NUMERICAL DIFFERENTIATION BY INTEGRATION

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Abstract. Based on the Lanczos methods revived by Groetsch, a method of differentiation by integration is presented to approximate derivatives of approximately specified functions. The method is applicable for any point in a finite closed interval. Convergence estimates in $C[a, b]$ and $L^p[a, b]$ are given. Numerical examples show that the method is simple and applicable.

1. Introduction

The problem of numerical differentiation is: Given $y = f(x)$ or values for $y = f(x)$ at $x = x_0, x_1, \ldots, x_n$, find approximations for $f'(x)$. As a continuous function can be obtained in the whole interval by the linear interpolation, we first only consider the former case in this paper. In practice, data will almost never be exactly available, only a noisy observation $f_δ$ instead of $f$ is known. In this case, the problem of numerical differentiation is known to be ill-posed in the sense that small perturbations of the function may lead to large errors in the computed derivative (see [1]). However, in many applications it is necessary to estimate the derivative of a function given noisy values of this function. Applications range from biology (see [2]), chemistry (see [3]), and mathematics (see [4]) to a variety of problems in physical applications (see [5]). In order to approximate $f'(x)$ in a stable way, special methods should be applied.

A number of methods have been developed for numerical differentiation. These methods fall into three categories: finite difference methods (see [6]–[8]), general regularization methods (see [4], [9], [10], [11], [12]), and integral methods (see [13]).

Within the framework of the finite-difference method, the approximate value of the derivative $f'(x)$ is calculated as

\begin{equation}
\frac{f'(x)}{h} \approx \frac{1}{h} \sum_{j=-l}^{l} a_j^l f_δ(x + jh).
\end{equation}

Where $a_j^l$ are some fixed real numbers, and $h$ is a step-size. For $l = 1$, $a_{-1}^1 = 0$, $a_0^1 = -1$, $a_1^1 = 1$, the finite-difference method (1.1) gives us the well-known forward
difference approximation

\[ f'(x) \approx \frac{f_\delta(x + h) - f_\delta(x)}{h}. \]  

(1.2)

The difference scheme (1.1) results in a stable regularizing algorithm only if the step-size \( h \) is chosen properly (see \([7]\)).

The second category of numerical differentiation methods expresses the derivative of a smooth function \( y = f(x) \) as the solution \( z(\cdot) \) of a Volterra integral equation:

\[ (Tz)(x) := \int_a^x z(t) dt = f(x) - f(a), \quad a \leq x \leq b. \]  

(1.3)

It is clear that \( z = f'(x) \) is the unique solution of (1.3). The regularization solution of equation

\[ \int_a^x z(t) dt = f_\delta(x) - f_\delta(a), \quad a \leq x \leq b \]  

(1.4)

is taken as an approximation for \( f'(x) \). There are a variety of regularization methods for (1.4), for example iterative regularization methods, TSVD regularization methods and Tikhonov regularization methods. An example of the Tikhonov regularization methods can be found in \([4]\), where a derivative \( S'_n(x) \) of a natural cubic spine \( S_n(x) \) solving the minimization problem

\[ \frac{1}{n-1} \sum_{i=1}^{n-1} (f_\delta(x_i) - S_n(x_i))^2 + \alpha \| S''_n \|^2 \rightarrow \min \]  

(1.5)

is taken as an approximation for \( f'(x) \) under the assumption that \( f_\delta(x_0) = f(x_0) \), \( f_\delta(x_n) = f(x_n) \). In equation (1.5), \( \alpha > 0 \) is a regularization parameter.

The Lanczos method, as interpreted by Groetsch \([13]\) as a regularization method, consists of approximating of \( f'(x) \) by

\[ (R_h f_\delta)(x) = \frac{3}{2h^3} \int_{-h}^{h} tf_\delta(x + t) dt, \quad x \in [a + h, b - h]. \]  

(1.6)

If \( f(x) \in C^3[a,b] \), the error of approximation can be estimated as follows:

\[ \| R_h f_\delta - f' \|_{\infty} \leq \frac{\| f'' \|_{\infty}}{10} h^2 + \frac{3\delta}{2h}, \]

where \( h > 0 \) is a regularization parameter (see \([13]\)).

The numerical realization of an integral method is very simple and does not require the solution a system of linear algebraic equations. However, the approximation of the derivative at the end points and points near to the end points of the interval cannot be calculated. In this paper, an integral method is proposed to approximate derivatives of approximately specified functions, and the method is applicable for any point in a finite closed interval.

This paper is organized as follows. In Section 2 an integral operator \( D_h f \) is proposed, \( (D_h) f(x) \) can be used for approximating the derivative of \( f(x) \) as \( h \to 0 \). When \( f'_+ \) and \( f'_- \) exist we show the convergence behavior of \( D_h f \) which generalizes a result of Groetsch \([13]\). In Section 3 convergence estimates in \( C[a,b] \) are given. If \( f''(x) \in C^{k,\alpha}[a,b] \) (\( k = 0, 1 \)), the corresponding convergence rate is \( O(\delta^{\frac{3}{k+1}}) \) by an a priori choice of regularization parameter \( h \). In Section 4 convergence estimates
in $L^p[a,b]$ are given. If $f(x) \in AC[a,b] \cap H^{k,p}(a,b)$ ($k = 2, 3$), the corresponding convergence rate is $O(\delta^{k+1})$ by an a priori choice of regularization parameter $h$. Numerical tests are given in Section 5 to verify the efficiency of the proposed method.

