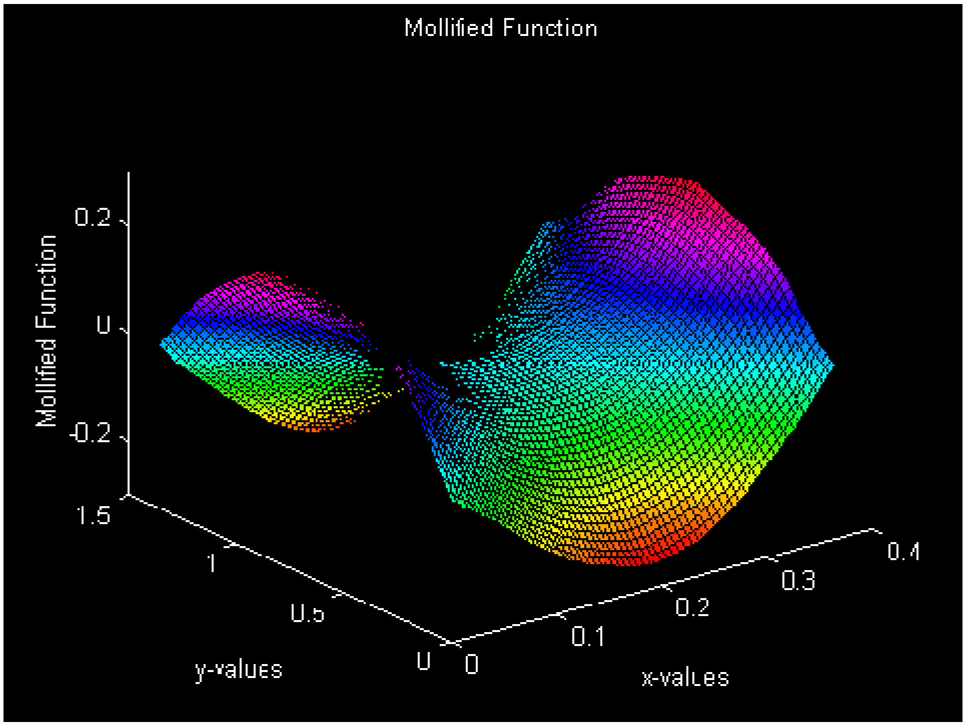
Michigan State University, 1994.

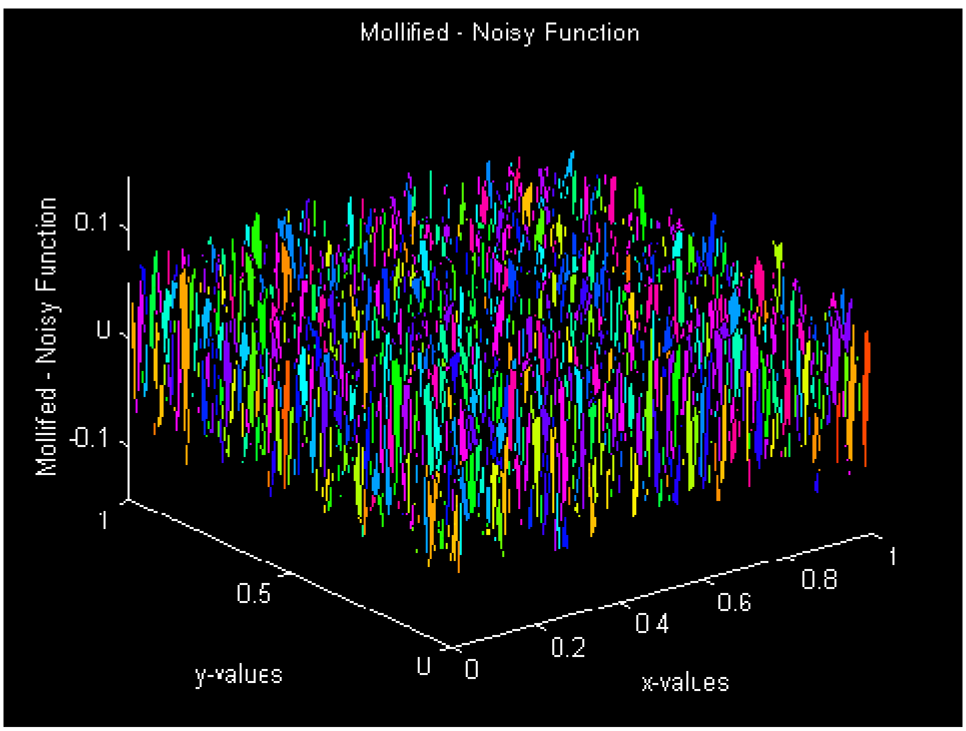

Features
Automatic
Robust
Efficient
No need for noise information
Entire domain reconstruction of the derivative including the boundary

