Inverse Problems Light: Numerical Differentiation

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1. INTRODUCTION. Reliable numerical simulations of technical processes require detailed knowledge of the underlying physical models. Consider the simulation of heat transport in a one-dimensional homogeneous medium, where the heat conductivity depends on the temperature. In this case the temperature distribution u is the solution of a one-dimensional parabolic differential equation

$$u_t = \big(a(u)u_x\big)_x, \qquad 0 < x < 1\,,\; 0 < t < T, \tag{1.1}$$

involving a nonlinear diffusion coefficient $a : \mathbb{R} \to \mathbb{R}^+$. Problem (1.1) also serves as a model for the saturation of porous media by liquid flow, in which case $a(u)$ is related to the capillary pressure of the pores.

In certain industrial applications a numerical simulation may require solving (1.1) for u. We call this the *direct problem*. In these simulations it is crucial that a coefficient $a(u)$ be used that is not only qualitatively correct but also reasonably accurate. Unfortunately, tabulated values for $a(u)$ from the literature often provide only a rough guess of the true coefficient; in this case simulations are not likely to be reliable.

Consequently, identification of the diffusion coefficient $a(u)$ from experimental data (typically, $u(x, t)$ for some abscissa $x \in (0, 1)$ and $0 < t < T$) is often the first hurdle to clear. This is the associated *inverse problem*.

A standard method to solve the inverse problem is the *output least squares method*, which tries to match the given data with simulated quantities using a gradient or Newton type method for updating the diffusion coefficient. Alternatively, one can consider (1.1) as a linear equation for $a(u)$. To set up this equation requires numerical differentiation of the data [**6**]. This approach is called the *equation error method.*

It must be emphasized that inverse problems are often very *ill-conditioned*: for example, small changes in $a(\cdot)$ have little effect on the solution u in (1.1), and consequently one cannot expect high resolution reconstructions of a in the presence of measurement errors in u. Indeed, small errors in u may cause large errors in the computed a if they are not taken into account appropriately.

Numerical differentiation of the data encompasses many subtleties and pitfalls that a complex (linear) inverse problem can exhibit; yet it is very easy to understand and analyze. For this reason one could say that numerical differentiation itself is an ideal model for inverse problems in a basic numerical analysis course.

To support this statement we revisit a well-known algorithm for numerical differentiation of noisy data and present a new error bound for it. The method and the error bound can be interpreted as an instance of one of the most important results in *regularization theory* for ill-posed problems. Still, our presentation is on a very basic level and requires no prior knowledge besides standard n-dimensional calculus and the notion of cubic splines.

Groetsch's book [**4**] presents other realistic inverse problems on an elementary technical level. Further examples and a rigorous introduction to regularization theory for the computation of stable solutions to these examples can be found in [**1**].

2. SETTING OF THE PROBLEM. Suppose $y = y(x)$ is a smooth function on $0 \le x \le 1$ and noisy samples $\tilde{y}_i$ of the values $y(x_i)$ are known at the points of a uniform grid $\Delta = \{0 = x_0 < x_1 < \cdots < x_n = 1\}$. Let $h = x_{i+1} - x_i$ be the mesh size of the grid and suppose

$$|\tilde{y}_i - y(x_i)| \le \delta, \tag{2.1}$$

where δ is a known level of noise in the data. For the moment we assume that the boundary data are known exactly:

$$\tilde{y}_0 = y(0) \quad \text{and} \quad \tilde{y}_n = y(1).$$

We are interested in finding a *smooth* approximation $f'(x)$ of $y'(x)$, defined for all $x \in [0, 1]$, from the given data $\tilde{y}_i$, with some guaranteed (best possible) accuracy.

If this material is to be presented in class, the precise notion of smoothness depends on the level of the course. In principle, the Sobolev space $H^2[0, 1]$ of all functions $f \in C^1[0, 1]$ with square integrable second derivative is the appropriate choice. However, $C^2[0, 1]$ would also be all right (see Section 3), but then the following error bounds are no longer optimal.