2. Differentiation by Integration

In this section an integral operator $D_h f$ is proposed, when $f'_+$ and $f'_-$ exist we show the convergence behavior of $D_h f$. $(D_h) f(x)$ can be used for approximating the derivative of $f(x)$ as $h \to 0$.

Assume that $f(x) \in C[a,b] \cap H^1_p(a,b)$ ($p \geq 1$) such that its derivative is in $L^p[a,b]$, and endow $C[a,b]$ with the uniform norm

$$\|z\|_{\infty} := \sup_{\tau \in [a,b]} |z(\tau)|$$

and $L^p[a,b]$ with the norm

$$\|z\|_p := (\int_a^b |z(\tau)|^p d\tau)^{1/p}.$$ 

In practice $f(x)$ is known through some experimental data: instead of $f(x)$ only an approximation $f_\delta(x)$ is available such that

(2.1) \hspace{1cm} \|f - f_\delta\|_{\infty} \leq \delta.

Let

$$F(x) = f(x) - \frac{f(b) - f(a)}{b - a}(x - a) - f(a)$$

and

$$F_\delta(x) = f_\delta(x) - \frac{f_\delta(b) - f_\delta(a)}{b - a}(x - a) - f_\delta(a).$$

Then $F(x)$ and $F_\delta(x)$ satisfy the initial conditions [15]

$$F(a) = F(b) = 0, \quad F_\delta(a) = F_\delta(b) = 0,$$

and clearly,

(2.2) \hspace{1cm} \|F - F_\delta\|_{\infty} \leq 2\delta.

Let $j(x) \in C^1_0(R)$ be an even function satisfying:

(1) \hspace{1cm} j(x) \geq 0;
(2) \hspace{1cm} \int_{-1}^1 j(x) dx = 1;
(3) \hspace{1cm} j(x) = 0, x \notin [-1, 1];
(4) \hspace{1cm} j'(x) = 0, x \notin [-1, 1].

Such functions $j(x)$ exist, for example:

$$j(x) = \begin{cases} \frac{1}{\Gamma_{1-k}^2(1-t^2)^k dt} (1 - x^2)^k, & x \in [-1, 1] \\ 0, & x \notin [-1, 1] \end{cases} \quad (k \geq 2, k \in N).$$

Let

$$\psi^h(x, t) = \frac{j(x-t)}{\int_a^b j(x-t) dt}$$

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and

$$\psi_t^h(x, t) = -\frac{1}{h} j \left( \frac{x-t}{h} \right),$$

it is obvious that

$$\int_a^b \psi_t^h(x, t) dt = \int_a^b \frac{j \left( \frac{x-t}{h} \right)}{\int_a^b j \left( \frac{x-t}{h} \right) dt} dt = \frac{1}{\int_a^b j \left( \frac{x-t}{h} \right) dt} \int_a^b j \left( \frac{x-t}{h} \right) dt = 1.$$

By substitution,

$$\int_a^b \psi_t^h(x, t) dt = \int_a^b \frac{j \left( \frac{x-t}{h} \right)}{\int_a^b j \left( \frac{x-t}{h} \right) dt} dx = \frac{2}{h} \int_a^b j \left( \frac{x-t}{h} \right) dx. $$

Notice $j(x)$ is an even function, it also holds that $\frac{1}{2} h \leq \int_a^b j \left( \frac{x-t}{h} \right) dx \leq h$. So we have the property that

$$\int_a^b \psi_t^h(x, t) dx \leq 2.$$

Let

$$K_f = \frac{f(b) - f(a)}{b - a}$$

and

$$K_{f_\delta} = \frac{f_\delta(b) - f_\delta(a)}{b - a}.$$

Define the integral operator

$$(D_h f)(x) = K_f - \int_{[a, b]} \psi^h_t(x, t) F(t) dt, \quad x \in [a, b],$$

where $h > 0$ is the regularization parameter. We use $(D_h f)(x)$ for approximating the derivative of $f(x)$ as $h \to 0$.

It is clear that

$$(D_h f)(x) = K_f + (D_h F)(x)$$

and

$$(D_h F)(x) = - \int_{[a, b]} \psi^h_t(x, t) F(t) dt.$$

Let $u = \frac{x-t}{h}$, then

$$(D_h f)(x) = K_f + \frac{1}{\int_{[a, b]} j \left( \frac{x-t}{h} \right) dt} \int_{\left[ \frac{x-b}{h}, \frac{x-a}{h} \right]} j'(u) F(x - hu) du$$

and

$$(D_h F)(x) = \frac{1}{\int_{[a, b]} j \left( \frac{x-t}{h} \right) dt} \int_{\left[ \frac{x-b}{h}, \frac{x-a}{h} \right]} j'(u) F(x - hu) du.$$
Denote by $f'_+(a)$ and $f'_-(b)$ the right-hand and left-hand derivatives of $f$ in the classical sense. Such derivatives could not even exist under the assumption $f \in C[a, b] \cap H^{1,p}(a, b)$. However, if $f'_+$ and $f'_-$ exist we note that $D_h f$ has the following convergence behavior, which generalizes a result of Groetsch [13].

