Numerical derivatives from one-dimensional scattered noisy data

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Abstract. Based on the cubic spline theory, we propose in this paper a regularization method for reconstructing numerical differentiation from one-dimensional scattered noisy data. Under two different choice rules for a suitable regularization parameter, the regularized solutions can be derived. Convergence results for the approximate derivative are given. Numerical experiments verify that the proposed strategy with the Morozov’s discrepancy principle for the choice of regularization parameter is effective and stable.

1. Introduction
The reconstruction of numerical derivatives from scattered noisy data is an important problem in scientific research and engineering disciplines. For instance, solutions related to problems in image process [4], solving Volterra integral equation [5] can be much improved if accurate approximation for derivative is available. The problem of numerical differentiation is well known to be ill-posed in the sense that a small error for measurement values on specified points may induce a large error in the computed derivatives. Some computational methods have been suggested in the works of [2,3,6,7,10]. These works mainly fall into two categories: difference methods [2,6,10] and Tikhonov regularization methods [3,7]. The difference method is simple and effective for precise data but the stepsize, being a regularization parameter, must depend on the level of noise and hence the specified points can not be too dense. This hinders the application of the difference method to reconstruct numerical derivatives from scattered noisy data. To solve effectively the ill-posed problems, Tikhonov regularization methods play an important role [11]. Most of the regularization procedures for numerical differentiation make use of variational approach to get a regularized solution. Once the regularization parameter is chosen, the approximation to the unknown function and its derivative can be obtained. Unfortunately, the determination of the minimizer for a smoothing functional and the optimal regularization parameter are generally a nontrivial task.

Based on the work of Hickernell and Hon on radial basis functions approximation [8], we use a semi-norm in the global space as a stabilizer which is different from the one defined by Wang et. al. [12] on a finite interval. This modification allows us to represent the minimizer of the objective functional by a linear combination of cubic splines and polynomials. Following the proofs given in [9], we then deduce convergence estimates under an a priori and an a posteriori choice rules for the regularization parameter. Numerical tests show that the proposed method with the a posteriori choice strategy is effective and stable.
2. Formulation and solution of the problem

Let \( y = y(x) \) be a function in \( \mathbb{R} \) and \( \{a = x_1 < x_2 < \cdots < x_n = b\} \) be a set of scattered points on \([a, b]\) with \( n \geq 2 \). Denote \( h_i = x_i - x_{i-1} \) for \( i = 2, \cdots, n \), and \( h_1 = 0, h_{n+1} = 0 \) be the stepsizes for a partition of \([a, b]\). Let \( h = \max_{2 \leq i \leq n} h_i \) be the maximum of these stepsizes. Denote \( \eta_i = \frac{2}{h_i + h_{i+1}} \) for \( i = 1, 2, \cdots, n \).

Consider the following numerical differentiation problem: given noisy samples \( \tilde{y}_i \) of an unknown function \( y(x) \) with values \( y(x_i) \) satisfying

\[
|\tilde{y}_i - y(x_i)| \leq \sigma_i \leq \delta, \quad i = 1, 2, \cdots, n,
\]

where \( \delta \) is called a noise level. The numerical differentiation problem is to find a function \( f_*^{(x)} \) such that \( f'_*(x) \) can be an approximation of the unknown derivative function \( y'(x) \). Here \( f_*^{(x)} \) denotes the first derivative with respect to \( x \).

Let \( I_\varepsilon = \{ i \mid \sigma_i = 0 \} \) be an index set of points with exact measurement values and \( I_a = \{1, 2, \cdots, n\} \setminus I_\varepsilon \) is an index set of points with noisy data.

Let \( X = \{ f \mid f \in C^1(\mathbb{R}), f'' \in L^2(\mathbb{R}) \} \) and \( Y = \{ f \mid f \in X, f(x_i) = y(x_i), i \in I_\varepsilon \} \).

Define a smoothing functional:

\[
\Phi(f) = \frac{1}{b-a} \sum_{i \in I_a} \frac{h_i + h_{i+1}}{2} \left( \frac{f(x_i) - \tilde{y}_i}{\sigma_i} \right)^2 + \alpha \|f''\|_{L^2(\mathbb{R})},
\]

where \( \alpha \) is a positive parameter and \( \alpha \sigma_i^2 \) are regularization parameters under the Tikhonov regularization sense.