Many textbooks on numerical analysis lack a satisfactory treatment of numerical differentiation. Usually, the treatment is restricted to the consistency error of sophisticated finite difference quotients while the stability problem due to error propagation is often ignored. Combining consistency error and propagation error for one-sided finite differences, one arrives at the bound

$$\left| \frac{\tilde{y}_{i+1} - \tilde{y}_i}{h} - y'(x) \right| \le O(h + \delta/h), \qquad x_i \le x \le x_{i+1}, \tag{2.2}$$

for the total error provided that $y \in C^2[0, 1]$; for a very nice pedagogical treatment of this subject, see [**3**]. The right-hand side of (2.2)—as a function of h—is plotted in Figure 1 (solid line): it attains a minimal value of $O(\sqrt{\delta})$ for $h \sim \sqrt{\delta}$. When h is smaller, the bound (2.2) deteriorates.

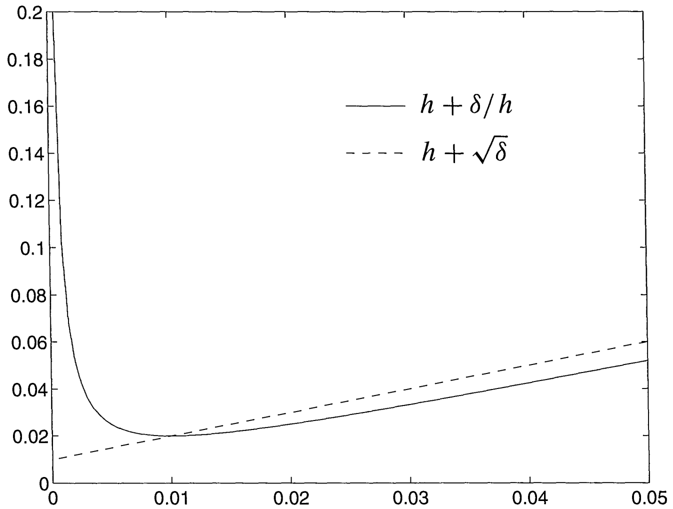

Figure 1. Qualitative behavior of the error bounds (2.2) and (2.7) versus h for fixed $\delta = 10^{-4}$.

There is a trivial solution to the stability problem: discard data until the spacing between the grid points is about $\sqrt{\delta}$ (this is sometimes called *regularization by coarse discretization*). This is not very satisfactory. Each datum carries information that should somehow be put to work. Another shortcoming of finite difference schemes is the lack of smoothness of the resulting approximations of y': the finite difference approximations are only piecewise constant functions.

We therefore take a different approach—one that uses all the data and leads to a smooth approximation. Let

$$\|g\| = \left(\int_0^1 g^2(x)\,dx\right)^{1/2}$$

denote the $\mathcal{L}^2$-norm of a square integrable function over (0, 1). With the aim of taming the wild oscillations in the approximate derivative that typically appear when differentiating noisy data, it appears natural to pose the numerical differentiation problem as a constrained optimization problem:

Problem I. *Minimize* $\|f''\|$ *among all smooth functions* f *satisfying* $f(0) = y(0)$, $f(1) = y(1)$, *and*

$$\frac{1}{n-1}\sum_{i=1}^{n-1}\big(\tilde{y}_i - f(x_i)\big)^2 \le \delta^2 . \tag{2.3}$$

Then, take the derivative f_*' *of the minimizing element* f_* *as an approximation of* y'.

It is important that the exact solution y belongs to the class of smooth functions over which the minimum is taken. In fact, given the uncertainty in the data, all functions f satisfying (2.3) can be considered as solution candidates. The minimizer of Problem I is the particular candidate that is 'smoothest'.