**Theorem 2.1.** If $f'_+(a)$ and $f'_-(b)$ exist, $f'_+(x)$ and $f'_-(x)$ exist for $x \in (a, b)$, then

$\lim_{h \to 0^+} (D_h f)(x) = \begin{cases} \frac{1}{2} (f'_+(x) + f'_-(x)) & x \in (a, b), \\ f'_+(a) & x = a, \\ f'_-(b) & x = b. \end{cases}$

**Proof.** Notice that for $f'_+(x) = K_f + F'_+(x)$, $f'_-(x) = K_f + F'_-(x)$ and (2.6), we only need to prove that

$$\lim_{h \to 0^+} (D_h F)(x) = \begin{cases} \frac{1}{2} (F'_+(x) + F'_-(x)) & x \in (a, b), \\ F'_+(a) & x = a, \\ F'_-(b) & x = b. \end{cases}$$

(1) We first prove that $\lim_{h \to 0^+} (D_h F)(x) = \frac{1}{2} (F'_+(x) + F'_-(x))$, $x \in (a, b)$. For $x \in (a, b)$, there exist $\delta_1 > 0$ such that $\frac{x-a}{h} > 1$ and $\frac{b-x}{h} > 1$ for $h < \delta_1$. In this case, by (2.3) and (2.8),

$$(D_h F)(x) = \frac{1}{h} \int_{[-1,1]} j'(u) F(x - hu) du.$$ 

According to the definition of $F'_\pm(x)$,

$$\lim_{y \to 0^+} \left( \frac{F(x + y) - F(x)}{y} - F'_\pm(x) \right) = 0,$$

for a given $\varepsilon > 0$, there exist $0 < \delta_2 < \delta_1$ such that

$$\left| \frac{F(x + y) - F(x)}{y} - F'_\pm(x) \right| < \frac{1}{\int_{[-1,1]} |u j'(u)| du} \varepsilon, \text{ as } 0 < y < \delta_2;$$

that is,

$$|F(x + y) - F(x) - F'_\pm(x)y| < \frac{\varepsilon y}{\int_{[-1,1]} |u j'(u)| du}, \text{ as } 0 < y < \delta_2.$$

At the same time,

$$\int_{[-1,0]} j'(u) F(x - hu) du$$

$$= \int_{[-1,0]} j'(u)[F(x - hu) - F(x) + F'_+(x)hu + F(x) - F'_+(x)hu] du$$

$$= \int_{[-1,0]} j'(u)[F(x - hu) - F(x) + F'_+(x)hu] du + F(x) \int_{[-1,0]} j'(u) du + \frac{1}{2} h F'_+(x)$$

and similarly,

$$\int_{[0,1]} j'(u) F(x - hu) du$$

$$= \int_{[0,1]} j'(u)[F(x - hu) - F(x) + F'_-(x)hu] du + F(x) \int_{[0,1]} j'(u) du + \frac{1}{2} h F'_-(x).$$
We then have:

\[
(D_hF)(x) = \frac{1}{h} \int_{[-1,0]} j'(u)[F(x-hu) - F(x) + F'_+(x)hu]du \\
+ \frac{1}{h} \int_{[0,1]} j'(u)[F(x-hu) - F(x) + F'_-(x)hu]du + \frac{1}{2}(F'_+(x) + F'_-(x)).
\]

So, if \( h < \delta_2 \), then

\[
\left| (D_hF)(x) - \frac{1}{2}(F'_+(x) + F'_-(x)) \right| \\
\leq \frac{1}{h} \int_{[-1,0]} |j'(u)||F(x-hu) - F(x) + F'_+(x)hu| du \\
+ \frac{1}{h} \int_{[0,1]} |j'(u)||F(x-hu) - F(x) + F'_-(x)hu| du \\
\leq \varepsilon \int_{[-1,0]} |uj'(u)| du \\
+ \varepsilon \int_{[0,1]} |uj'(u)| du \\
= \varepsilon.
\]

(2) We next prove that \( \lim_{h \to 0^+} (D_hF)(a) = F'_+(a) \) and \( \lim_{h \to 0^+} (D_hF)(b) = F'_-(b) \).