Consider the following two questions: (1) How to find \( f_\alpha \in Y \) such that \( \Phi(f_\alpha) \leq \Phi(f) \), for all \( f \in Y \). (2) If such \( f_\alpha \) has been obtained, how to choose a good parameter \( \alpha^* \) such that \( f_\alpha^{(x)}(x) \) converges to the exact function \( y'(x) \) with a high convergence order?

To answer the first question, a simple proof based on mathematical analysis is given in the following theorem. The convergence results will be given in next section.

**Theorem 2.1** Denote

\[
f_\alpha(x) = \sum_{j=1}^n c_j |x - x_j|^3 + d_1 + d_2 x,
\]

with coefficients \( \{c_j\}_1^n \) and \( \{d_j\}_1^n \) satisfying

\[
\begin{align*}
&f_\alpha(x_i) + 12(b-a)\alpha \eta_i \sigma_i^2 c_i = \tilde{y}_i, \quad i \in I_\varepsilon, \\
&f_\alpha(x_i) = y(x_i), \quad i \in I_a, \\
&\sum_{j=1}^n c_j = \sum_{j=1}^n c_j x_j = 0.
\end{align*}
\]

The function \( f_\alpha \) is then a minimizer of the smoothing functional (2), i.e., \( \Phi(f_\alpha) = \min_{f \in Y} \Phi(f) \leq \Phi(y) \).

**Proof:** It is clear that \( f_\alpha(x) \in C^2(\mathbb{R}) \). From (3), the second order derivative of \( f_\alpha(x) \) can be calculated as

\[
f''_\alpha(x) = 6 \sum_{j=1}^n c_j |x - x_j|.
\]

Due to condition (6), we know that \( f''_\alpha^{(2+j)}(x) = 0 \) for \( x \leq x_1 \) or \( x \geq x_n \) where \( j \geq 0 \) is an integer. Hence, \( f_\alpha \in X \). Considering condition (5), we then have \( f_\alpha \in Y \).
Furthermore, the third order derivative of \( f_\alpha(x) \) is given by

\[
f^{(3)}_\alpha(x) = \begin{cases} 
0, & x < x_1 \text{ and } x > x_n; \\
6 \left( \sum_{j=1}^{i-1} c_j - \sum_{j=i}^{n} c_j \right), & x_{i-1} < x < x_i; \\
6 \left( \sum_{j=1}^{i} c_j - \sum_{j=i+1}^{n} c_j \right), & x_i < x < x_{i+1}. 
\end{cases}
\]

Therefore, we have

\[
f^{(3)}_\alpha(x_{i+}) - f^{(3)}_\alpha(x_{i-}) = 12c_i, \quad i = 1, 2, \ldots, n,
\]

where \( f^{(3)}_\alpha(x_{i-}) \) and \( f^{(3)}_\alpha(x_{i+}) \) are respectively the left- and right-hand limits of function \( f^{(3)}_\alpha(x) \) at point \( x_i \). From condition (4), we obtain

\[
f^{(3)}_\alpha(x_{i+}) - f^{(3)}_\alpha(x_{i-}) = \frac{1}{\alpha(b - a)\eta_i\sigma_i^2} (\tilde{y}_i - f_\alpha(x_i)), \quad i \in I_a.
\]

Since

\[
\Phi(f) - \Phi(f_\alpha) = \frac{1}{b - a} \sum_{i \in I_a} \left( \frac{(f(x_i) - \tilde{y}_i)^2 - (f_\alpha(x_i) - \tilde{y}_i)^2}{\eta_i\sigma_i^2} \right) + \alpha \int_\mathbb{R} \left( (f''(x))^2 - (f''_\alpha(x))^2 \right) dx
\]

