THE MOLLIFICATION METHOD AND THE NUMERICAL SOLUTION OF ILL-POSED PROBLEMS

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To the musicians in my life:
Diego S., Veronica, and Francis.
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During the last 20 years, the subject of ill-posed problems has expanded from a collection of individual techniques to a highly developed and rich branch of applied mathematics. This textbook essentially builds, from basic mathematical concepts, the understanding of the most important aspects of the numerical treatment of the applied inverse theory.

The subject has grown—and continues to grow—at such a fast pace that it is impossible to offer a complete treatment in an introductory textbook and all that can be done is to discuss a few important and interesting topics. Inevitably, in making the selection, I have been influenced by my own interests which, on the other hand, allowed me the pleasure to write about the particular problems with which I am most familiar. This book is intended to be a self-contained presentation of practical computational methods which have been extensively and successfully applied to a wide range of ill-posed problems. The nature of the subject demands the application of special mathematical techniques—rarely seen in typical science courses and strange to normal engineering curricula—with which it is initially difficult to relate the steps of a calculation with the more classical concepts of stability and accuracy. This book is intended to solve the problem by giving an account of the theory that builds from the phenomena to be explained, keeping everything in as elementary a level as possible, making it useful to a wide circle of readers.

The primary goal of this book is to provide an introduction to a number of essential ideas and techniques for the study of inverse problems that are ill posed. There is a clear emphasis on the mollification method and its multiple applications when implemented as a space marching algorithm. As such, this book is intended to be an outline of the numerical results obtained with the
mollification method and a manual of various other methods which are also used in arriving at some of these results. Although the presentation concentrates mostly on problems with origins in mechanical engineering, many of the ideas and methods can be easily applied to a broad class of situations.

This book—an outgrowth of classes that the author has taught at the University of Cincinnati for several years in the Seminar of Applied Mathematics—is organized around a series of specific topics aimed at upper-level undergraduates and first-year graduate students in applied mathematics, the sciences, and engineering. It may be used as a primary test for a course on computational methods for inverse ill-posed problems or as a reference work for professionals interested in modeling inverse phenomena in general.

The treatment is strongly computational, with many examples and exercises, and truly interdisciplinary. There is more than enough material in the book to be covered in a semester or two-quarters-long course. Although all the problems considered are physically motivated, a knowledge of the physics involved is not essential—but always very useful!—for the understanding of the mathematical aspects of these problems. It has been my experience, after teaching this material several times, that the subject is most appreciated by the students when they write programs of their own and see them work. This is the main reason for having computational exercises in the book. An "experimental" approach to numerical modeling—defining and carefully testing the new numerical methods on simple problems with known solutions, before attempting to formally prove their stability and accuracy—is often the best way to proceed. The students are advised to work on as many exercises as possible in each chapter, as this is the best way to learn the material and to check if students master the subject.

Chapter 1 begins with the classical topic of numerical differentiation as an inverse problem. The mollification method is then introduced and a thorough discussion of its numerical implementation follows.

In Chapter 2 we investigate Abel's integral equation—another classical problem of mathematical physics—and four different methods are developed and placed in their proper computational framework.

Chapter 3—the main thrust of the book—is devoted to the one-dimensional inverse heat conduction problem (IHCP). The discussion of several mathematical models and their pertinent numerical algorithms for the approximate determination of the unknown transient temperature and heat flux functions is developed here.

Chapter 4 on the two-dimensional IHCP is presented as an integral part of the text. It is in this topic area where the reader can find the most prolific and challenging source of new problems.

Chapter 5 contains three independent applications for space marching solutions of the IHCP: identification of boundary source functions and radiation laws, numerical solutions of the Stefan problem and inverse Stefan problem, and determination of the initial temperature distribution in a
one-dimensional conductor from transient measurements at interior locations.

Chapter 6 illustrates further applications of stable numerical differentiation techniques ranging from the determination of forcing terms in systems of ordinary differential equations to the identification of transmissivity coefficients in linear and nonlinear elliptic and parabolic equations in one space dimension.

Appendix A offers a selected overview of the essential mathematical tools used in these lectures. It should constitute a genuine aid for nonmathematicians.

Finally, Appendix B contains an up-to-date citing of the literature related to the IHCP. It might certainly be of value to graduate students and researchers interested in the subject.

Diego A. Murio
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D. A. M.
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In several practical contexts, it is sometimes necessary to estimate the derivative of a function whose values are given approximately at a finite number of discrete points. It is easy to imagine many different situations—mostly involving integral equations and ordinary and partial differential equations—related with the question of numerical differentiation of measured (noisy) data. Several interesting applications of this basic problem will be investigated in the following chapters.