For \( x = a \), there exist \( \delta_3 > 0 \) such that \( \frac{b-a}{h} > 1 \) for \( h < \delta_3 \), in this case, by (2.3) and (2.8),

\[
(D_hF)(a) = \frac{2}{h} \int_{[-1,0]} j'(u)F(a-hu)du.
\]

According to the definition of \( F'_+(a) \), for a given \( \varepsilon > 0 \), there exist \( \delta_4 < \delta_3 \) such that

\[
|F(a+y) - F(a) - F'_+(a)y| < \frac{\varepsilon y}{\int_{[-1,1]} |uj'(u)| du}, \text{ for } 0 < y < \delta_4.
\]

Notice that \( F(a) = 0 \), and

\[
(D_hF)(a) = \frac{2}{h} \int_{[-1,0]} j'(u)[F(a-hu) - F(a) + F'_+(a)hu]du \\
+ \frac{2}{h} \int_{[-1,0]} j'(u)[F(a) - F'_+(a)hu]du \\
= \frac{2}{h} \int_{[-1,0]} j'(u)[F(a-hu) - F(a) + F'_+(a)hu]du + F'_+(a).
\]

So, if \( h < \delta_4 \), then

\[
\left| (D_hF)(a) - F'_+(a) \right| \\
\leq \frac{2}{h} \int_{[-1,0]} |j'(u)||F(a-hu) - F(a) + F'_+(a)hu| du \\
\leq \frac{2\varepsilon \int_{[-1,0]} |uj'(u)| du}{\int_{[-1,1]} |uj'(u)| du} \\
= \varepsilon.
\]

Similarly, we have \( \lim_{h \to 0^+} (D_hF)(b) = F'_-(b) \).
3. Convergence estimates in \( C[a, b] \)

In this section we give convergence estimates of \( D_h f_\delta \) under the assumption \( f' \in C[a, b] \).

Define

\[
(\rho h g)(x) = \int_{[a, b]} \psi^h(x, t) g(t) dt
\]
and

\[
\varpi(g, h) := \sup_{|t-\tau| \leq h, t, \tau \in [a, b]} |g(\tau) - g(t)|.
\]

**Proposition 3.1.** If \( g(x) \in C[a, b] \), then

\[
\|\rho_h g - g\|_\infty \leq \varpi(g, h).
\]

**Proof.** Observe that

\[
(\rho h g)(x) - g(x) = \int_{[a, b]} \psi^h(x, t) [g(t) - g(x)] dt.
\]

Therefore, we have

\[
|\rho_h g(x) - g(x)| \\
\leq \int_{[a, b]} \psi^h(x, t) |g(t) - g(x)| dt \\
= \int_{[a, b] \cap [x-h, x+h]} \psi^h(x, t) |g(t) - g(x)| dt \\
\leq \varpi(g, h) \int_{[a, b] \cap [x-h, x+h]} \psi^h(x, t) dt \\
= \varpi(g, h).
\]

If \( f(x) \in C^1[a, b] \), then \( F(x) \in C^1[a, b] \), and notice that \( F(a) = F(b) = 0 \). By (2.5) and the formula of integration by parts, we get

\[
(D_h f)(x) = (\rho h f')(x) = \int_{[a, b]} \psi^h(x, t) f'(t) dt.
\]

The following corollary is then a consequence of Proposition 3.1.

**Corollary 3.1.** If \( f(x) \in C^1[a, b] \), then

\[
\|D_h f - f'\|_\infty \leq \varpi(f', h).
\]

Clearly, if \( f(x) \in C^1[a, b] \), then \( \|D_h f - f'\|_\infty \to 0 \) as \( h \to 0 \). From Corollary 3.1, we obtain

**Lemma 3.1.** If \( f' \) is Hölder continuous with exponent \( \alpha \) (\( 0 < \alpha \leq 1 \)) and constant \( C_1 \), that is,

\[
|f'(t) - f'(\tau)| \leq C_1 |t - \tau|^\alpha, \quad t, \tau \in [a, b],
\]
then

\[
\|D_h f - f'\|_\infty \leq C_1 h^\alpha.
\]

In particular, if \( f(x) \in C^2[a, b] \), then \( \|D_h f - f'\|_\infty \leq \|f''\|_\infty h \).
Proof. By the definition of \( \varpi(f', h) \),
\[ \varpi(f', h) = \sup_{|t-\tau| \leq h} |f'(\tau) - f'(t)| \leq \sup_{t, \tau \in [a, b]} C_1 |\tau - t| \leq C_1 h. \]
\hfill \Box

Lemma 3.2. If \( f'' \) is Hölder continuous with exponent \( \alpha \) (\( 0 < \alpha \leq 1 \)), there is a constant \( C_2 \) such that
\[ |f''(t) - f''(\tau)| \leq C_2 |t - \tau|^\alpha, \quad t, \tau \in [a, b]. \]

If \( h < \frac{1}{2}(b - a) \), then
\[ \|D_h f - f'\|_{\infty, [a + h, b - h]} \leq \frac{2^{\alpha-1}}{1 + \alpha} C_2 h^{1+\alpha}. \]

