

# INVERSE PROBLEMS LIGHT: NUMERICAL DIFFERENTIATION

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**Abstract.** We present an error analysis for the numerical differentiation of noisy data via smoothing cubic splines. Our treatment is elementary enough to be included in a course on numerical analysis. Still, it accounts for many numerical problems that arise in the solution of much more complex ill-posed inverse problems.

**Key words.** Numerical differentiation, cubic splines, Tikhonov regularization, discrepancy principle

**AMS subject classifications.** 65-01, 65D07, 65D25, 41A15, 65J20

**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

$$u_t = (a(u)u_x)_x, \quad 0 < x < 1, \quad 0 < t < T, \quad (1.1)$$

involving some nonlinear diffusion coefficient  $a : \mathbb{R} \rightarrow \mathbb{R}^+$ . 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 the numerical simulation may consist in solving (1.1) for  $u$ . We call this the *direct problem*. In these simulations it is crucial that a coefficient  $a(u)$  be used which 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 will not be reliable.

Consequently, the 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 approach for solving 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 the numerical differentiation of the data, cf., e.g., [6]. This approach is called *equation error method*.

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

Taking the equation error approach the conditioning issue for the inverse problem (1.1) can be tied down via its connection to numerical differentiation. In fact, numerical differentiation encompasses many subtleties and pitfalls that a complex

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(linear) inverse problem can exhibit; yet it is very easy to understand and analyze. For this reason one could say that numerical differentiation is ideally suited as a model for inverse problems in a basic numerical analysis course.

To support this statement we are going to revisit in the sequel 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 the center of a mathematical specialization known as *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.

We mention that Groetsch's book [4] presents other realistic inverse problems on an elementary technical level. Further examples and a rigorous introduction into 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  $0 \leq x \leq 1$  and noisy samples  $\tilde{y}_i$  of the values  $y(x_i)$  are known at the points of a uniform grid  $\Delta = \{0 = x_0 < x_1 < \dots < x_n = 1\}$ . Let  $h = x_{i+1} - x_i$  be the mesh size of the grid and suppose

$$|\tilde{y}_i - y(x_i)| \leq \delta, \quad (2.1)$$

where  $\delta$  is a known level of noise in the data. For the moment we shall 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 satisfying 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

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

for the total error provided that  $y \in C^2[0, 1]$ ; for a very nice pedagogical treatment of this subject, see Groetsch [3]. The right-hand side of (2.2) – as a function of  $h$  – is plotted in Figure 2.1 (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.

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 really satisfying. Each datum carries information which 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*

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

*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 very 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 which 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’

$$\ell(x) = y(0) + x(y(1) - y(0)), \quad (2.4)$$

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,  $f_t$  will also satisfy 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. Note that this case occurs, if and only if  $\ell$  satisfies the constraint (2.3).

Excluding this trivial case, the minimizer  $f_*$  will satisfy (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*

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

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

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

*The derivative  $f'_*$  of the minimizing function is then an approximation of  $y'$ .*

Problem II is a special instance of a general method known as *Tikhonov regularization*; in this context  $\alpha$  is called the regularization parameter, and the way  $\alpha$  is chosen in Problem II is called the *discrepancy principle* (cf. Groetsch [2]).

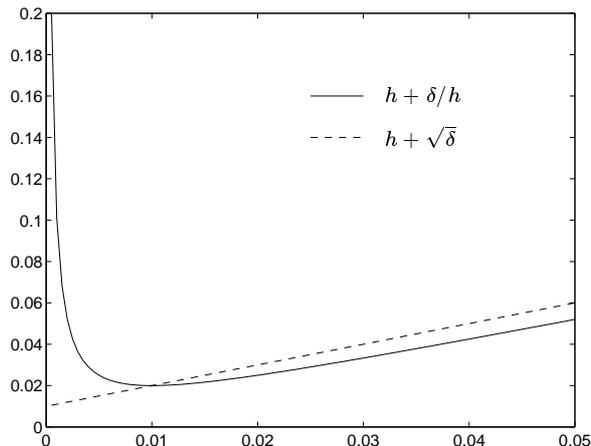


FIG. 2.1. Qualitative behavior of the error bounds (2.2) and (2.7) versus  $h$  for fixed  $\delta = 10^{-4}$ .

