Numerical differentiation of noisy, nonsmooth data

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Abstract

We consider the problem of differentiating a function specified by noisy data. Regularizing the differentiation process avoids the noise amplification of finite-difference methods. We use total-variation regularization, which allows for discontinuous solutions. The resulting simple algorithm accurately differentiates noisy functions, including those which have a discontinuous derivative.

1 Introduction

In many scientific applications, it is necessary to compute the derivative of functions specified by data. Conventional finite-difference approximations will greatly amplify any noise present in the data. Denoising the data before or after differentiating does not generally give satisfactory results. (See an example in Section 4.)

A method which does give good results is to regularize the differentiation process itself. This guarantees that the computed derivative will have some degree of regularity, to an extent that is often under control by adjusting parameters. A common framework for this is Tikhonov regularization [12] of the corresponding inverse problem. That is, the derivative of a function f, say on $[0, L]$, is the minimizer of the functional

$$F(u) = \alpha R(u) + DF(Au - f), \tag{1}$$

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where $R(u)$ is a regularization or penalty term that penalizes irregularity in u, $Au(x) = \int_0^x u$ is the operator of antidifferentiation, $DF(Au - f)$ is a data fidelity term that penalizes discrepancy between Au and f, and α is a regularization paramater that controls the balance between the two terms. $DF(\cdot)$ is most commonly the square of the L^2 norm, $DF(\cdot) = \int_0^L |\cdot|^2$, as is appropriate if f has additive, Gaussian noise. (See [8] for an alternative in the case of Poisson noise.) In [12], the regularization term is the squared L^2 norm; this controls the size of u, without forcing minimizers to be regular. Tikhonov regularization was first applied to numerical differentiation by Cullum [4], where the regularization is the squared H^1 norm, $R(u) = \int_0^L |u'|^2$. This forces minimizers to be continuous, as is required for the H^1 norm to be finite. This prevents the accurate differentiation of functions with singular points.

Other variational methods have the same drawback of forcing smoothness. An approach that penalizes the L^2 norm of u'' forces the minimizer to be a cubic spline (see [11, 9, 6]). The variational approach of Knowles and Wallace [7] does not fall into the category of Tikhonov regularization, but explicitly assumes that u is smooth.

2 Total-variation regularization

We propose to use total-variation regularization in (1). We will thus compute the derivative of f on $[0, L]$ as the minimizer of the functional

$$F(u) = \alpha \int_0^L |u'| + \frac{1}{2} \int_0^L |Au - f|^2. \tag{2}$$

We assume $f \in L^2$ (an empty assumption in the discrete case), and for convenience that $f(0) = 0$. (In practice we simply subtract $f(0)$ from f.) The functional F is defined on $BV[0, L]$, the space of functions of bounded variation. It is in fact continuous on BV, as BV is continuously embedded in L^2, and A is continuous on L^2 (being an integral operator with bounded kernel). Existence of a minimizer for F follows from the compactness of BV in L^2 [1, p. 152] and the lower semicontinuity of the BV seminorm [1, p. 120]. This and the strict convexity of F are sufficient to guarantee that F has a unique minimizer u_*.

Use of total variation accomplishes two things. It suppresses noise, as a noisy function will have a large total variation. It also does not suppress jump discontinuities, unlike typical regularizations. This allows for the computation of discontinuous derivatives, and the detection of corners and edges in noisy data.

Total-variation regularization is due to Rudin, Osher, and Fatemi in [10]. It has since found many applications in image processing. Replacing A in the two-dimensional analog of (2) with the identity operator gives a method for denoising an image f. See [3, 2] for an example where A is the Abel transform, giving a method for regularizing Abel inversion.

3 Numerical implementation

A simple approach to minimizing (2) is gradient descent. This amounts to evolving to stationarity the PDE obtained from the Euler-Lagrange equation:

$$u_t = \alpha \frac{d}{dx} \frac{u'}{|u'|} - A^*(Au - f), \tag{3}$$

where $A^* v(x) = \int_x^L v$ is the L^2-adjoint of A. Replacing the $|u'|$ in the denominator with $\sqrt{(u')^2 + \epsilon}$ for some small $\epsilon > 0$ avoids division by zero. Typically, (3) is implemented with explicit time marching, with u_t discretized as $(u_{n+1} - u_n)/\Delta t$ for some fixed Δt.