Proof. In equation (3.3), let \( u = \frac{x-t}{h} \), then
\[ (3.4) \quad (D_h f)(x) - f'(x) = h \int_{\mathbb{R}} \psi_h(x, x - hu)[f'(x - hu) - f'(x)]du. \]
If \( a + h \leq x \leq b - h \), then \( [\frac{x-b}{h}, \frac{x-a}{h}] \cap [-1, 1] = [-1, 1] \), and from (3.4),
\[ (D_h f)(x) - f'(x) = h \int_{[-1, 1]} \psi_h(x, x - hu)[f'(x - hu) - f'(x)]du \]
\[ = \int_{[-1, 1]} j(u)[f'(x - hu) - f'(x)]du. \]
Since \( j(u) \) is an even function, then
\[ (3.5) \quad (D_h f)(x) - f'(x) = \int_{[0, 1]} j(u)[f'(x + hu) + f'(x - hu) - 2f'(x)]du. \]
Note that
\[ f'(x + hu) + f'(x - hu) - 2f'(x) = \int_{[0, hu]} [f''(x + s) - f''(x - s)]ds, \]
and hence by (3.5):
\[ |(D_h f)(x) - f'(x)| \]
\[ \leq \int_{[0, 1]} j(u)(\int_{[0, hu]} |f''(x + s) - f''(x - s)|ds)du \]
\[ \leq \int_{[0, 1]} j(u)(\int_{[0, h]} |f''(x + s) - f''(x - s)|ds)du \]
\[ \leq \int_{[0, 1]} j(u)du (C_2 \int_{[0, h]} (2s)^\alpha ds). \]
Note that since \( \int_{[0, 1]} j(u)du = \frac{1}{2} \), we have
\[ \|D_h f - f'\|_{\infty, [a + h, b - h]} \leq \frac{2^{\alpha-1}}{1 + \alpha} C_2 h^{1+\alpha}. \]
\hfill \Box

If \( f(x) \in C^3[a, b] \) and \( h < \frac{1}{2}(b - a) \), then by Lemma 3.2,
\[ \|D_h f - f'\|_{\infty, [a + h, b - h]} \leq \frac{1}{2} \|f''\|_{\infty} h^2. \]
**Lemma 3.3.** If \( h < \frac{1}{2}(b - a) \), then

\[
\|D_h f_\delta - D_h f\|_\infty \leq \frac{2\delta}{b - a} + \frac{4M}{h}\delta,
\]

where \( M = \int_{[-1,1]} |j'(u)| \, du \).

**Proof.** From (2.5), we have

\[
|(D_h f_\delta)(x) - (D_h f)(x)| \leq |K_f - K_{f_\delta}| + \int_{[a,b]\cap[x-h,x+h]} |\psi^h_t(x,t)| |F_\delta(t) - F(t)| \, dt.
\]

The first term satisfies:

\[
(3.6) \quad |K_f - K_{f_\delta}| \leq \frac{2\delta}{b - a}.
\]

By (2.2), the second term satisfies:

\[
\int_{[a,b]\cap[x-h,x+h]} |\psi^h_t(x,t)| |F_\delta(t) - F(t)| \, dt
\]

\[
\leq 2\delta \int_{[a,b]\cap[x-h,x+h]} |\psi^h_t(x,t)| \, dt
\]

\[
= \frac{2\delta}{h} \int_a^b j\left(\frac{x-t}{h}\right) \, d\tau \left(\int_{[a,b]\cap[x-h,x+h]} |j'(\frac{x-t}{h})| \, dt\right).
\]

Note that \( \int_{[a,b]\cap[x-h,x+h]} |j'(\frac{x-t}{h})| \, dt \leq h \int_{[-1,1]} |j'(u)| \, du \), and by (2.3), we get

\[
(3.7) \quad \int_{[a,b]\cap[x-h,x+h]} |\psi^h_t(x,t)| |F_\delta(t) - F(t)| \, dt \leq \frac{4\int_{[-1,1]} |j'(u)| \, du}{h} \delta.
\]

By (3.6) and (3.7), we have

\[
\|D_h f_\delta - D_h f\|_\infty \leq \frac{2\delta}{b - a} + \frac{4M}{h}\delta.
\]

The method \( D_h \) produces the approximation

\[
(D_h f_\delta)(x) = K_{f_\delta} - \int_{[a,b]\cap[x-h,x+h]} \psi^h_t(x,t)F_\delta(t) \, dt, \ x \in [a,b].
\]

The error in this approximation can be bounded as follows:

\[
(3.8) \quad \|D_h f_\delta - f'\|_\infty \leq \|D_h f_\delta - D_h f\|_\infty + \|D_h f - f'\|_\infty.
\]

This inequality and the lemmas above give the following convergence rates for \( D_h f_\delta \).

**Theorem 3.1.** (1) If \( f(x) \in C^1[a,b] \) and \( h < \frac{1}{2}(b - a) \), then

\[
\|D_h f_\delta - f'\|_\infty \leq \frac{2\delta}{b - a} + \frac{4M}{h}\delta + \varpi(f', h).
\]

If we choose \( h = h(\delta) \) satisfies \( h(\delta) \to 0 \) and \( \frac{\delta}{h(\delta)} \to 0 \) as \( \delta \to 0 \), then

\[
\|D_h f_\delta - f'\|_\infty \to 0, \text{ as } \delta \to 0.
\]