\[
= \frac{1}{b - a} \sum_{i \in I_a} \frac{(f(x_i) - f_\alpha(x_i))^2}{\eta_i\sigma_i^2} + \alpha \|f'' - f''_\alpha\|_{L^2(\mathbb{R})}^2 + \frac{2\alpha}{\eta_i\sigma_i^2} \int_\mathbb{R} f''(x) \left( f''(x) - f''_\alpha(x) \right) dx
\]

and

\[
\int_\mathbb{R} f''(x) \left( f''(x) - f''_\alpha(x) \right) dx = \int_{x_1}^{x_n} f''(x) \left( f''(x) - f''_\alpha(x) \right) dx
\]

\[
= (-1) \int_{x_1}^{x_n} f^{(3)}_\alpha(x) (f'(x) - f'_\alpha(x)) dx
\]

\[
= \sum_{i=1}^{n} \left( f^{(3)}_\alpha(x_{i+}) - f^{(3)}_\alpha(x_{i-}) \right) (f(x_i) - f_\alpha(x_i))
\]

\[
= \sum_{i \in I_a} \left( f^{(3)}_\alpha(x_{i+}) - f^{(3)}_\alpha(x_{i-}) \right) (f(x_i) - f_\alpha(x_i)),
\]

combining (7) and (9) into (8) we then have

\[
\Phi(f) - \Phi(f_\alpha) = \frac{1}{b - a} \sum_{i \in I_a} \left( \frac{(f(x_i) - f_\alpha(x_i))^2}{\eta_i\sigma_i^2} \right) + \alpha \|f'' - f''_\alpha\|_{L^2(\mathbb{R})}^2 \geq 0. \tag{10}
\]

This proves that \( f_\alpha \) is a minimizer of the functional \( \Phi \).

Furthermore, if there exists another function \( f_* \in Y \) such that \( \Phi(f_*) = \Phi(f_\alpha) \). Then, by (10) and (5), we have

\[
\|f''_* - f''_\alpha\|_{L^2(\mathbb{R})}^2 = 0, \quad f_*(x_i) = f_\alpha(x_i), \quad i = 1, 2, \ldots, n.
\]

Hence, \( f_* - f_\alpha \) is a linear polynomial. Since \( n \geq 2, f_* = f_\alpha \), i.e. the minimizer of functional (2) is uniquely determined by (3) and (4)-(6).
3. Convergence results
In this section, we consider an \textit{a priori} choice strategy and an \textit{a posteriori} choice rule to find the parameter \(\alpha\) respectively. The \textit{a priori} rule takes \(\alpha = 1\) and the \textit{a posteriori} rule is Morozov’s discrepancy principle, i.e. choosing \(\alpha\) from the following equation

\[
\frac{1}{b-a} \sum_{i \in I_n} \frac{h_i + h_{i+1}}{2} \left( \frac{f_\alpha(x_i) - \tilde{y}_i}{\sigma_i} \right)^2 = 1.
\]  

(11)

Under each choice of the parameter, convergence estimates can be obtained and will be given in Theorem 3.2 and 3.4. The proof of Theorem 3.2 will use the following lemma generalized from Lemma 2.2 in Powell’s paper [9].

**Lemma 3.1** Let \(\{\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_m\}, m \geq 2\) be any finite set of points in \(\mathbb{R}\) that are all different and let \(\{\hat{c}_1, \hat{c}_2, \ldots, \hat{c}_m\}\) be any real multipliers that satisfy the conditions

\[
\sum_{i=1}^{m} \hat{c}_i = \sum_{i=1}^{m} \hat{c}_i \hat{x}_i = 0.
\]

Furthermore, let \(g\) be any function from \(\mathbb{R}\) to \(\mathbb{R}\) that has square integrable second order derivative. Then, the linear functional

\[
L(g) = \sum_{i=1}^{m} \hat{c}_i g(\hat{x}_i)
\]

has the property

\[
|L(g)| \leq 12^{-1} C(\hat{c})^{1/2} \|g''\|_{L^2(\mathbb{R})},
\]

(12)

where

\[
C(\hat{c}) = 12 \sum_{i=1}^{m} \sum_{j=1}^{m} \hat{c}_i \hat{c}_j |\hat{x}_i - \hat{x}_j|^3 \geq 0.
\]