The problem with (3) is that convergence is slow. A faster algorithm is the lagged diffusivity method of Vogel and Oman [14]. The idea is to replace at each iteration of (3) the nonlinear differential operator $u \mapsto \frac{d}{dx}\frac{u'}{|u'|}$ with the linear operator $u \mapsto \frac{d}{dx}\frac{u'}{|u'_n|}$. The algorithm has been proven to converge to the minimizer of F [5].

Our discrete implementation of the algorithm is straightforward, and follows [13]. We assume that u is defined on a uniform grid $\{x_i\}_0^L = \{0, \Delta x, 2\Delta x, \ldots, L\}$. Derivatives of u are computed halfway between grid points as centered differences. Integrals of u are likewise computed halfway between grid points, using the trapezoid rule. The matrix of the differentiation operator is denoted D; the matrix of the antidifferentiation operator A is denoted K. Let E_n be the diagonal matrix whose ith entry is $\left((u_n(x_i) - u_n(x_{i-1}))^2 + \epsilon\right)^{-1/2}$. Let $L_n = \Delta x D^t E_n D$, $H_n = K^t K + \alpha L_n$. The matrix H_n is an approximation to the Hessian of F at u_n. The update $s_n = u_{n+1} - u_n$ is the solution to $H_n s_n = -g_n$, where $g_n = K^t(Ku_n - f) + \alpha L_n u_n$.

Less straightforward is the choice of the regularization parameter α. We use the discrepancy principle: the mean-squared difference between Au_* and

f should equal the variance of the noise in f. This has the effect of choosing the most regular solution to the ill-posed inverse problem $Au = f$ that is consistent with the data f. In practice, the noise in f is not generally known, so we estimate the noise variance by comparing f with a smoothed version of f.

4 Example

Let $f_0(x) = |x - 1/2|$ on $[0, 1]$. We define f at 100 evenly-spaced points in $[0, 1]$, and add Gaussian noise of standard deviation 0.05. Figure 1 shows the resulting f.

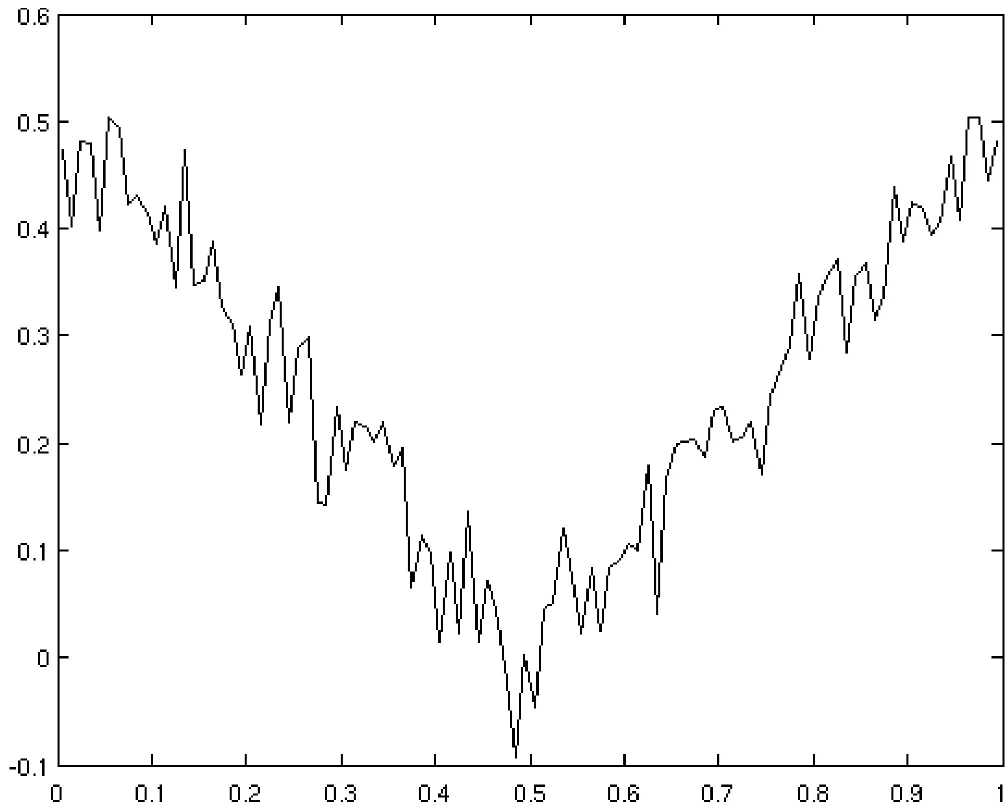

Figure 1: The function f, obtained from $|x - 1/2|$ by adding Gaussian noise of standard deviation 0.05.