If the minimizing element f_* of Problem I satisfies the constraint (2.3) with strict inequality (i.e., the constraint (2.3) is *inactive*) then f_* must be the 'trivial solution'

$$\ell(x) = y(0) + x\big(y(1) - y(0)\big), \tag{2.4}$$

i.e., the straight line interpolating the two boundary values. To see this consider $f_t = (1-t)f_*$ for sufficiently small nonnegative t: by assumption, f_t satisfies the constraint (2.3), and $\|f_t''\| = (1-t)\|f_*''\|$ so that $\|f_*''\|$ must vanish in order to be minimal. This shows that f_* is the linear interpolant of the given boundary data. This case occurs if and only if ℓ satisfies the constraint (2.3).

Excluding this trivial case, the minimizer f_* satisfies (2.3) with equality, and hence, can be calculated using the method of Lagrange. If $1/\alpha$ denotes the corresponding Lagrange multiplier for constraint (2.3), the equivalent formulation of Problem I is:

Problem II. *Minimize*

$$\Phi[f] \equiv \frac{1}{n-1}\sum_{i=1}^{n-1}\big(\tilde{y}_i - f(x_i)\big)^2 + \alpha\|f''\|^2 \tag{2.5}$$

among all smooth functions f satisfying $f(0) = y(0)$, $f(1) = y(1)$, where α is such that the minimizing element f_α of (2.5) *satisfies*

$$\frac{1}{n-1}\sum_{i=1}^{n-1}\left(\tilde{y}_i - f_\alpha(x_i)\right)^2 = \delta^2. \tag{2.6}$$

The derivative f_*' of the minimizing function f_* is then an approximation of y'.

Problem II is a special instance of a general method known as *Tikhonov regularization*; in this context α is called the *regularization parameter*, and the way α is chosen in Problem II is called the *discrepancy principle* [**2**].

Except for the interpolatory constraints at the boundary of the interval, (2.5) has been investigated and solved by Schoenberg [**10**] and Reinsch [**8**], who showed that the solution of Problem II is a natural cubic spline over the grid Δ. Reinsch also gives a constructive algorithm for calculating this spline. The whole algorithm including the determination of the Lagrange multiplier $1/\alpha$ takes only $O(n)$ operations, but this is a different story that could fill another note.

Our main interest is the error $f_*' - y'$, i.e., the error of this particular way of numerical differentiation. We have the following result, which appears to be new; a proof is given in Section 5.

Theorem 2.1. *Let y'' be square integrable over* $(0, 1)$ *and let f_* be the minimizer of Problem II. Then*

$$\|f_*' - y'\| \le \sqrt{8}\left(h\,\|y''\| + \sqrt{\delta}\,\|y''\|^{1/2}\right). \tag{2.7}$$

The theorem says that, as long as $h > (\delta/\|y''\|)^{1/2}$, the error bound is of the same order as that for finite differences; see (2.2). However, the bound (2.7) remains of order $O(\sqrt{\delta})$ when $h \to 0$, without the need to discard any information. The error estimate (2.7) is sharp in the sense that for $\delta = 0$, i.e., noise-free data, the right-hand side coincides up to a multiplicative constant with the best-possible worst case bound for the interpolating spline; see Lemma 4.2. We can also give a hand-waving argument to illustrate the sharpness of the second term on the right-hand side of (2.7) as $h \to 0$. To this end we integrate by parts and use the boundary values of f_* to obtain

$$\|f_*' - y'\|^2 = \int_0^1 (f_*' - y')^2\,dx = -\int_0^1 (f_* - y)(f_*'' - y'')\,dx. \tag{2.8}$$

The Cauchy-Schwarz inequality ensures that the right-hand side of (2.8) is bounded by $\|f_* - y\|\,\|f_*'' - y''\|$; the first factor is approximately δ as h becomes small, while the second factor is bounded by $2\|y''\|$ because of the triangle inequality and the setting of Problem I.

Although Theorem 2.1 may not surprise those who are acquainted with the literature on Tikhonov regularization, we emphasize that the standard theory in [**1**] and [**2**] does not cover a result like this. The reason is the somewhat nonstandard combination of the penalty term $\|f''\|$ in (2.5) and the smoothness assumption on the exact solution y.