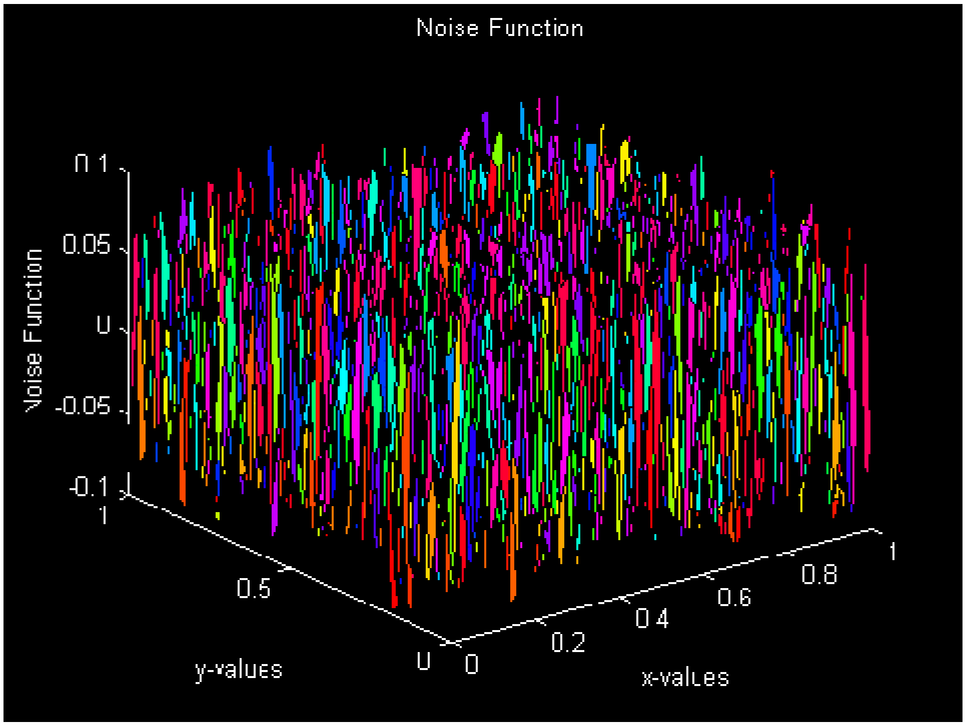

Surface Fitting
Example No. 1
Number of data points in [0,1] x [0,1]: 128 x 128
Maximum data noise: 0.1
Relative l2-error mollified data in [0,1] x [0,1]: 0.00469

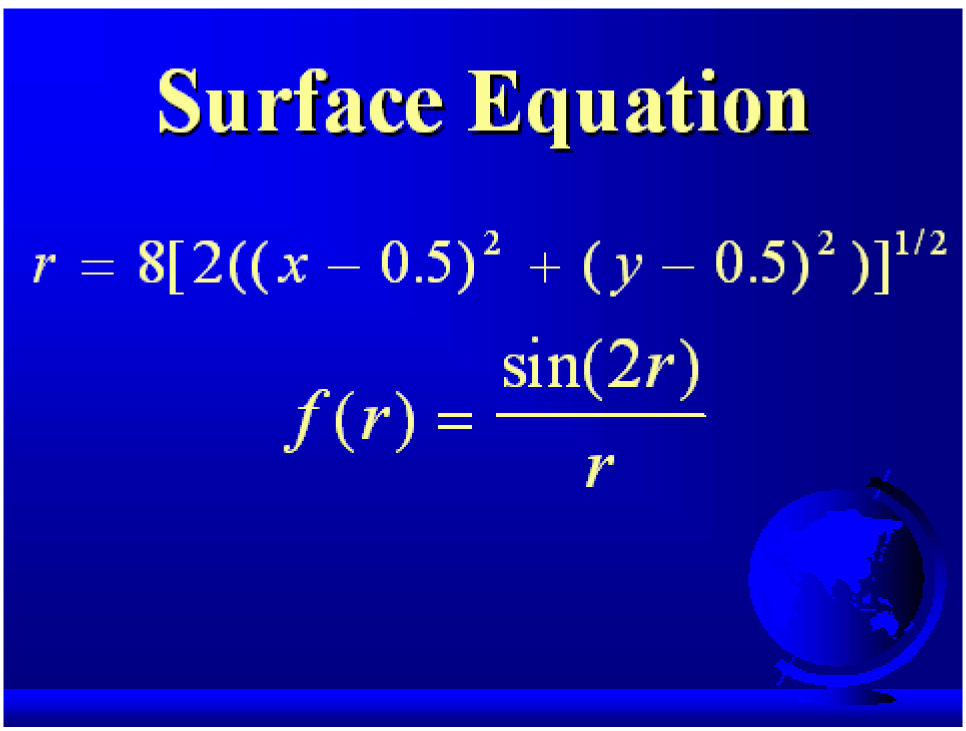

Surface Equation
$r = x - 0.5$
$s = y - 0.5$
$f(r,s) = r^2 - s^2$

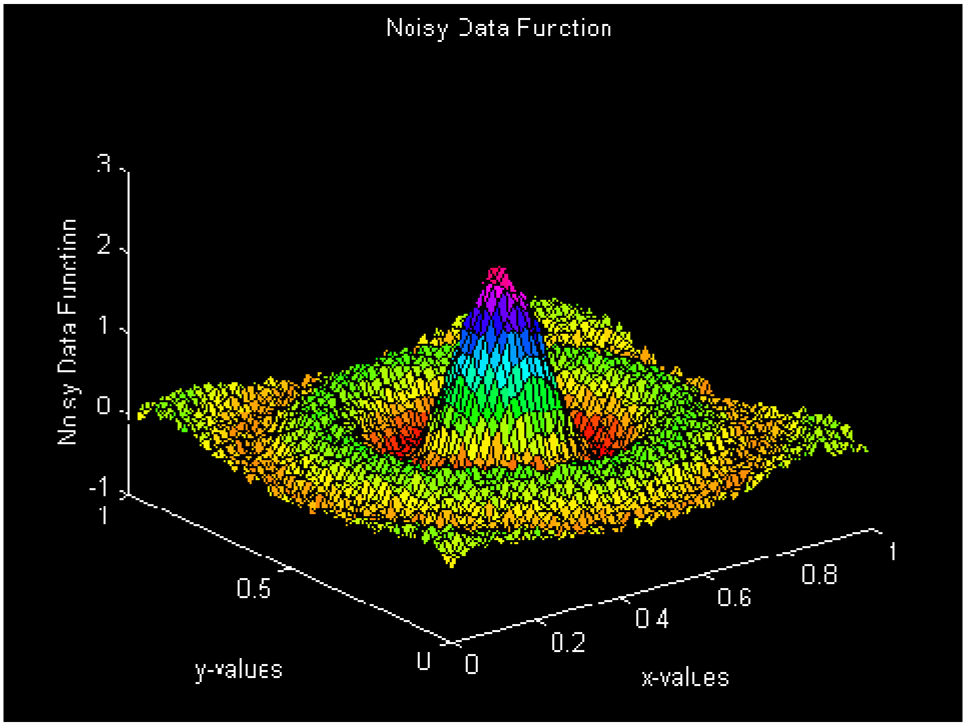

Noisy Data Function
Noisy Data Function
0.4
0.2
0
-0.2
-0.4
1
0.5
0
y-values
0
0.2
0.4
0.6
0.8
1
x-values