First, we show in Figure 2 the result of computing f' by simple centered differencing. The noise has been greatly amplified, so much that denoising the result is hopeless.

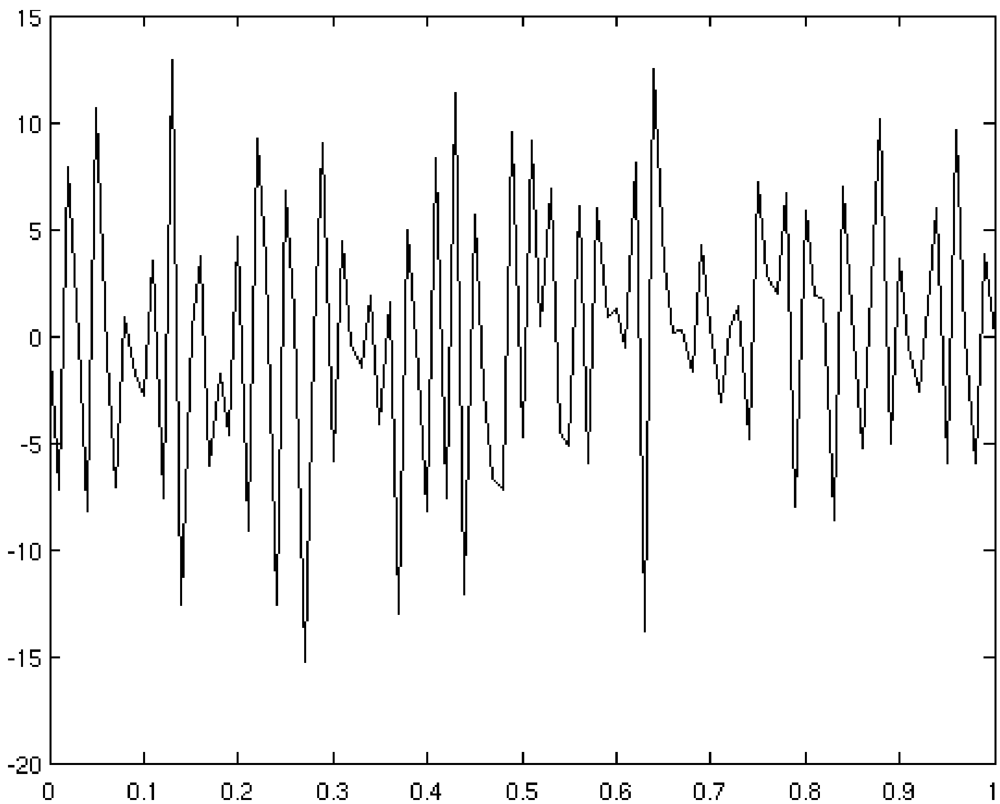

Figure 2: Computing f' with finite differences greatly amplifies noise.

We compare with this the result in Figure 3 of denoising f before computing f' by differencing. The denoising is done by total variation regularization, as in (2) but with A replaced by the identity operator. The residual noise in the denoised f is still amplified enough by the differentiation process to give an unsatisfactory result.