The remainder of this article is organized as follows. In Section 3 we prove that the minimizing element f_* is a natural cubic spline over the grid Δ. Section 4 summarizes basic error estimates in spline approximation. A proof of Theorem 2.1 is contained in Section 5. Finally, numerical results and comments are given in Section 6.

3. THE MINIMIZING SPLINE. There are two ways to prove existence and uniqueness of the minimizing element f_* of (2.5). One possibility is to consider this problem as a differentiable optimization problem over a convex domain in $H^2[0,1]$. This approach is technical and requires involved mathematical prerequisites if the derivation is to be rigorous. The technique that we use verifies directly the optimality of the corresponding spline function. The shortcoming of our approach is that the characterization (3.1) of the minimizing element f_* seems to appear from nowhere, but we feel that the simplicity of our treatment is fair compensation for this.

Let f_* be a natural cubic spline over Δ, i.e., a function that is twice continuously differentiable over $[0, 1]$ with $f_*''(0) = f_*''(1) = 0$, and coincides on each subinterval $[x_{i-1}, x_i]$ of Δ with some cubic polynomial. We show that the minimizer f_* is uniquely determined by connecting the jumps of f_*''' at the interior nodes $x = x_i$ with the values $f_*(x_i)$ through

$$f_*'''(x_i+) - f_*'''(x_i-) = \frac{1}{\alpha(n-1)}\big(\tilde{y}_i - f_*(x_i)\big), \qquad i = 1, \dots, n-1. \tag{3.1}$$

The boundary values of f_* have been fixed to be $f_*(0) = \tilde{y}_0$ and $f_*(1) = \tilde{y}_n$. For a constructive algorithm for computing f_* see **[8]**.

For any function g with square integrable second derivative and boundary values $g(0) = g(1) = 0$, integration by parts yields

$$\int_0^1 g'' f_*''\,dx = g'(1)f_*''(1) - g'(0)f_*''(0) - \int_0^1 g' f_*'''\,dx = -\sum_{i=1}^{n}\int_{x_{i-1}}^{x_i} g' f_*'''\,dx$$

$$= -\sum_{i=1}^{n} f_*'''\Big|_{[x_{i-1},x_i]} g(x)\Big|_{x=x_{i-1}}^{x_i},$$

where we have used the properties of the natural spline f_*. Since g vanishes at the boundary, this simplifies to

$$\int_0^1 g'' f_*''\,dx = \sum_{i=1}^{n-1} g(x_i)\big(f_*'''(x_i+) - f_*'''(x_i-)\big).$$

Using (3.1), this yields

$$2\alpha\int_0^1 g'' f_*''\,dx = \frac{2}{n-1}\sum_{i=1}^{n-1} g(x_i)\big(\tilde{y}_i - f_*(x_i)\big). \tag{3.2}$$

Now let f be any function with square integrable second derivative and boundary values $f(0) = \tilde{y}_0$ and $f(1) = \tilde{y}_n$. Then, the functional Φ defined in (2.5) satisfies

$$\Phi[f] - \Phi[f_*] = \frac{1}{n-1}\sum_{i=1}^{n-1}\big(f(x_i) - f_*(x_i)\big)\big(f(x_i) + f_*(x_i) - 2\tilde{y}_i\big)$$

$$+\,\alpha\,\|f'' - f_*''\|^2 + 2\alpha\int_0^1 (f'' - f_*'')f_*''\,dx.$$

Inserting (3.2) with $g = f - f_*$ for the last integral on the right-hand side gives

$$\Phi[f] - \Phi[f_*] = \frac{1}{n-1}\sum_{i=1}^{n-1}\big(f(x_i) - f_*(x_i)\big)\big(f(x_i) + f_*(x_i) - 2\tilde{y}_i\big)$$

$$+\alpha\,\|f'' - f_*''\|^2 + \frac{2}{n-1}\sum_{i=1}^{n-1}\big(f(x_i) - f_*(x_i)\big)\big(\tilde{y}_i - f_*(x_i)\big)$$

$$= \frac{1}{n-1}\sum_{i=1}^{n-1}\big(f(x_i) - f_*(x_i)\big)^2 + \alpha\,\|f'' - f_*''\|^2.$$