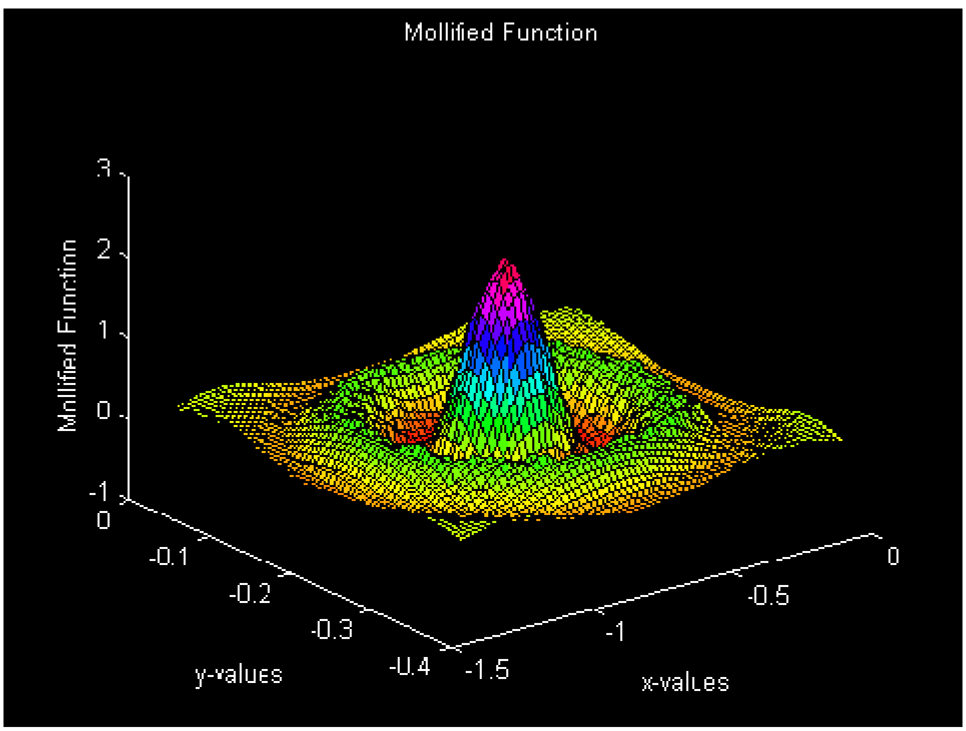

Mollified Function
Mollified Function
0.2
0
-0.2
1.5
1
0.5
0
y-values
0
0.1
0.2
0.3
0.4
x-values

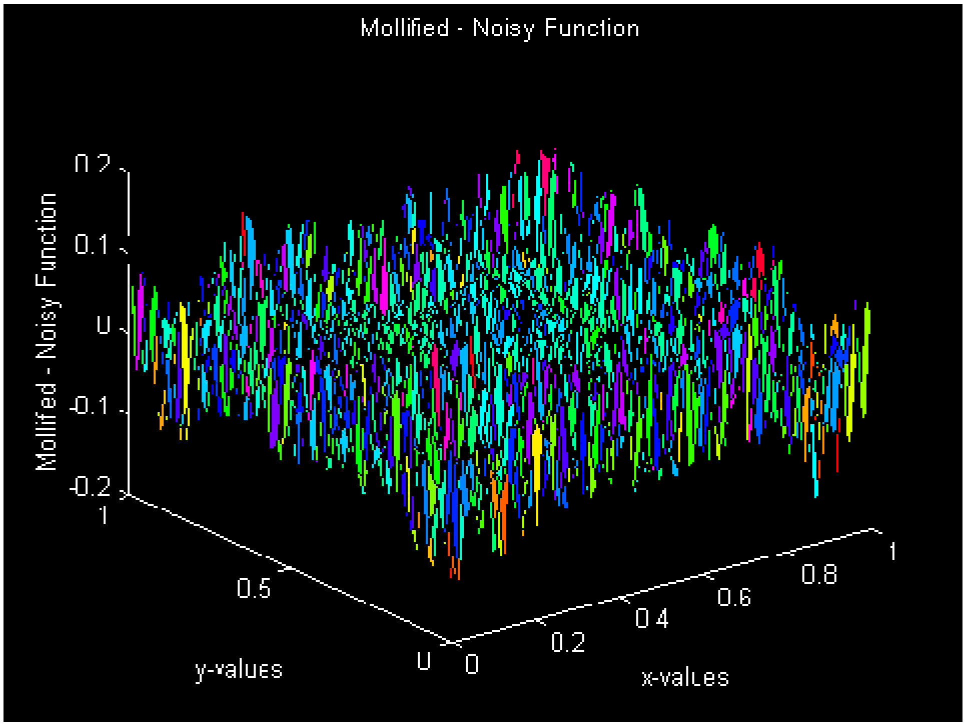

Mollified - Noisy Function
Mollifed - Noisy Function
0.1
0
-0.1
1
0.5
0
y-values
0
0.2
0.4
0.6
0.8
1
x-values