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  $\Delta$ . Reinsch also gives a constructive algorithm for calculating this spline. We mention that the whole algorithm including the determination of the Lagrange multiplier  $1/\alpha$  only takes  $O(n)$  operations, but this is a different story which 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; the proof is given in Section 5.

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

$$\|f'_* - y'\| \leq \sqrt{8} \left( h \|y''\| + \sqrt{\delta} \|y''\|^{1/2} \right). \quad (2.7)$$

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  $h \rightarrow 0$ , without the need to discard any information. It should be mentioned that 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 below). 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  $h \rightarrow 0$ . To this end we integrate by parts and use the boundary values of  $f_*$  to obtain

$$\|f'_* - y'\|^2 = \int_0^1 (f'_* - y')^2 dx = - \int_0^1 (f_* - y)(f''_* - y'') dx.$$

By the Cauchy-Schwarz inequality the right-hand side is bounded by  $\|f_* - y\| \|f''_* - y''\|$ ; the first factor is approximately  $\delta$  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, 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 paper is organized as follows. In Section 3 we provide a proof that the minimizing element  $f_*$  is a natural cubic spline over the grid  $\Delta$ . 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 a number of 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 the treatment is fair compensation for this.

So, let  $f_*$  be a natural cubic spline over  $\Delta$ , i.e., a function which is twice continuously differentiable over  $[0,1]$  with  $f_*''(0) = f_*''(1) = 0$ , and which coincides on each subinterval  $[x_{i-1}, x_i]$  of  $\Delta$  with some cubic polynomial. We shall see 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

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

Recall that 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  $f_*$  compare [8].

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

$$\begin{aligned} \int_0^1 g'' f_*'' dx &= g'(1) f_*''(1) - g'(0) f_*''(0) - \int_0^1 g' f_*''' dx = - \sum_{i=1}^n \int_{x_{i-1}}^{x_i} g' f_*''' dx \\ &= - \sum_{i=1}^n f_*''' \Big|_{[x_{i-1}, x_i]} g(x) \Big|_{x=x_{i-1}}, \end{aligned}$$

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

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

Using (3.1), this yields

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

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  $\Phi$  defined in (2.5) satisfies

$$\begin{aligned}\Phi[f] - \Phi[f_*] &= \frac{1}{n-1} \sum_{i=1}^{n-1} (f(x_i) - f_*(x_i))(f(x_i) + f_*(x_i) - 2\tilde{y}_i) \\ &\quad + \alpha \|f'' - f_*''\|^2 + 2\alpha \int_0^1 (f'' - f_*'') f_*'' dx.\end{aligned}$$

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

$$\begin{aligned}\Phi[f] - \Phi[f_*] &= \frac{1}{n-1} \sum_{i=1}^{n-1} (f(x_i) - f_*(x_i))(f(x_i) + f_*(x_i) - 2\tilde{y}_i) \\ &\quad + \alpha \|f'' - f_*''\|^2 + \frac{2}{n-1} \sum_{i=1}^{n-1} (f(x_i) - f_*(x_i)) (\tilde{y}_i - f_*(x_i)) \\ &= \frac{1}{n-1} \sum_{i=1}^{n-1} (f(x_i) - f_*(x_i))^2 + \alpha \|f'' - f_*''\|^2.\end{aligned}$$

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  $\Phi$  is pretty standard and applies to any quadratic functional.

**4. Preliminaries on spline approximation.** Before proving Theorem 2.1, we collect a number of 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 which interpolates the exact data  $y(x_i)$  at  $x = x_i$ ,  $i = 0, \dots, n$ . Then  $s''$  is the best approximation of  $y''$  in  $\mathcal{L}^2(0, 1)$  from the space of linear splines over  $\Delta$ , i.e.,*

$$\|s'' - y''\|^2 + \|s''\|^2 = \|y''\|^2. \quad (4.1)$$

*Proof.* See Hämmerlin and Hoffmann [5, Section 6.2.1].  $\square$

LEMMA 4.2. *Let  $s$  be the natural cubic spline over  $\Delta$  which interpolates the exact data  $y(x_i)$  at  $x = x_i$ ,  $i = 0, \dots, n$ . Then,*