(2) If \( f' \) is Hölder continuous with exponent \( \alpha \) (\( 0 < \alpha \leq 1 \)), there is a constant \( C_1 \) such that

\[
|f'(t) - f'({\tau})| \leq C_1 |t - \tau|^{\alpha}, \quad t, \tau \in [a,b].
\]
If $h < \frac{1}{2} (b - a)$, then
\[ \| D_h f_\delta - f' \|_\infty \leq \frac{2\delta}{b - a} + \frac{4M}{h} \delta + C_1 h^\alpha. \]

If $h = h(\delta)$ is chosen a priori by $h \sim \delta^{\frac{1}{\alpha+1}}$, then
\[ \| D_{h(\delta)} f_\delta - f' \|_\infty = O(\delta^{\frac{\alpha+1}{\alpha+2}}). \]

(3) If $f''$ is Hölder continuous with exponent $\alpha$ ($0 < \alpha \leq 1$), there is a constant $C_2$ such that
\[ |f''(t) - f''(\tau)| \leq C_2 |t - \tau|^\alpha, \quad t, \tau \in [a, b]. \]

If $h < \frac{1}{2} (b - a)$, then
\[ \| D_h f_\delta - f' \|_\infty, [a + h, b - h] \leq \frac{2\delta}{b - a} + \frac{4M}{h} \delta + \frac{2^{\alpha-1}}{1 + \alpha} C_2 h^{1+\alpha}. \]

If $h = h(\delta)$ is chosen a priori by $h \sim \delta^{\frac{1}{\alpha+2}}$, then
\[ \| D_{h(\delta)} f_\delta - f' \|_\infty, [a + h, b - h] = O(\delta^{\frac{\alpha+1}{\alpha+2}}). \]

Proof. The error between $D_h f_\delta$ and $f'$ can be bounded as (3.8). From Lemma 3.3, the first term on the right side of (3.8) satisfies
\[ \| D_h f_\delta - D_h f \|_\infty \leq \frac{2\delta}{b - a} + \frac{4M}{h} \delta. \]

The second term on the right side of (3.8) can be estimated by Corollary 3.1, Lemma 3.1 and Lemma 3.2. Then, the convergence rates results are obvious by appropriate choice of parameter $h$. \hfill \Box

4. CONVERGENCE ESTIMATES IN $L^p[a, b]$

In this section we give convergence estimates of $D_h f_\delta$ under the assumption $f' \in L^p[a, b].$

Proposition 4.1. If $g(x) \in C^1[a, b]$, then
\[ \| \rho_h g - g \|_p \leq 2 \| g' \|_p h. \]

Proof. If $g(x) \in C^1[a, b]$, let
\[ \varpi(x) = \begin{cases} g'(x) & x \in [a, b], \\ 0 & x \notin [a, b]. \end{cases} \]

Then
\[ |(\rho_h g)(x) - g(x)| \leq h \int_{[\frac{x-h}{h}, \frac{x}{h}]} \psi^h(x, x - hu) \int_{[0, -hu]} \varpi(x + s) ds \, du \]

(4.1)
and by Hölder’s inequality, we get
\[
\int_\Omega \psi^h(x, x - hu) \left| \int_{[0, -hu]} \varpi(x + s) \, ds \right| \, du
\]
\[
= \int_\Omega \left[ \psi^h(x, x - hu) \right]^{\frac{1}{p}} \left[ \psi^h(x, x - hu) \right]^{\frac{1}{q}} \left| \int_{[0, -hu]} \varpi(x + s) \, ds \right| \, du
\]
\[
\leq \left( \int_\Omega \psi^h(x, x - hu) \, du \right)^{\frac{1}{q}} \left( \int_\Omega \left| \int_{[0, -hu]} \varpi(x + s) \, ds \right|^{p} \, du \right)^{\frac{1}{p}},
\]
where \( \frac{1}{p} + \frac{1}{q} = 1 \), \( \Omega = \left[ \frac{x-h}{h}, \frac{x-a}{h} \right] \cap [-1, 1] \). Note that \( h \int_\Omega \psi^h(x, x - hu) \, du = 1 \) and, by (4.1),
\[
\left| (\rho_h g)(x) - g(x) \right|^p \leq h \int_{\frac{x-h}{h}, \frac{x-a}{h}} \psi^h(x, x - hu) \left| \int_{[0, -hu]} \varpi(x + s) \, ds \right|^{p} \, du
\]
\[
\leq h \int_{[-1,0]} \psi^h(x, x - hu) \left| \int_{[0, h]} \varpi(x + s) \, ds \right|^{p} \, du
\]
\[
+ h \int_{[0,1]} \psi^h(x, x - hu) \left| \int_{[-h,0]} \varpi(x + s) \, ds \right|^{p} \, du.
\]
However, \( h \int_{[0,1]} \psi^h(x, x - hu) \, du \leq 1 \) and \( h \int_{[-1,0]} \psi^h(x, x - hu) \, du \leq 1 \), and so,
\[
\left| (\rho_h g)(x) - g(x) \right|^p \leq \int_{[-h,h]} \varpi(x + s) \, ds \right|^{p}.
\]
By Hölder’s inequality, we get
\[
\left[ \int_{[-h,h]} \varpi(x + s) \, ds \right]^{p} \leq \left[ \int_{[-h,h]} \varpi(x + s) \, ds \right]^{p} \left[ \int_{[-h,h]} 1^q \, ds \right]^{\frac{p}{q}}
\]
\[
= (2h)^{\frac{p}{q}} \int_{[-h,h]} \varpi(x + s) \, ds \]
and, therefore,
\[
\int_{[a,b]} \left| (\rho_h g)(x) - g(x) \right|^p \, dx
\]
\[
\leq (2h)^{\frac{p}{q}} \int_{[a,b]} \left[ \int_{[-h,h]} \varpi(x + s) \, ds \right]^{p} \, dx
\]
\[
= (2h)^{\frac{p}{q}} \int_{[-h,h]} \left[ \int_{[a,b]} \varpi(x + s) \, ds \right]^{p} \, dx
\]
\[
\leq (2h)^{\frac{p}{q}} \int_{[-h,h]} \left[ \int_{[a-h,b+h]} \varpi(x) \, dx \right]^{p} \, dx
\]
\[
= (2h)^{\frac{p}{q} + 1} \int_{[a-h,b+h]} \varpi(x) \, dx.
\]
Note that \( \int_{[a-h,b+h]} \varpi(x) \, dx = \int_{[a,b]} \left| g'(x) \right|^p \, dx \), and hence,
\[
\left\| \rho_h g - g \right\|_p \leq 2 \left\| g' \right\|_p h. \]
Proposition 4.2. If \( g(x) \in C^2[a, b] \) and \( h < \frac{1}{2}(b - a) \), then