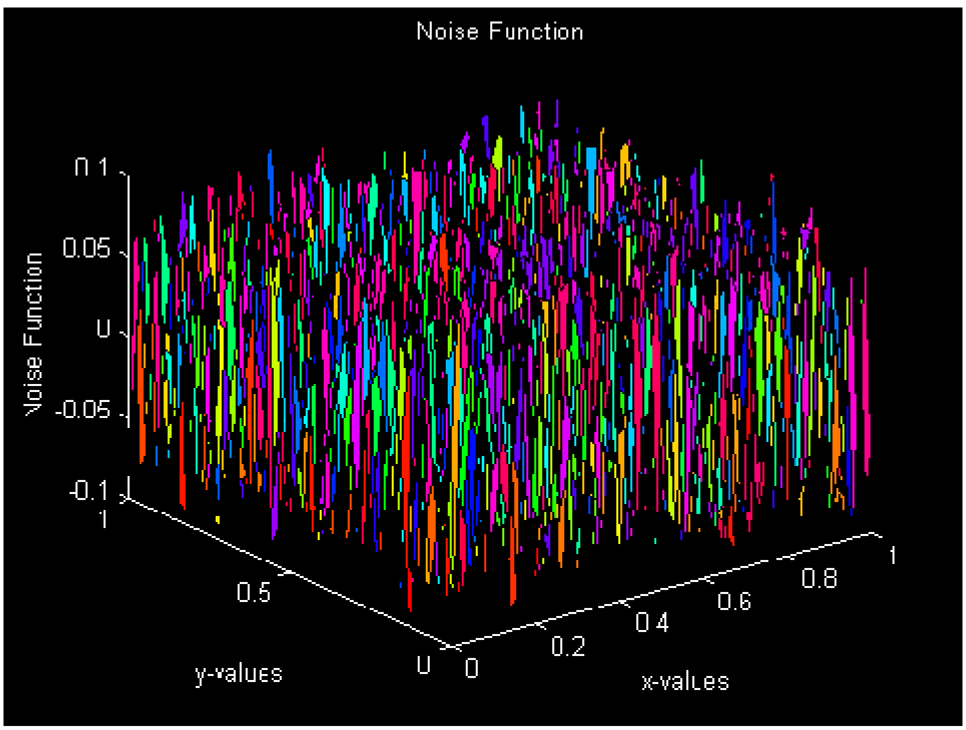

Noise Function
Noise Function
0.1
0.05
0
-0.05
-0.1
1
0.5
0
y-values
0
0.2
0.4
0.6
0.8
1
x-values

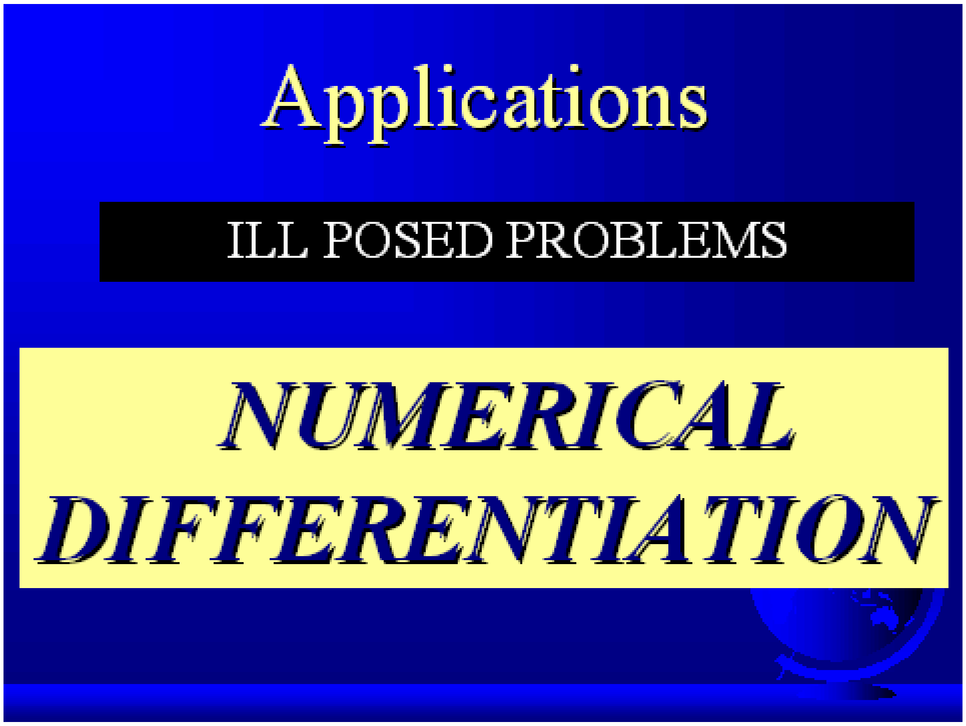

Surface Equation
$r = 8[2((x-0.5)^2 + (y-0.5)^2)]^{1/2}$
$f(r) = \frac{\sin(2r)}{r}$