**Proof:** Denote

\[
t(x) = \sum_{i=1}^{m} \hat{c}_i |x - \hat{x}_i|^{3}, \quad x \in \mathbb{R}.
\]

We have

\[
L(g) = \sum_{i=1}^{m} \hat{c}_i g(\hat{x}_i) = 12^{-1} \sum_{i=1}^{m} \left( t^{(3)}(\hat{x}_i+) - t^{(3)}(\hat{x}_i-) \right) g(\hat{x}_i)
\]

\[
= 12^{-1} \int_{\mathbb{R}} g'' t'' dx.
\]

Thus,

\[
|L(g)| \leq 12^{-1} \|g''\|_{L^2(\mathbb{R})} \|t''\|_{L^2(\mathbb{R})},
\]

(13)

where

\[
C(\hat{c}) = \|t''\|_{L^2(\mathbb{R})}^2 = 12 \sum_{i=1}^{m} \sum_{j=1}^{m} \hat{c}_i \hat{c}_j |\hat{x}_i - \hat{x}_j|^3 \geq 0.
\]

(14)

Combining (14) and (13), then (12) is proved.

Hereafter, denote \(\|\cdot\|\) to be the \(L^2(\mathbb{R})\) norm.
Furthermore, from Lemma 3.1, we obtain
\[ \|f_{\alpha_1} - y\|_{L^2(a,b)} \leq 12^{-1/2}(b-a)^{1/2}\left(1 + 2^{1/2}\|y''\|\right)h^{3/2} + 4(b-a)^{1/2}\left(2^{1/2} + \|y''\|\right)\delta. \]

Furthermore, if \(\alpha = \alpha_2\) is obtained from (11), then we have
\[ \|f_{\alpha_2} - y\|_{L^2(a,b)} \leq 6^{-1/2}(b-a)^{1/2}\|y''\|h^{3/2} + 4\sqrt{2}(b-a)^{1/2}\delta. \]

**Proof:** For any \(x \in [x_i, x_{i+1}]\), \(x\) can be expressed as \(x = \lambda x_i + (1 - \lambda)x_{i+1}, 0 \leq \lambda \leq 1\). The conditions of Lemma 3.1 are satisfied if we let \(m = 3, \hat{c}_1 = \lambda, \hat{c}_2 = 1 - \lambda, \hat{c}_3 = -1\) and \(\hat{x}_1 = x_i, \hat{x}_2 = x_{i+1}, \hat{x}_3 = x\). Let \(e\) be the error function \(e = f_\alpha - y\). We then have
\[ L(e) = \sum_{i=1}^{3} \hat{c}_i e(\hat{x}_i) = \lambda e(x_i) + (1 - \lambda)e(x_{i+1}) - e(x). \]

Furthermore, from Lemma 3.1, we obtain
\[ |e(x)| \leq |L(e)| + |\lambda e(x_i) + (1 - \lambda)e(x_{i-1})| \leq 12^{-1}|C(\lambda)|^{1/2}|e''| + 2^{1/2}[e^2(x_i) + e^2(x_{i-1})]^{1/2}, \]
where
\[ C(\lambda) = 12 \sum_{i=1}^{3} \sum_{j=1}^{3} \hat{c}_i \hat{c}_j |\hat{x}_i - \hat{x}_j|^3 \]
\[ = 12\left[2\lambda(1 - \lambda)|x_i - x_{i+1}|^3 - 2\lambda|x - x_i|^3 - 2(1 - \lambda)|x - x_{i+1}|^3\right] \]
\[ = 12h_{i+1}^3[2\lambda(1 - \lambda)]^2 \leq 3h^3. \]

Integrating the square of (15) on \([x_i, x_{i+1}]\) yields
\[ \int_{x_i}^{x_{i+1}} e^2(x)dx \leq 24^{-1}h^3h_{i+1}|e''|^2 + 4e^2(x_i)h_{i+1} + 4e^2(x_{i+1})h_{i+1}. \]