\[
\|\rho_h g - g\|_{p, [a + h, b - h]} \leq \left( \frac{1}{p + 1} \right)^{\frac{1}{p}} \|g''\|_p h^2.
\]

Proof. If \( g(x) \in C^2[a, b] \) and \( a + h \leq x \leq b - h \), note that

\[
g(x + hu) + g(x - hu) - 2g(x) = \int_{[0, hu]} [g''(x + s) + g''(x - s)](hu - s)ds.
\]

By (3.3) and (3.5),

\[
|\langle \rho_h g \rangle(x) - g(x)| \leq \int_{[0, 1]} j(u)(\int_{[0, hu]} (|g''(x + s)| + |g''(x - s)|)(hu - s)ds)du
\]

\[
\leq \int_{[0, 1]} j(u)(\int_{[0, h]} (|f'''(x + s)| + |f'''(x - s)|)(h - s)ds)du
\]

\[
= \left( \int_{[0, 1]} j(u)du \right) \left( \int_{[0, h]} (|g''(x + s)| + |g''(x - s)|)(h - s)ds \right).
\]

However, \( \int_{[0, 1]} j(u)du = \frac{1}{2} \), and hence,

\[
|\langle \rho_h g \rangle(x) - g(x)| \leq \frac{1}{2} \int_{[0, h]} (|g''(x + s)| + |g''(x - s)|)(h - s)ds.
\]

Minkowski’s inequality then gives

\[
\|\rho_h g - g\|_p \leq \frac{1}{2} \left( \left\| \int_{[0, h]} |g''(x + s)| (h - s)ds \right\|_p \right)
\]

\[
+ \left\| \int_{[0, h]} |g''(x - s)| (h - s)ds \right\|_p
\]

and by Hölder’s inequality, we get

\[
\left( \int_{[0, h]} |g''(x + s)| (h - s)ds \right)^p \leq (\int_{[0, h]} |g''(x + s)|^p (h - s)ds)(\int_{[0, h]} 1^q ds)^{\frac{p}{q}}
\]

\[
= h^\frac{p}{q} \int_{[0, h]} |f'''(x + s)|^p (h - s)^p ds.
\]
Therefore,
\[
\left\| \int_{[0,h]} (|g''(x + s)| (h - s)) ds \right\|_{p, [a + h, b - h]} \\
\leq h^{\frac{1}{p}} \left( \int_{[a + h, b - h]} \left( \int_{[0,h]} |g''(x + s)|^p (h - s)^p ds dx \right)^{\frac{1}{p}} \right) \\
= h^{\frac{1}{p}} \left( \int_{[0,h]} (h - s)^p \left( \int_{[a + h, b - h]} |g''(x + s)|^p ds dx \right)^{\frac{1}{p}} \right) \\
\leq h^{\frac{1}{p}} \left( \int_{[0,h]} (h - s)^p \left( \int_{[a,b]} |g''(x)|^p dx ds \right)^{\frac{1}{p}} \right) \\
\leq (\frac{1}{p + 1})^{\frac{1}{p}} \|g''\|_p h^2.
\]

Similarly,
\[
\left\| \int_{[0,h]} (|g''(x + s)| (h - s)) ds \right\|_{p, [a + h, b - h]} \leq (\frac{1}{p + 1})^{\frac{1}{p}} \|g''\|_p h^2.
\]

By (4.3) we then have
\[
\|\rho_h g - g\|_{p, [a + h, b - h]} \leq (\frac{1}{p + 1})^{\frac{1}{p}} \|g''\|_p h^2. \quad \square
\]