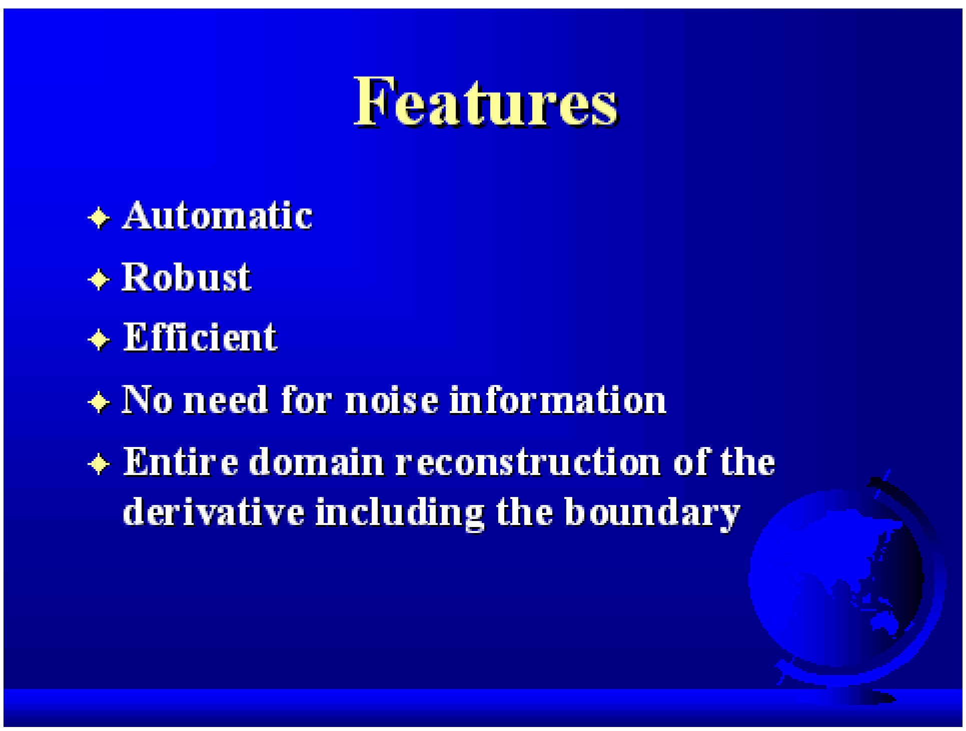

Noisy Data Function
Noisy Data Function
3
2
1
0
-1
1
0.5
0
y-values
0
0.2
0.4
0.6
0.8
1
x-values

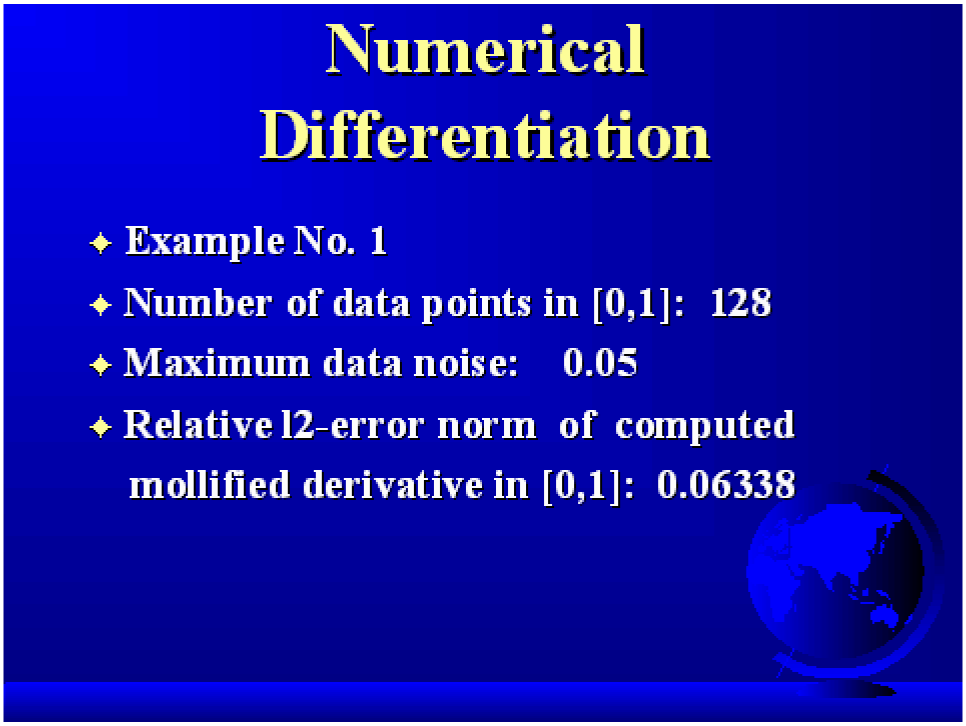

Mollified Function
Mollified Function
3
2
1
0
-1
0
-0.1
-0.2
-0.3
-0.4
y-values
-1.5
-1
-0.5
0
x-values

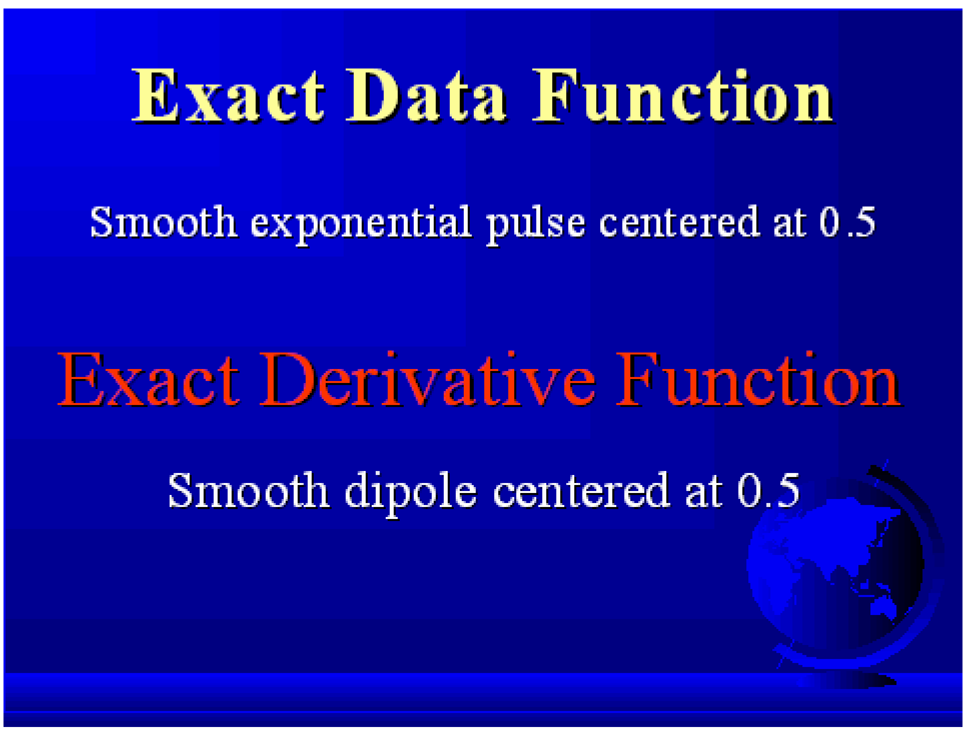

Mollified - Noisy Function
Mollifed - Noisy Function
0.2
0.1
0
-0.1
-0.2
1
0.5
0
y-values
0
0.2
0.4
0.6
0.8
1
x-values