1.1 DESCRIPTION OF THE PROBLEM

In order to gain some insight on the underlying principles, let us analyze first the ideal situation where we seek an approximation to the derivative function $f'(x)$ under the assumption that the exact (errorless) data function $f(x)$ is sufficiently smooth on a given interval $[a, b]$. For example, if we assume that $f \in C^3([a, b])$—third derivative continuous on $[a, b]$—and satisfies the uniform bound

$$
\|f'''\|_{\infty, [a, b]} = \max_{a < x < b} |f'''(x)| \leq M_3,
$$

it is possible to approximate the derivative $f'(x)$ by the centered difference

$$
D_0f(x) = \frac{f(x + h) - f(x - h)}{2h}, \quad a \leq x - h < x < x + h \leq b.
$$
NUMERICAL DIFFERENTIATION

We can estimate the truncation error by Taylor's series. In fact, we have

\[
 f(x + h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(s_1), \quad x < s_1 < x + h, \\
 f(x - h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(s_2), \quad x - h < s_2 < x.
\]

Subtracting the last two expressions and dividing by 2h, we get

\[
 D_0(x) = f'(x) + \frac{h^2}{6}(f'''(s_1) + f'''(s_2))
\]

and

\[
 |D_0f(x) - f'(x)| \leq \frac{h^2}{3}M_3 = O(h^2). \tag{1.1}
\]

The approximation of the derivative by centered differences—in the absence of noise in the data—is a second-order consistent procedure, that is, as \( h \) approaches 0, \( D_0f(x) \) converges to \( f'(x) \) with rate proportional to \( h^2 \).

However, in real situations we deal with experimentally determined (measured) data that contain errors, systematic and random. The following discussion will assume that any systematic errors have been removed from the supplied data function. Consequently, instead of the ideal data function \( f(x) \), we consider a measured data function \( f_m(x) \) obtained by adding the random noise function \( N(x) \) to \( f(x) \). We also assume that the amplitude of the noise is bounded by \( \epsilon \). Thus,

\[
 f_m(x) = f(x) + N(x), \quad a \leq x \leq b,
\]

and

\[
 \|N(x)\|_{\infty,[a,b]} = \max_{a \leq x \leq b} |N(x)| \leq \epsilon.
\]

To illustrate the new situation, consider a smooth but arbitrary ideal data function \( f(x) \) and the also very smooth noisy function \( N(x) = \alpha \sin(wx) \), \( |\alpha| \leq \epsilon \), \( w \in \mathbb{R} \), defined on the entire real line. Then

\[
 f'_m(x) = f'(x) + \alpha w \cos(wx),
\]

and for small \( \alpha \) and large \( w \), the derivative error

\[
 f'_m(x) - f'(x) = \alpha w \cos(wx)
\]

is greatly amplified for \( x = \pm k\pi/w, k = 0, 1, 2, \ldots \).
In terms of centered differences,
\[ D_0 f_m(x) = D_0 f(x) + \frac{N(x + h) - N(x - h)}{2h} \]
\[ = D_0 f(x) + \frac{\alpha}{h} \sin(wh) \cos(wx). \]  
(1.2)

Now suppose that \( w \) is chosen, as a function of \( h \), to be \( w = \pi / 2h \). Hence, for each \( h \),

\[ D_0 f_m(x) = D_0 f(x) + \frac{\alpha}{h} \cos\left(\frac{\pi x}{2h}\right) \]

and the second term on the right-hand side—the rounding error—is inversely proportional to the interval of computation \( h \). Therefore, with a decrease in \( h \) the rounding error increases. This is indeed the case in general. Even if \( N(x) \) represents a random noise variable with amplitude \( |N(x)| \leq \varepsilon \), we have

\[ -\frac{\varepsilon}{h} \leq \frac{N(x + h) - N(x - h)}{2h} \leq \frac{\varepsilon}{h} \]

and whenever the numerator \( N(x + h) - N(x - h) \) is different from 0, the rounding error is greatly amplified for small values of \( h \).

From a more honest computational point of view, we would like to estimate the difference between the "ideal" derivative function \( f'(x) \)—a complete abstract object numerically—and the actual "computed" value \( D_0 f_m(x) \) obtained from the measured data using finite differences. We proceed as follows.