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

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

We will 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  $\chi$  be the best approximation in  $\mathcal{L}^2(0, 1)$  of  $g$  from the space of piecewise constant splines over  $\Delta$ . Then*

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

*Proof.* See Schumaker [11, Thm. 6.1].  $\square$

**5. Proof of Theorem 2.1.** In view of Lemma 4.2 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  $\chi$  of  $e'$  with respect to  $\mathcal{L}^2(0, 1)$ , i.e.,

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

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

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

where we have used that  $e(0) = e(1) = 0$  (since  $f_*$  and  $s$  interpolate  $y$  at the boundary). It remains to estimate 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

$$I_1 \leq \|e'\| \|e' - \chi\| \leq h \|e'\| \|e''\|.$$

The formulation of Problem I implies that  $\|f''_*\| \leq \|y''\|$ , and hence

$$\|e''\| \leq \|f''_*\| + \|s''\| \leq 2 \|y''\| \quad (5.3)$$

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

$$I_1 \leq 2h \|e'\| \|y''\|. \quad (5.4)$$

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

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

Note that, by construction,

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

and hence,

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

The last integral can be estimated using Cauchy-Schwarz and (5.3) again:

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

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

$$\|e'\|^2 \leq 2h\|e'\| \|y''\| + 8\delta\|y''\|.$$

Completing the squares this can be rewritten as

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

This yields

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

and from Lemma 4.2 we therefore obtain

$$\|f'_* - y'\| \leq \|e'\| + \|s' - y'\| \leq 2h\|y''\| + \sqrt{8}\sqrt{\delta}\|y''\|^{1/2} + \frac{h}{\pi}\|y''\|.$$

This completes the proof.

**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  $\delta$  is replaced by  $2\delta$  in Problems I and II then Theorem 2.1 yields the same bound as before for  $\|f'_* - Y'\|$ , and since  $\|Y' - y'\| = |\varepsilon| \leq 2\delta$  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 the knowledge of  $u_t(x_i, t)$ , i.e.,

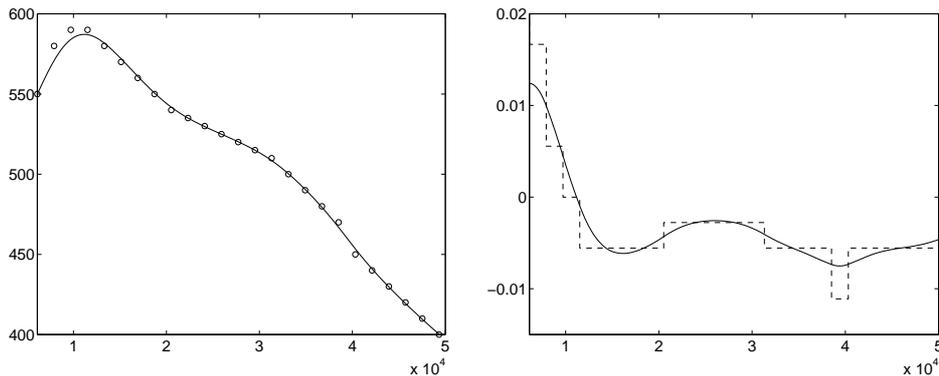


FIG. 6.1. Given data (left) and their numerical derivatives (right)

numerical differentiation of the given data. The left-hand side plot in Figure 6.1 shows the measurements  $u(0, t_j)$  (the circles) and the corresponding smoothing cubic spline. The right-hand side plot shows the numerical derivatives computed with finite differences (the dashed, piecewise constant function) and the smoothing spline (solid line), respectively.

For the purpose of reconstructing  $a$  the piecewise constant approximation is useless for its lack of smoothness; the exact solution  $u$  of this parabolic equation 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].

All temperature measurements turned out to be multiples of five ( $^{\circ}\text{C}$ ); consequently the finite difference quotient approximation of  $u_t$  only takes a few distinct values. On the other hand this allows an estimation of  $\delta$  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  $\delta$  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. Some of these works are related to ours in that they also address the problem of numerical differentiation. For example, see the book by Wahba [13], which summarizes her early work in this area, and also the paper by Rice and Rosenblatt [9].

Beyond the cubic spline setting there are lots of other approaches to the topic of this paper. A good place to search for additional literature is the book by Murio [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.

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