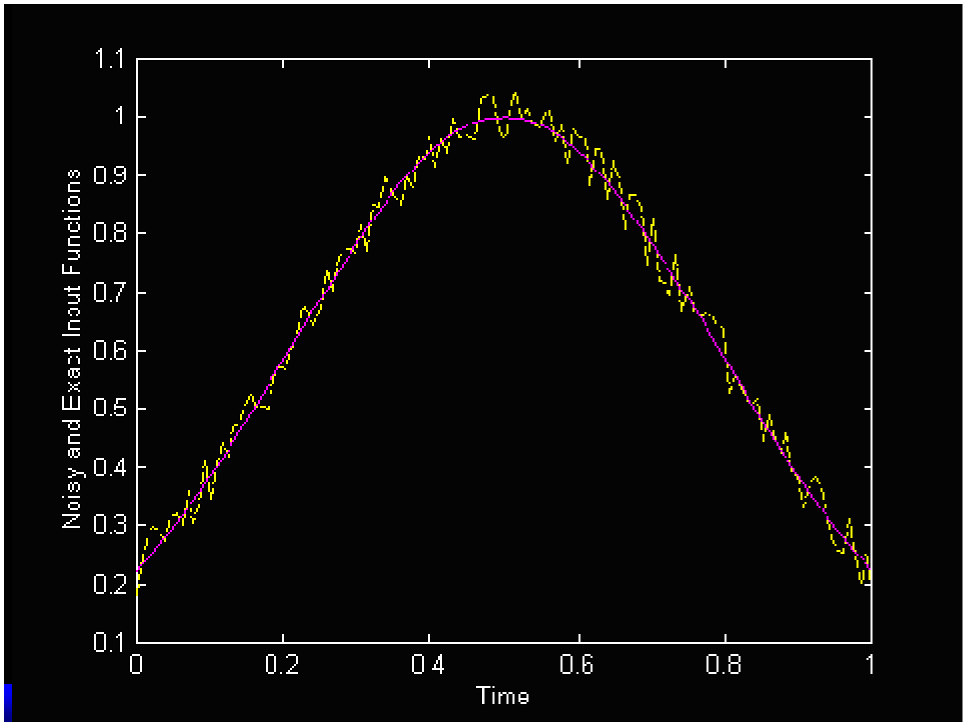

Noise Function
Noise Function
0.1
0.05
0
-0.05
-0.1
1
0.5
0
y-values
0
0.2
0.4
0.6
0.8
1
x-values