From

\[ f'(x) - D_0 f_m(x) = f'(x) - D_0 f(x) + D_0 f(x) - D_0 f_m(x), \]

using the triangle inequality, (1.1) and (1.2),

\[ |f'(x) - D_0 f_m(x)| \leq |f'(x) - D_0 f(x)| + |D_0 f(x) - D_0 f_m(x)| \]
\[ \leq \frac{h^2}{3} M_3 + \frac{|\alpha|}{h} |\sin(wh)| |\cos(wx)|. \]

If we consider, as before, the particular values \( w = \pi / 2h \), the estimate becomes

\[ |f'(x) - D_0 f_m(x)| \leq \frac{h^2}{3} M_3 + \frac{|\alpha|}{h} \left| \cos\left(\frac{\pi x}{2h}\right) \right|. \]
which strongly suggests choosing \( h \) so as to minimize the upper bound for the total error. This seems reasonable since, in general, as \( h \) decreases, the truncation error decreases and the rounding error increases.

The upper bound, achievable for some values of \( x \), shows that at least near those points it is not possible to approximate the ideal derivative function \( f'(x) \) by centered finite differences as in (1.1); now, as \( h \) approaches 0, the error blows up! This result is, of course, totally expected because the known instability of \( f_m'(x) \) is inherited by the finite-difference approximation \( D_0 f_m(x) \).

The preceding discussion shows that the process of differentiation is such that small errors in the data function might produce large errors in the derivative function, independently of how smooth the error function is. Moreover, the same occurrence is notably true in the context of discrete approximations for numerical differentiation with noisy data. This situation is also encountered in many other problems and justifies the following definition.

**DEFINITION 1.1 (Hadamard)** A mathematical problem is said to be well posed if it has a unique solution and the solution depends continuously on the data.

A problem which is not well posed is said to be ill posed. The differentiation problem is an example of the latter.

The conclusion is simple. The application of standard numerical techniques to the process of numerical differentiation might yield nonphysical "solutions." What can be done?

First of all, we need to characterize the source of ill-posedness for the differentiation problem. A new insight can be obtained by performing a Fourier analysis of the process. If \( f(x), f'(x) \in L^2(\mathbb{R}) \), then \( \hat{f}(w) = iw \hat{f}(w) \). This means that \( f \) is not just "a function in \( L^2(\mathbb{R}) \)"; its high-frequency behavior is such that \( ||\hat{f}|| \) decreases faster than \( ||w^{-1}|| \) as \( ||w|| \to \infty \). Now, even if we assume that the noise function \( N(x) \in L^2(\mathbb{R}) \), there is no reason to believe that the high-frequency components of \( \hat{N}(w) \) will be subject to such a rapidly decreasing behavior and we cannot, in general, guarantee that the product \((iw)\hat{N}(w)\) will be in \( L^2(\mathbb{R}) \).

We conclude that the differentiation problem, in this setting, is an ill-posed problem in the high-frequency components and any attempt to stabilize the problem—restore continuity with respect to the data—in order to be successful, must take this consideration into account.

### 1.2 STABILIZED PROBLEM

Let \( C^0(I) \) denote the set of continuous functions over the interval \( I = [0, 1] \) with \( ||f||_{\infty,I} = \max_{x \in I} |f(x)| < \infty \).
We consider the problem of estimating in $I$ the derivative $f'(x)$ of a function $f(x)$ defined on $I$ and observed with error. We assume that $f(x)$ is twice continuously differentiable on $I$. Instead of $f(x)$, we know some data function $f_m(x) \in C^0(I)$ such that $\|f_m - f\|_{\infty, i} \leq \epsilon$.

Our initial task is to stabilize the differential process. To that end, we first introduce the function

$$\rho_\delta(x) = \frac{1}{\delta \sqrt{\pi}} \exp \left( \frac{-x^2}{\delta^2} \right),$$

the Gaussian kernel of "blurring radius" $\delta$. We notice that $\rho_\delta$ is a $C^\infty$ (infinitely differentiable) function that falls to nearly 0 outside a few radii from its center ($\approx 3\delta$), is positive, and has total integral 1.

After extending the ideal data function $f(x)$ and the measured data function $f_m(x)$ to the interval $I_\delta = [-3\delta, 1 + 3\delta]$ in such a way that they decay smoothly to 0 in $[-3\delta, 0] \cup [1, 1 + 3\delta]$ and they are 0 in $\mathbb{R} - I_\delta$, the convolution

$$J_\delta f(x) = (\rho_\delta * f)(x) = \int_{-\infty}^{\infty} \rho_\delta(x - s)f(s)\, ds
\equiv \int_{x - 3\delta}^{x + 3\delta} \rho_\delta(x - s)f(s)\, ds, \quad (1.3)$$

defines a $C^\infty$ function in the entire real line.