Summating the above inequality for \(i = 1\) to \(n - 1\) gives
\[ \int_{a}^{b} e^2(x)dx \leq 24^{-1}(b-a)h^3|e''|^2 + 8\sum_{i=1}^{n} \frac{h_i + h_{i+1}}{2} e^2(x_i) \]
\[ \leq 24^{-1}(b-a)h^3|e''|^2 + 8\sum_{i \in I_a} \frac{h_i + h_{i+1}}{2} e^2(x_i). \]

If the \(a\ priori\) parameter \(\alpha = \alpha_1 = 1\) is chosen, note that \(\sum_{i \in I_a} \frac{h_i + h_{i+1}}{2} \leq b - a\), we then have
\[ \sum_{i \in I_a} \frac{h_i + h_{i+1}}{2}(f_{\alpha_1}(x_i) - y(x_i))^2 \]
This leads to

\[ \text{Hence, we have} \]

\[ \text{From} \]

\[ \frac{1}{h^2} \sum_{i \in I_n} \left( \frac{f_{\alpha_1}(x_i) - y(x_i)}{\sigma_i} \right)^2 \leq 2\delta^2 \left( \frac{1}{h^2} \sum_{i \in I_n} \left( \frac{f_{\alpha_1}(x_i) - \tilde{y}_i}{\sigma_i} \right)^2 + \left( \frac{\tilde{y}_i - y(x_i)}{\sigma_i} \right)^2 \right) \]

\[ \leq 2\delta^2 (b - a) \left( \Phi(y) + 1 \right) \]

\[ \leq 2\delta^2 (b - a) \left( 2 + \|y''\|^2 \right). \]

Since

\[ \|f'\| \leq \Phi(f_{\alpha_1}) \leq \Phi(y) \leq 1 + \|y''\|^2, \]

and

\[ \|f'' - y''\|^2 \leq 2 \left( \|f'\|^2 + \|y''\|^2 \right) \leq 2 \left( 1 + 2\|y''\|^2 \right). \]  \hspace{1cm} (19)

Combining (17), (18) and (19), we finally obtain the following error estimate

\[ \int_a^b (f_{\alpha_1} - y)^2 dx \leq 24^{-1}(b - a)\delta^2 \left( 1 + 2\|y''\|^2 \right) + 16\delta^2 (b - a) \left( 2 + \|y''\|^2 \right). \]

This leads to

\[ \|f_{\alpha_1} - y\|_{L^2(a,b)} \leq 12^{-1/2} (b - a)^{1/2} \left( 1 + 2\|y''\|^2 \right) \delta^{3/2} \]

\[ + 4(b - a)^{1/2} \left( 2^{1/2} + \|y''\|^2 \right) \delta. \]  \hspace{1cm} (20)

Furthermore, if \( \alpha = \alpha_2 \) is obtained by using the Morozov’s discrepancy principle (11), from (1) and (11) we have

\[ \frac{1}{b - a} \sum_{i \in I_n} \left( \frac{f_{\alpha_2}(x_i) - y(x_i)}{\sigma_i} \right)^2 \]

\[ \leq 2\delta^2 \left( \frac{1}{b - a} \sum_{i \in I_n} \left( \frac{f_{\alpha_2}(x_i) - \tilde{y}_i}{\sigma_i} \right)^2 + \left( \frac{\tilde{y}_i - y_i}{\sigma_i} \right)^2 \right) \leq 4\delta^2. \]  \hspace{1cm} (21)

From

\[ \alpha_2 \|f_{\alpha_2}''\|^2 = \Phi(f_{\alpha_2}) - \frac{1}{b - a} \sum_{i \in I_n} \left( \frac{f_{\alpha_2}(x_i) - \tilde{y}_i}{\sigma_i} \right)^2 \]

\[ \leq \Phi(y) - 1 \leq \alpha_2 \|y''\|^2, \]

we then have

\[ \|f_{\alpha_2}''\|^2 \leq \|y''\|^2, \]

and

\[ \|f_{\alpha_2}'' - y''\|^2 \leq 2 \|f_{\alpha_2}''\|^2 + \|y''\|^2 \leq 4\|y''\|^2. \]  \hspace{1cm} (22)