This proves that $\Phi[f] - \Phi[f_*] \geq 0$ for the whole class of candidates f allowed in Problem II. Furthermore, if equality holds, then $f - f_*$ must be a linear function with vanishing boundary values; hence, $f = f_*$. Consequently, f_* is the unique minimizer of Problem II.

The technique that we have employed to show that f_* is the minimizer of Φ is standard and applies to any quadratic functional.

4. PRELIMINARIES ON SPLINE APPROXIMATION. Before proving Theorem 2.1, we collect some preliminary results that provide background information on splines. Each of these facts is easy to prove, but for the reader's convenience we provide appropriate references.

Lemma 4.1. *Let s be the natural cubic spline that interpolates the exact data $y(x_i)$ at $x = x_i$, $i = 0, \ldots, n$. Then s'' is the best approximation of y'' in $\mathcal{L}^2(0,1)$ from the space of linear splines over Δ, i.e.,*

$$\|s'' - y''\|^2 + \|s''\|^2 = \|y''\|^2. \tag{4.1}$$

Proof. See [**5**, Section 6.2.1]. ∎

Lemma 4.2. *Let s be the natural cubic spline over Δ that interpolates the exact data $y(x_i)$ at $x = x_i$, $i = 0, \ldots, n$. Then*

$$\|s' - y'\| \leq \frac{h}{\pi}\|y''\|.$$

Proof. The proof follows that of Theorem 1.3 in [**12**]; it actually simplifies because in our context $s'' - y'' \in \mathcal{L}^2$. At the end of the proof one must apply the inequality $\|(s-y)''\| \leq \|y''\|$, which follows from Lemma 4.1. ∎

We also use the following approximation property of piecewise constant splines:

Lemma 4.3. *Let g have a square integrable derivative over $[0,1]$, and let χ be the best approximation in $\mathcal{L}^2(0,1)$ of g from the space of piecewise constant splines over Δ. Then*

$$\|g - \chi\| \leq h\,\|g'\|.$$

Proof. See [**11**, Thm. 6.1]. ∎

5. PROOF OF THEOREM 2.1. Lemma 4.2 ensures that it suffices to study the error $\|f_*' - s'\|$, where s is the interpolating natural cubic spline for the exact data $y(x_i)$, $i = 0, \dots, n$.

To this end, let $e = f_* - s$ and consider the best approximating piecewise constant spline χ of e' with respect to $\mathcal{L}^2(0, 1)$, i.e.,

$$\chi|_{(x_{i-1},x_i)} = \chi_i = \frac{1}{h}\int_{x_{i-1}}^{x_i} e'\,dx. \tag{5.1}$$

Rewrite $\|e'\|^2$ as

$$\begin{aligned}
\|e'\|^2 &= \int_0^1 e'(e'-\chi)\,dx + \int_0^1 e'\chi\,dx = \int_0^1 e'(e'-\chi)\,dx + \sum_{i=1}^{n}\chi_i\int_{x_{i-1}}^{x_i} e'\,dx \\
&= \int_0^1 e'(e'-\chi)\,dx + \sum_{i=1}^{n}\chi_i\big(e(x_i) - e(x_{i-1})\big) \\
&= \int_0^1 e'(e'-\chi)\,dx + \sum_{i=1}^{n-1} e(x_i)\big(\chi_i - \chi_{i+1}\big) + e(1)\chi_n - e(0)\chi_1 \\
&= \int_0^1 e'(e'-\chi)\,dx + \sum_{i=1}^{n-1} e(x_i)\big(\chi_i - \chi_{i+1}\big) =: I_1 + I_2,
\end{aligned} \tag{5.2}$$