The extensions can be easily accomplished, for instance, by defining

$$f_m(x) = f_m(0) \exp \left( \frac{x^2}{(3\delta)^2 - x^2} \right), \quad -3\delta \leq x \leq 0,$$

$$f_m(x) = f_m(1) \exp \left( \frac{(x - 1)^2}{(x - 1)^2 - (3\delta)^2} \right), \quad 1 \leq x \leq 1 + 3\delta. \quad (1.4)$$

$J_\delta f$ is the mollifier of $f$ and $\delta$ is the radius of mollification.

Notice that the Fourier transform of $J_\delta N(x)$ is given by

$$(J_\delta N)(w) = \hat{\rho}_\delta(w) \hat{N}(w) = \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{w^2 \delta^2}{4} \right) \hat{N}(w)$$

and damps those Fourier components of the noise $N$ with wavelength $2\pi/w$ much shorter than $2\pi\delta$; the longer wavelengths are damped hardly at all, as
required by our analysis in the previous section. We also observe that if \( f \) has compact support \( K \), the mollification function defined by (1.3) does not have compact support and, as such, does not verify Definition A.9. However, for all practical purposes we can consider its "numerical support" to be compact and extended up to approximately 3\( \delta \) units away from the boundary of \( K \).

Moreover, from the definition, it follows immediately that

\[
\frac{d}{dx} J_\delta f(x) = (\rho_\delta * f)'(x) = (\rho_\delta * f')(x) = (\rho_\delta * f)(x).
\]

The following two lemmas are fundamental for our results.

**Lemma 1.1** (Consistency) If \( \|f''\|_{\infty, I} \leq M_2 \), then

\[
\|(\rho_\delta * f)' - f'\|_{\infty, I} \leq 3\delta M_2.
\]

**Proof.** For \( x \in I \),

\[
(\rho_\delta * f)'(x) = \int_{-\infty}^{\infty} \rho_\delta(x - s)f'(s)\, ds
\]

and

\[
f'(x) = \int_{-\infty}^{\infty} \rho_\delta(x - s)f'(x)\, ds.
\]

Subtracting and using the mean value theorem,

\[
|(\rho_\delta * f)'(x) - f'(x)| \leq \int_{-\infty}^{\infty} \rho_\delta(x - s)|f'(s) - f'(x)|\, ds
\]

\[
\leq \int_{x-3\delta}^{x+3\delta} \rho_\delta(x - s)|f'(s) - f'(x)|\, ds
\]

\[
\leq 3\delta M_2.
\]

Thus,

\[
\|(\rho_\delta * f)' - f'\|_{\infty, I} \leq 3\delta M_2.
\]

**Lemma 1.2** (Stability) If \( f_m(x) \in C^0(I) \) and \( \|f_m - f\|_{\infty, I} \leq \varepsilon \), then

\[
\|(\rho_\delta * f_m)' - (\rho_\delta * f)'\|_{\infty, I} \leq \frac{2\varepsilon}{\delta \sqrt{\pi}}.
\]
Proof. For $x \in I$,

$$\left| (\rho_\delta * f_m)'(x) - (\rho_\delta * f)'(x) \right|$$

$$\leq \int_{-\infty}^{\infty} \left| \frac{d}{dx} \rho_\delta(x-s) \right| |f_m(s) - f(s)| \, ds$$

$$\leq \varepsilon \int_{-\infty}^{\infty} \left| \frac{d}{dx} \rho_\delta(x-s) \right| \, ds = 2\varepsilon \int_{0}^{\infty} \frac{d}{dx} \rho_\delta(x) \, dx = \frac{2\varepsilon}{\delta \sqrt{\pi}}.$$

Lemma 1.2 shows that attempting to reconstruct the derivative of the mollified data function is a stable problem with respect to perturbations in the data, in the maximum norm, and for $\delta$ fixed.

Theorem 1.1 (Error Estimate) Under the conditions of Lemmas 1.1 and 1.2,

$$\| (\rho_\delta * f_m)' - f' \|_{\infty, I} \leq 3\delta M_2 + \frac{2\varepsilon}{\delta \sqrt{\pi}}. \quad (1.5)$$

Proof. The estimate follows from Lemmas 1.1 and 1.2 and the triangle inequality. ☐

We observe that the error estimate (1.5) is minimized by choosing $\delta = \bar{\delta} = [2\varepsilon / 3M_2 \sqrt{\pi}]^{1/2}$. For this "optimal" choice of the radius of mollification, the error estimate becomes

$$\| (\rho_\delta * f_m)' - f' \|_{\infty, I} \leq 2\pi^{-1/4} \sqrt{6M_2 \varepsilon},$$

and we obtain uniform convergence as $\varepsilon \to 0$—as the quality of the data improves—with rate $O(\varepsilon^{1/2})$.

