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Heuristic regularization methods for numerical differentiation

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ABSTRACT

In this paper, we use smoothing splines to deal with numerical differentiation. Some heuristic methods for choosing regularization parameters are proposed, including the *L*-curve method and the de Boor method. Numerical experiments are performed to illustrate the efficiency of these methods in comparison with other procedures.

1. Introduction

Numerical differentiation is the problem of approximating the derivatives of a certain function. It frequently arises in practice as well as in theory. For example, the inverse problem of calculating engineering loads from strain data requires the second-order differentiation of bending moment of a beam, [1]. Other examples can be found e.g. in [2–6] and the references therein.

Suppose that $f(x)$ is a function defined on $[0, 1]$. Often we obtain the values of $f(x)$ at particular points by measurement which encounters unavoidable errors. Hence let us denote the measured function by $f^\delta(x)$, where the so-called noise level $\delta > 0$ is such that $\|f - f^\delta\| < \delta$, ($\|\cdot\|$ is a certain norm, e.g., the L^2-norm). From f^δ, we aim to approximate the derivatives of f of some orders. This problem, which we call numerical differentiation, is well-known to be ill-posed in the sense of Hadamard. This means that a small noise in the measured data, i.e., small δ, may cause intolerable errors in the computed derivatives.

Various techniques have been proposed for stable numerical differentiation (see [2–11] for further references and surveys). We can classify them into two groups:

(1) Methods which are based on knowledge or good estimate of the noise level δ.

(2) Methods which do not require knowledge of δ, but seek to extract this information from the nature of the problem and the data.

Methods in the second group are often called *heuristic methods*. Since the noise level δ or prior information about the exact solution is not always available, it is pragmatic to develop heuristic methods for choosing regularization parameters. In the literature, there are a number of such methods such as the *L*-curve method [12,13] and the generalized cross validation method (GCV for short) [3] which have been demonstrated to be fairly satisfactory. However, for numerical differentiation,

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the use of such methods is rather sparse. To the best of our knowledge, the most comprehensive analysis is the use of GCV in [3].

For numerical differentiation, smoothing splines are recognized to be useful objects. A breakthrough in using smoothing splines was made with the work of Schoenberg and Reinsch in 1960s (see [14] and references therein). They proved that the minimizer of problem (1) (see Section 2) is a spline of order $2k$. After that, there were some papers dealing with the issue of choosing the regularization parameter. One of the most prominent methods is the generalized cross validation method (GCV) which was investigated thoroughly by Craven and Wahba (see [3]). Another popularly cited paper was due to Hanke and Scherzer [4]. In their paper, with the choice $\alpha = \delta^2$, they proved the convergence result for using cubic smoothing spline to approximate derivatives. Following this paper, several authors dealt with higher smoothing splines with the same parameter choice, e.g., [6]. Parallel to the development of using splines is the implementation in Matlab with the Spline Toolbox by de Boor [15]. In this toolbox, the author implemented the procedure for choosing the regularization parameter by the discrepancy principle and remarkably, the heuristic method based on trace balance which we call later the ad hoc procedure, or *the de Boor method*. The users can also find various applications of splines in this toolbox.

In this paper, we are particularly interested in heuristic methods for choosing regularization parameters in smoothing splines. By working with the Matlab program, especially the Spline Toolbox of de Boor [15] and the Regularization Toolbox [12] by Hansen, we see the possibility of using smoothing splines for numerical differentiation with heuristic strategies for choosing the regularization parameters, including the L-curve method and the so-called ad hoc procedure (or de Boor method). We implement the L-curve method (which makes use of the regularization package of Hansen) for smoothing splines and modify the idea of trace balance of de Boor for higher smoothing splines. We also combine these methods to choose more suitable regularization parameters.

This paper is organized as follows. In Section 2, we formulate the problem and recall some well-known results on smoothing splines. Section 3 illustrates these results by examining the cases when $k = 2$ and 3 and devises some heuristic methods for choosing the regularization parameters, including the L-curve method and the de Boor method. Numerical examples are presented in Section 4. In the course of experiments, we find these methods satisfactory and, in some cases, even better than methods using knowledge of the noise level.

2. Preliminaries

Let us formulate the problem of smoothing splines and state some previous results (see [6]). Suppose that $y = y(x)$ is a function from [0, 1] into $\mathbb{R}$. Let n be a natural number,

$$\Delta = \{0 = x_0 < x_1 < x_2 < \cdots < x_n = 1\}$$

a grid on [0, 1], and δ a given constant which indicates the level of noise in the data. Denote step sizes by

$$h_i = x_{i+1} - x_i, \quad i = 0, 1, 2, \ldots, n-1.$$

Next, by measurement, we have a number of noisy samples y_i of the values $y(x_i)$ satisfying

$$|y_i - y(x_i)| \le \delta, \quad i = 0, 1, 2, \ldots, n.$$

From these samples, we aim to construct approximations of the function, as well as its derivatives of some orders. To this end, we seek for a solution of the variational problem

$$\Phi(f) = \frac{1}{n-1}\sum_{j=1}^{n-1}(y_j - f(x_j))^2 + \alpha\int_0^1 f^{(k)}(x)^2dx = \min! \tag{1}$$

over the admissible set

$$\Lambda = \left\{f \in H^k(0, 1), f(0) = y_0, f(1) = y_n\right\},$$

where the Sobolev space $H^k(0, 1)$ is defined by (see, [2,3,5,6])

$$H^k(0, 1) = \left\{f \in C^{k-1}[0, 1], f^{(k-1)}(x) = a + \int_0^x \psi(s)ds, a \in \mathbb{R}, \psi \in L^2(0, 1)\right\}.$$

Here $\alpha > 0$, called a regularization parameter, controls the infidelity of the computed function to the data, presented by the term $\frac{1}{n-1}\sum_{j=1}^{n-1}(y_j - f(x_j))^2$ and its roughness, represented by the term $\int_0^1 f^{(k)}(x)^2dx$. The minimizer, denoted by f_α, turns out to be a spline of order $2k$. Its derivatives with respect to some suitable α are then used to approximate the derivatives (up to order $k-1$) of the original function. Observe that, for $\alpha = 0$, the minimizer f_0 is the spline that interpolates the data while, as $\alpha \to \infty$, the minimizers approach the straight line that best fits the data.

Sometimes the noise level δ can be estimated accurately. However, in general, we can neither estimate this quantity nor understand its behavior. This motivates computational methods which do not depend on the knowledge the noise level.

Problem (1) was investigated thoroughly in [6] (see also [4]). It is stated that the minimizer f_* can be given by

$$f_*(x) = c_{j,1} + c_{j,2}x + \cdots + c_{j,2k}x^{2k}, \quad x \in [x_j, x_{j+1}), \tag{2}$$