where we have used the fact that $e(0) = e(1) = 0$ (since f_* and s interpolate y at the boundary). It remains to bound the two terms I_1 and I_2 in (5.2). For the first term we use the Cauchy-Schwarz inequality and Lemma 4.3 to obtain

$$I_1 \le \|e'\|\,\|e'-\chi\| \le h\,\|e'\|\,\|e''\|.$$

The formulation of Problem I implies that $\|f_*''\| \le \|y''\|$, and hence

$$\|e''\| \le \|f_*''\| + \|s''\| \le 2\|y''\| \tag{5.3}$$

by Lemma 4.1. Therefore we obtain the following bound for I_1:

$$I_1 \le 2h\,\|e'\|\,\|y''\|. \tag{5.4}$$

Next we bound I_2 using the Cauchy-Schwarz inequality in $\mathbb{R}^{n-1}$ and (5.1). This yields

$$\begin{aligned}
I_2^2 &\le \sum_{i=1}^{n-1} e^2(x_i)\sum_{i=1}^{n-1}\big(\chi_i - \chi_{i+1}\big)^2 \\
&= \sum_{i=1}^{n-1} e^2(x_i)\sum_{i=1}^{n-1}\frac{1}{h^2}\left(\int_{x_{i-1}}^{x_i}\big(e'(x) - e'(x+h)\big)\,dx\right)^2.
\end{aligned}$$

By construction,

$$\sum_{i=1}^{n-1} e^2(x_i) = \sum_{i=1}^{n-1}\big(f_*(x_i) - y(x_i)\big)^2 \le 4n\delta^2,$$

and hence

$$I_2^2 \le 4n^3\delta^2 \sum_{i=1}^{n-1} \left(\int_{x_{i-1}}^{x_i} \int_x^{x+h} |e''(t)|\, dt\, dx \right)^2 \le 4n^3\delta^2 \sum_{i=1}^{n-1} \left(\int_{x_{i-1}}^{x_i} \int_{x_{i-1}}^{x_{i+1}} |e''(t)|\, dt\, dx \right)^2$$
$$\le 4n\delta^2 \sum_{i=1}^{n-1} \left(\int_{x_{i-1}}^{x_{i+1}} |e''(t)|\, dt \right)^2 .$$

This last integral can be bounded using Cauchy-Schwarz and (5.3) again:

$$I_2^2 \le 4n\delta^2 \sum_{i=1}^{n-1} \int_{x_{i-1}}^{x_{i+1}} |e''(t)|^2\, dt \int_{x_{i-1}}^{x_{i+1}} dt \le 8\,\delta^2 2\,\|e''\|^2 \le 64\,\delta^2\,\|y''\|^2.$$

Inserting this and (5.4) into (5.2) we finally obtain

$$\|e'\|^2 \le 2h\,\|e'\|\,\|y''\| + 8\delta\,\|y''\|. \tag{5.5}$$

Completing the squares permits us to conclude from (5.5) that

$$\left(\|e'\| - h\,\|y''\|\right)^2 \le \left(h\,\|y''\| + \sqrt{8}\sqrt{\delta}\,\|y''\|^{1/2}\right)^2.$$

This yields

$$\|e'\| \le 2h\,\|y''\| + \sqrt{8}\sqrt{\delta}\,\|y''\|^{1/2},$$

and Lemma 4.2 implies that

$$\|f_*' - y'\| \le \|e'\| + \|s' - y'\| \le 2h\,\|y''\| + \sqrt{8}\sqrt{\delta}\,\|y''\|^{1/2} + \frac{h}{\pi}\,\|y''\|. \qquad \blacksquare$$