However, in practical computations we have to solve the problem with a fixed upper bound $\varepsilon$, and the choice $\delta = \bar{\delta}$ is impossible because $M_2$ is not known, in general.

Before discussing the selection of the radius of mollification, let us summarize our approach. This same basic strategy will be used again and again to solve different ill-posed problems and with different methods.

First, we replace the original ill-posed problem of finding $f'$ by the new problem of finding $J_{\delta \xi} f'$. The new problem is well posed, depends on a parameter $\delta > 0$, and, in the absence of noise in the data, is consistent with the original problem (Lemma 1.1).

Second, in the presence of noise in the data, with a fixed value of the parameter $\delta > 0$, we solve the new problem—not the original one—which is stable with respect to perturbations in the data (Lemma 1.2).
It is customary to say that the family $J_\delta f', \delta > 0$—satisfying Lemmas 1.1 and 1.2—is a *regularizing family* for the differentiation problem.

Figures 1.1 and 1.2 illustrate a random noise function of amplitude 0.1 added to $f(x) = 1$ in real $x$ space, its Fourier transform, the mollified (filtered) version in the frequency space, and the mollified noise function back in real space, respectively. Observe carefully the relationships among the high-frequency components before and after the filtering procedure.

**Remarks**

1. It is a simple task to estimate the error between the exact derivative $f'$ restricted to the grid points and the centered-difference approximation $D_0(\rho_\delta * f_m)$. Given that $(\rho_\delta * f_m) \in C^3(I)$, if $M_{3,\delta}$ denotes a uniform upper bound for its third derivative, we simply combine estimates (1.1)
and (1.2) using the triangle inequality to obtain
\[ \| D_0(\rho_\delta * f_m) - f' \| \leq \frac{h^2}{3} M_{3,6} + 3\delta M_2 + \frac{2\varepsilon}{\delta\sqrt{\pi}}. \]

2. For the analysis of a totally discretized approach of the mollification method, the reader is referred to the exercises in Sec. 1.7.

1.3 DIFFERENTIATION AS AN INVERSE PROBLEM

Consider a Fredholm linear integral equation of the first kind
\[ f(x) = \int_0^1 k(x, s) g(s) \, ds, \quad (1.6) \]
where the kernel function \( k \) is square integrable in \([0, 1] \times [0, 1]\) and the only solution of the homogeneous problem

\[
0 = \int_0^1 k(x, s) g(s) \, ds
\]

is \( g(x) = 0, \, 0 \leq x \leq 1. \)

Ordinarily, \( k \) and \( g \) are known functions and we are asked to determine the solution function \( f \) so as to satisfy (1.6). So posed, this is a direct problem.

There is, however, an interesting inverse problem that can be formulated. The objective of this new problem is to determine part of the "structure" of the system represented by the prototype Fredholm equation. In our case, we would like to find the function \( g(x) \) from experimental information given by the approximate knowledge of the solution of the direct problem \( f(x) \).

From the physical point of view, the distinction between a direct (going from \( g \) to \( f \)) and an inverse problem (going from \( f \) to \( g \)) is of a phenomenological nature. Actual experiments are associated only with direct problems (cause-effect relationship); there are no physical experiments directly linked to inverse problems. It is this unavoidable and natural physical fact that it is sometimes hidden in the mathematical model. This means that in order to experimentally validate the solution of an inverse problem, it is necessary to use this solution a posteriori, as data for the experiment associated with the direct problem. As an example, consider the solution of the heat equation forward in time with initial (time 0) and boundary conditions as the usual direct problem. There are several inverse problems associated with this direct problem—some of them to be discussed later—but, for the moment, we can restrict our attention to the inverse problem (backward in time) of attempting to recover the initial condition from knowledge of the boundary conditions and the temperature distribution at some time \( t > 0 \). It is clear that the inverse problem cannot be directly validated by an experiment because it is impossible to physically reverse the flow of time.

The preceding discussion, obviously, does not apply to mathematical modeling. In the much simpler situation of numerical differentiation, we point out that if in (1.6) the kernel \( k \) is given by

\[
k(x, s) = \begin{cases} 
0, & x < s, \\
1, & x \geq s,
\end{cases}
\]

then solving for \( g \) with \( f \) as data is equivalent to differentiating \( g \), that is, \( g(x) = f'(x) \).