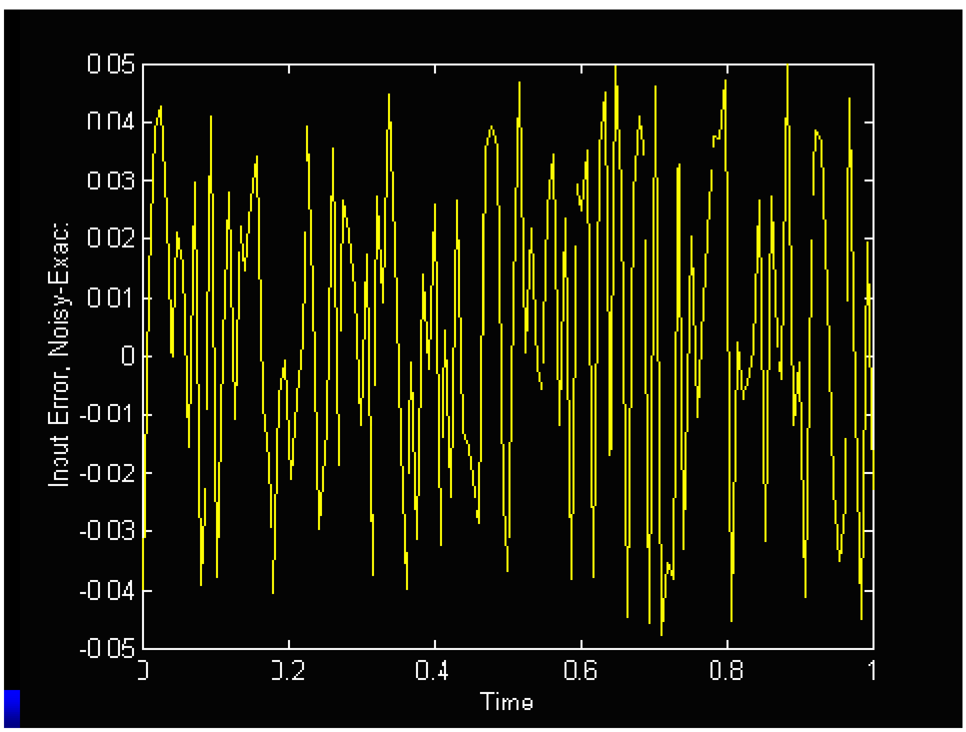

Applications
ILL POSED PROBLEMS
NUMERICAL
DIFFERENTIATION

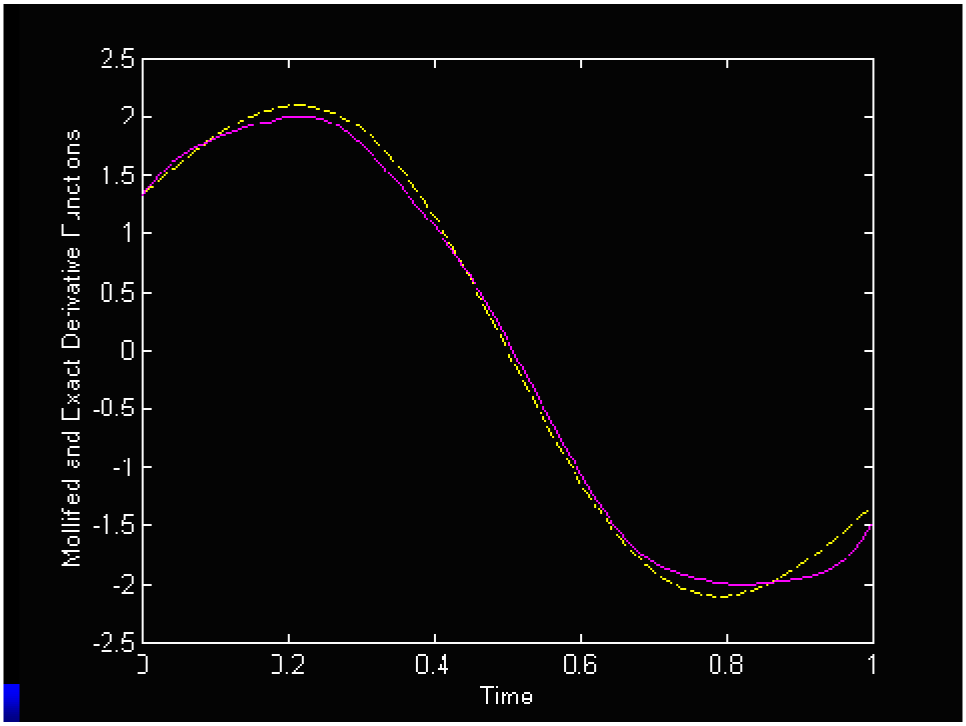

Features
Automatic
Robust
Efficient
No need for noise information
Entire domain reconstruction of the
derivative including the boundary

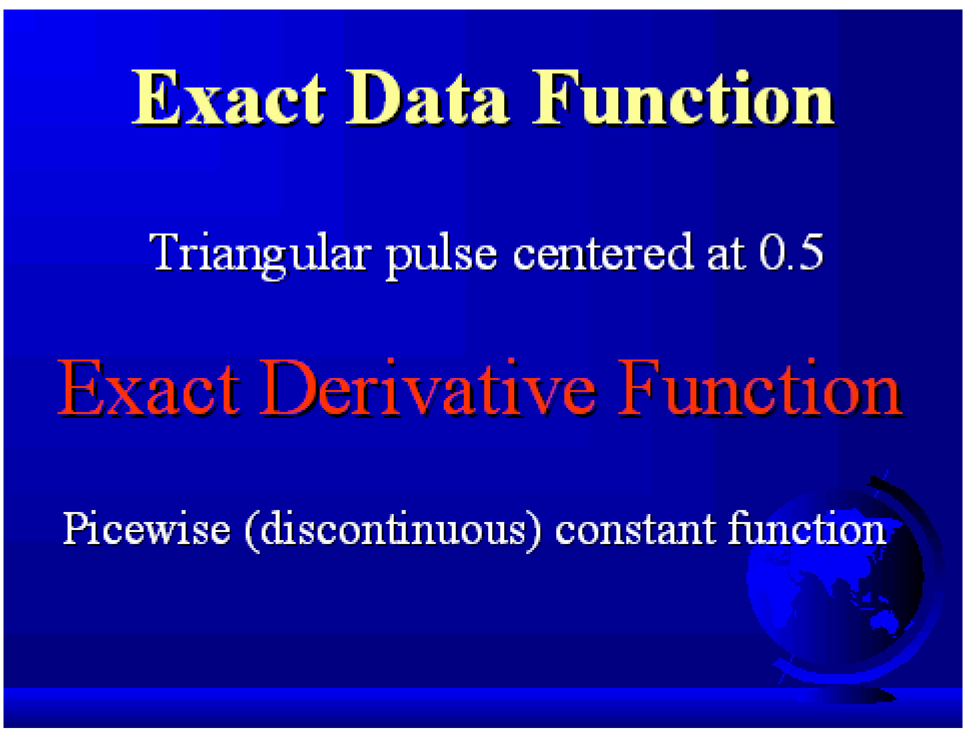

Numerical Differentiation
Example No. 1
Number of data points in [0,1]: 128
Maximum data noise: 0.05
Relative l2-error norm of computed mollified derivative in [0,1]: 0.06338

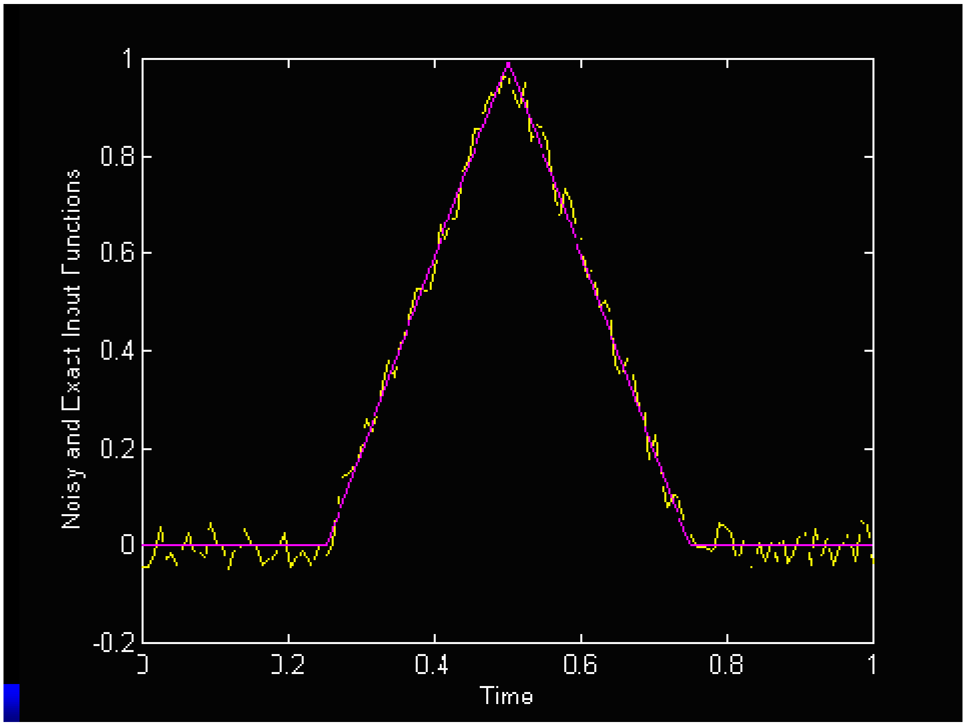

Exact Data Function
Smooth exponential pulse centered at 0.5
Exact Derivative Function
Smooth dipole centered at 0.5