6. NUMERICAL RESULTS AND CONCLUDING REMARKS. Theorem 2.1 extends in a straightforward way to the situation when the boundary data of y are also perturbed. In this case one can consider the function

$$Y(x) = y(x) + \tilde{y}_0 - y(0) + \varepsilon x\,,$$

where $\varepsilon = \tilde{y}_n - y(1) + y(0) - \tilde{y}_0$. Then $Y(0) = \tilde{y}_0$ and $Y(1) = \tilde{y}_n$, and hence Theorem 2.1 applies to Y. Note that $Y'' = y''$. Consequently, if δ is replaced by 2δ in Problems I and II then Theorem 2.1 yields the same bound as before for $\|f_*' - Y'\|$, and since $\|Y' - y'\| = |\varepsilon| \le 2\delta$ the same type of bound results for $\|f_*' - y'\|$ as well.

For the inverse problem of determining the diffusion coefficient $a(\cdot)$ in (1.1), considered in [**6**], an industrial client provided temperature measurements of $u(x_i, t_j)$ at a few thermocouples at locations x_i and equidistant times $t_j \in [0, T]$. A crucial step of the equation error method used in [**6**] requires knowledge of $u_t(x_i, t)$, i.e., numerical differentiation of the given data. The left-hand plot in Figure 2 shows the measurements $u(0, t_j)$ (the circles) and the corresponding smoothing cubic spline. The right-hand plot shows both the numerical derivatives computed with finite differences (the dashed, piecewise constant function) and the smoothing spline (solid line).

For the purpose of reconstructing a, the piecewise constant approximation is useless for its lack of smoothness; the exact solution u of the parabolic equation (1.1) is known to be smooth so that a cubic spline approximation is much more appropriate. The entire algorithm for reconstructing the diffusion coefficient is described in [**6**].

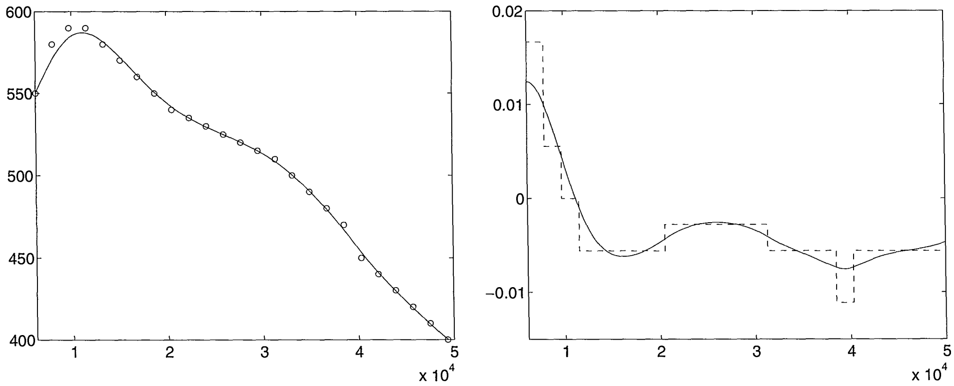

Figure 2. Given data (left) and their numerical derivatives (right)

All temperature measurements turned out to be multiples of five °C; consequently the finite difference quotient approximation of u_t takes only a few distinct values. On the other hand, this allows an estimation of δ in (2.1); we took $\delta = 2.5$ presuming a rounding to the closest multiple of five in the measuring process. With this value of δ the Lagrange multiplier $1/\alpha$ was tuned so as to satisfy (2.6).

The idea of smoothing data by cubic splines has a long tradition, especially among statisticians; see [**13**], which summarizes early work in this area, and also [**9**].

Beyond the cubic spline setting there are many other approaches to the topic of this paper. A good place to search for additional literature is [**7**], which focuses on the mollification method. We caution, however, that many numerical schemes impose artificial boundary conditions on y, which may lead to annoying boundary artifacts for practical data sets.

ACKNOWLEDGMENT. This work was inspired by a note of Chuck Groetsch [**3**]. We are very grateful for his careful reading of our manuscript and his editorial suggestions, which improved the paper a lot.

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