Substituting inequalities (22), (21) into (17) yields

\[ \int_{\Omega} (f_{\alpha_2} - y)^2 dx \leq 24^{-1}(b - a)\delta^2 \|y''\|^2 + 32(b - a)\delta^2. \]

Hence, we have

\[ \|f_{\alpha_2} - y\|_{L^2(a,b)} \leq 6^{-1/2}(b - a)^{1/2}\|y''\|^2 \delta^{3/2} + 4\sqrt{2}(b - a)^{1/2}\delta. \]

We need the following interpolation theorem [1] for the error estimate on the first order derivative.
Lemma 3.3 Let $-\infty < a < b < \infty$. For $0 < \varepsilon \leq 1$ and every function $f$ twice continuously differentiable on the open interval $(a, b)$, there exists a constant $K$ such that

$$
\int_a^b |f'(x)|^2 \, dx \leq K \varepsilon \int_a^b |f''(t)|^2 \, dt + K \varepsilon^{-1} \int_a^b |f(t)|^2 \, dt.
$$

(23)

Theorem 3.4 For any $y \in X$, suppose that $f_{\alpha}$ is given by Theorem 2.1. Taking $\alpha = \alpha_1 = 1$ or $\alpha = \alpha_2$ by Mozorov’s discrepancy principle (11), then for sufficiently small $\delta$ and $h$ we have

$$
\|f_{\alpha_i} - y\|_{L^2(a,b)} \leq C_i h^{3/4} + D_i \delta^{1/2}, \quad i = 1, 2,
$$

where $C_1, C_2$ and $D_1, D_2$ are constants depending on $\|y''\|$ and $b - a$.

Figure 1. Plots of function $y'(x)$ and its approximation $f'_{\alpha}(x)$ for scattered noisy data while $\delta = 0.01$. 

(a) no regularization

(b) a priori rule

(c) a posteriori rule
The derivative of $f^{\alpha}(x)$ and $y(x)$

Parameter $\alpha = 1$

(a) a priori rule

Parameter $\alpha = 0.0084$

(b) a posteriori rule

Figure 2. Plots of function $y'(x)$ and its approximation $f^{\alpha}(x)$ for scattered noisy data while $\delta = 0.1$.

**Proof:** For sufficiently small $\delta$ and $h$, it follows from Theorem 3.2 that $\|f^{\alpha_i} - y\|_{L^2(a,b)} \leq 1$. Setting $\varepsilon = \|f^{\alpha_i} - y\|_{L^2(a,b)}$ in Lemma 3.3 and using Theorem 3.2, we have

$$
\|f^{\alpha_i}' - y'\|_{L^2(a,b)}^2 \leq K\left[\|f^{\alpha_i}'' - y''\|_{L^2(a,b)}^2 + 1\right] \|f^{\alpha_i} - y\|_{L^2(a,b)} \tag{25}
$$

where $C_1, C_2$ and $D_1, D_2$ are constants depending on $\|y''\|$ and $b - a$. Then square root for inequality above gives the conclusion.

**4. Numerical example**

Choose a smooth exact function $y = \sin(2\pi x)e^{-x^2}$ in the following numerical experiments. Generate 101 scattered points on $[-2, 2]$. The noisy data are generated by adding uniform random numbers in $[-0.01, 0.01]$. Computational results are displayed in Figure 1 where the dotted line represents $f^{\alpha}$ and the solid line represents $y'$. In Figure 1(a), we take $\alpha = 0$ which means we do not use any regularization. In Figure 1(b), $\alpha = \alpha_1 = 1$ and in Figure 1(c), $\alpha = \alpha_2$ given by discrepancy principle. When the noise are generated by uniform distribution in $[-0.1, 0.1]$, computational results are displayed in Figure 2.

It is observed that for the small noise level, the approximation $f^{\alpha}$ matches the exact function $y'$ quite well for the a priori and the a posteriori choice of the parameter. However for a bit larger noise level, the discrepancy principle works more effective.

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**6. Conclusion**

In this paper, we investigate a classical ill-posed problem—numerical differentiation by using cubic spline approximation and Tikhonov regularization. Convergence results under two choice rules for regularization parameter are given. Numerical results show that the proposed method is effective and stable.
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