Now we implement our total-variation regularized differentiation, (2). The result is in Figure 4. The overall shape of f_0' is captured almost perfectly. The jump is correctly located. The one inaccuracy is the size of the jump: there is a loss of contrast, which is typical of total-variation regularization in the presence of noise. Decreasing the size of the jump reduces the penalty

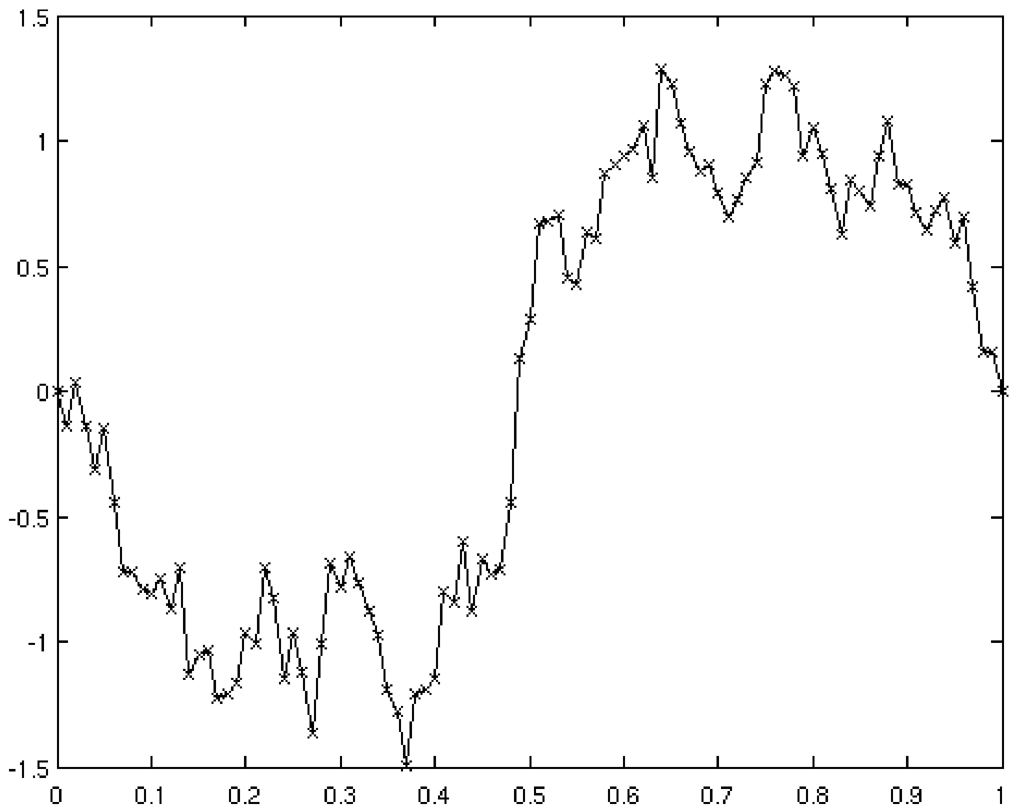

Figure 3: The function f is denoised, then differentiated with finite differences. The result is noisy and inaccurate.

term in (2), at the expense of increasing the data-fidelity term. We also show the result of applying the antidifferentiation operator to the computed f', and compare with f_0 in Figure 5. The corner is sharp and the lines are straight, though a little too flat.

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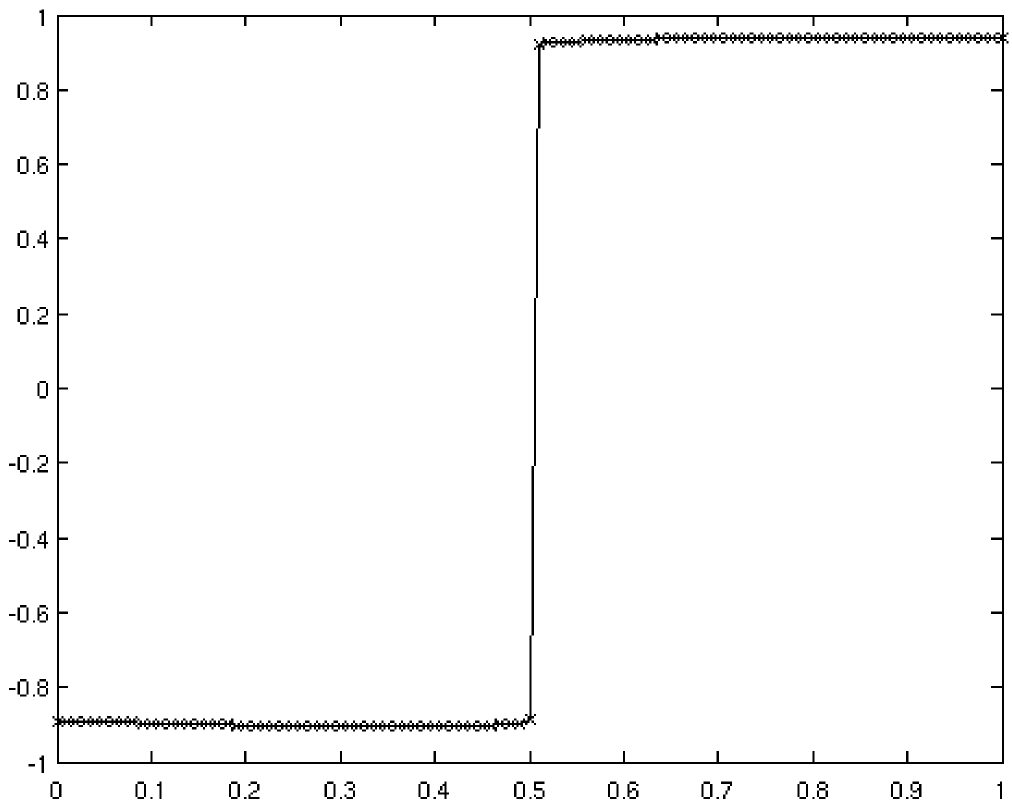