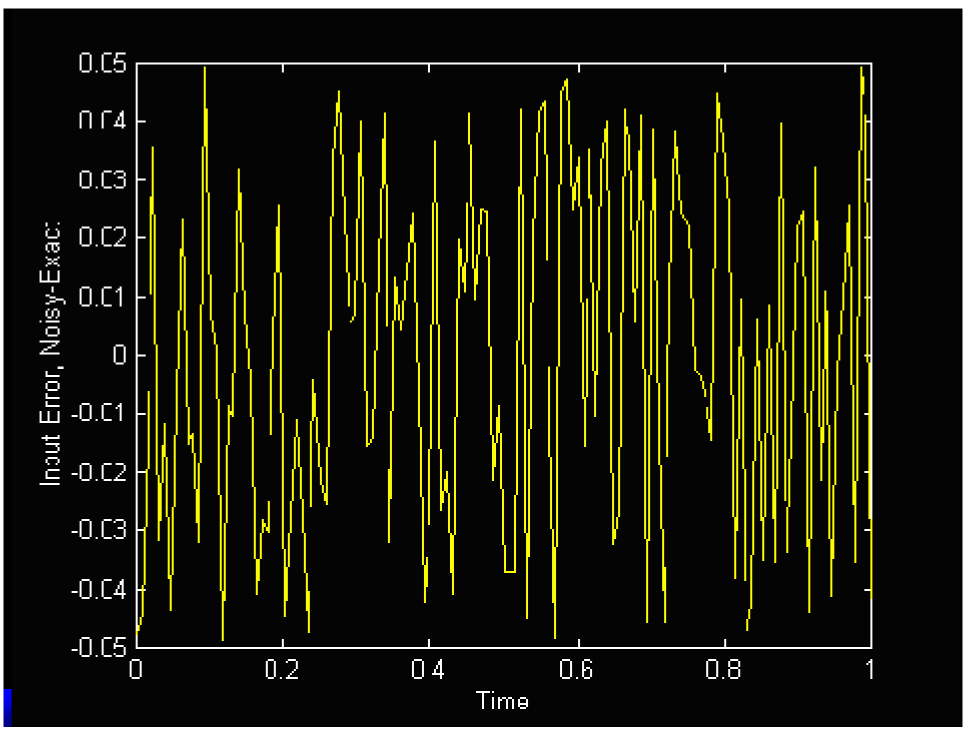

Noisy and Exact Inout Functions
Time
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.2
0.4
0.6
0.8
1

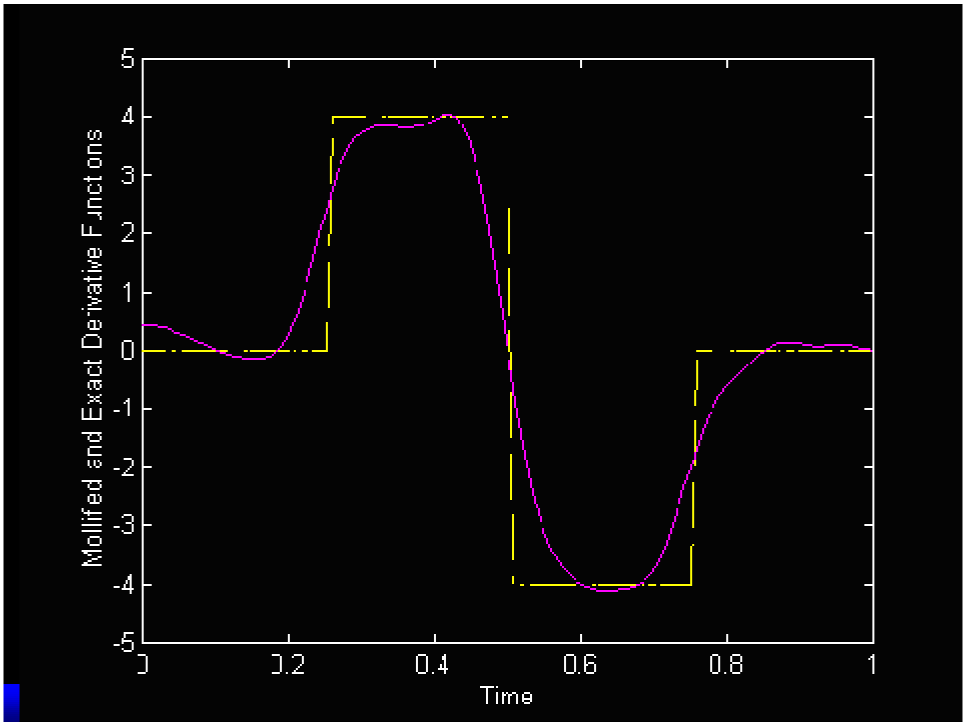

Inout Error, Noisy-Exac
Time
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
0.2
0.4
0.6
0.8
1


2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
0
0.2
0.4
0.6
0.8
1
Time
Mollifed and Exact Derivative Functions


Exact Data Function
Triangular pulse centered at 0.5
Exact Derivative Function
Picewise (discontinuous) constant function


Noisy and Exact Input Functions
Time
1
0.8
0.6
0.4
0.2
0
-0.2
0
0.2
0.4
0.6
0.8
1


Input Error, Noisy-Exact
Time
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
0
0.2
0.4
0.6
0.8
1


Mollifed and Exact Derivative Functions
Time
5
4
3
2
1
0
-1
-2
-3
-4
-5
0
0.2
0.4
0.6
0.8
1