Figure 4: Regularizing the differentiation process with total-variation produces a noiseless derivative with a correctly located, sharp jump. The discrepancy of the values from ± 1 are due to contrast loss, an artifact of total variation methods in the presence of noise.

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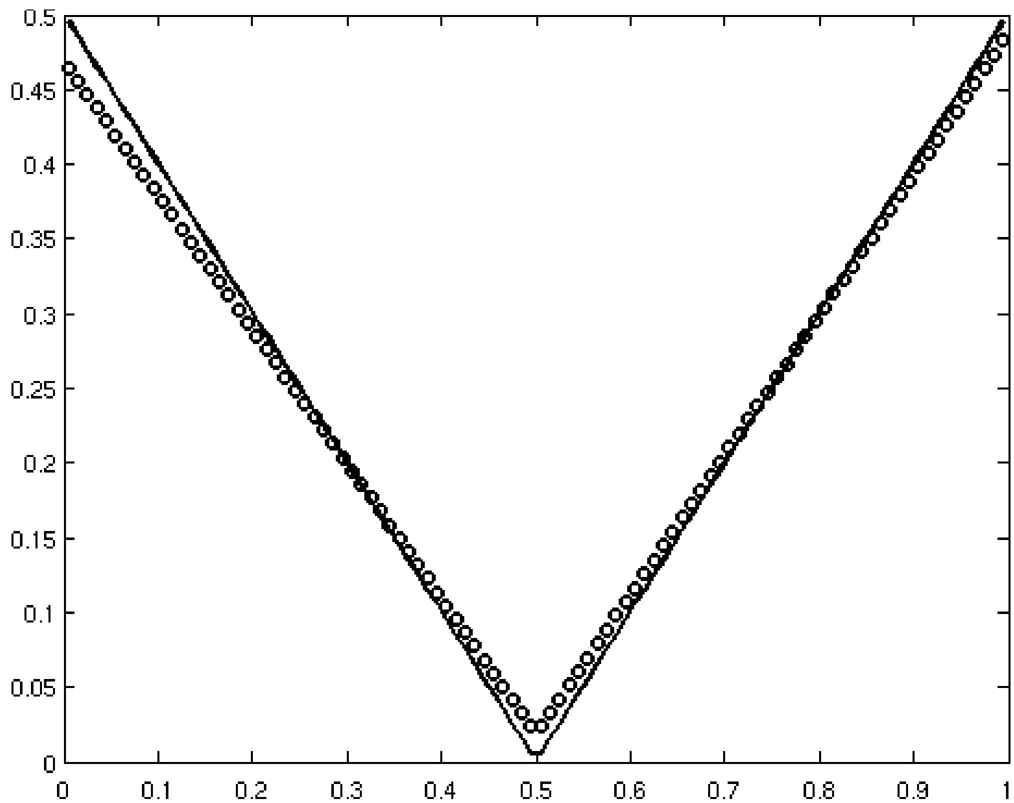

Figure 5: The function f_0 (solid line) and the antidifferentiated numerical derivative (circles). The numerically computed function is very similar to the exact one.

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