**Proposition 4.3.** If \( g(x) \in L^p[a,b] \), then
\[
\|\rho_h g\|_p \leq 2^{\frac{1}{p}} \|g\|_p.
\]

**Proof.** In equation (3.1), let \( u = \frac{x - t}{h} \). Then
\[
(\rho_h g)(x) = h \int_{[\frac{x-h}{h}, \frac{x-a}{h}] \cap [-1,1]} \psi^h(x, x - hu) g(x - hu) du.
\]
Let
\[
\omega(x) = \begin{cases} 
  g(x) & x \in [a,b], \\
  0 & x \notin [a,b],
\end{cases}
\]
then
\[
|(\rho_h g)(x)| = h \left| \int_{[\frac{x-h}{h}, \frac{x-a}{h}] \cap [-1,1]} \psi^h(x, x - hu) \omega(x - hu) du \right| \\
\leq h \int_{[\frac{x-h}{h}, \frac{x-a}{h}] \cap [-1,1]} \psi^h(x, x - hu) |\omega(x - hu)| du.
\]

By Hölder’s inequality,
\[
|(\rho_h g)(x)| \\
\leq h \int_{\Omega} [\psi^h(x, x - hu)]^{\frac{1}{p}} |\psi^h(x, x - hu)|^{\frac{1}{p}} |\omega(x - hu)| du \\
\leq h \left( \int_{\Omega} \psi^h(x, x - hu) du \right)^{\frac{1}{p}} \left( \int_{\Omega} |\psi^h(x, x - hu)|^{p} du \right)^{\frac{1}{p}},
\]
where \( \Omega = \left[ \frac{x-b}{h}, \frac{x-a}{h} \right] \cap [-1, 1] \). Note that \( h \int_{\left[ \frac{x-b}{h}, \frac{x-a}{h} \right] \cap [-1, 1]} \psi^h(x, x-hu)du = 1 \) and \( h\psi^h(x, x-hu) \leq 2j(u) \), then

\[
|\langle \rho_h g \rangle (x) \rangle |^p \leq 2 \int_{[-1,1]} j(u) |\omega(x-hu)|^p du.
\]

From (4.4), we have

\[
\int_{[a,b]} |\langle \rho_h g \rangle (x) \rangle |^p dx \leq 2 \int_{[a,b]} \int_{[-1,1]} j(u) |\omega(x-hu)|^p du dx
\]

\[
= 2 \int_{[-1,1]} \int_{[a,b]} j(u) |\omega(x-hu)|^p dx du
\]

\[
\leq 2 \int_{[-1,1]} \int_{[a-h, b+h]} j(u) |\omega(x)|^p dx du.
\]

Note that \( \int_{[-1,1]} j(u) du = 1 \), and so,

\[
\|\rho_h g\|_p \leq 2^{\frac{1}{p}} \left( \int_{[a-h, b+h]} |\omega(x)|^p dx \right)^{\frac{1}{p}} = 2^{\frac{1}{p}} \|g\|_p. \quad \square
\]

We denote the space of absolutely continuous functions on \([a, b]\) by \( AC[a,b] \).

**Lemma 4.1.** If \( f(x) \in AC[a, b] \), then

\[
\|D_h f - f'\|_p \to 0, \quad as h \to 0.
\]

**Proof.** If \( f(x) \in AC[a, b] \), then \( f' \in L^p[a, b] \) and notice \( F(a) = F(b) = 0 \). By (2.5) and the formula of integration by parts,

\[
(D_h f)(x) = \langle \rho_h f' \rangle (x) = \int_{[a, b] \cap [x-h, x+h]} \psi^h(x, t) f'(t) dt.
\]

Since \( C[a, b] \) is dense in \( L^p[a, b] \), for all \( \eta > 0 \), there exists \( \Phi \in C[a, b] \) such that

\[
\|\Phi - f'\|_p < \frac{\eta}{2^{1+\frac{1}{p}} + 2}.
\]

By Proposition 3.1, \( \|\rho_h \Phi - \Phi\|_p \leq (b-a)^{\frac{1}{p}} \varpi(\Phi, h) \), and hence there exists \( h_0 \) such that for \( 0 < h < h_0 \),

\[
\|\rho_h \Phi - \Phi\|_p < \frac{\eta}{2}.
\]

By Proposition 4.3 and (4.5),

\[
\|D_h f - \rho_h \Phi\|_p = \|\rho_h f' - \rho_h \Phi\|_p \leq 2^{\frac{1}{p}} \|f' - \Phi\|_p,
\]

thus,

\[
\|D_h f - f'\|_p \leq \|\rho_h f' - \rho_h \Phi\|_p + \|\rho_h \Phi - \Phi\|_p + \|\Phi - f'\|_p
\]

\[
\leq (2^{\frac{1}{p}} + 2) \|\Phi - f'\|_p + \|\rho_h \Phi - \Phi\|_p \leq \eta. \quad \square
\]

**Lemma 4.2.** If \( f(x) \in AC[a, b] \cap H^{2,p}(a, b) \), then

\[
\|D_h f - f'\|_p \leq 2 \|f''\|_p h.
\]

**Proof.** If \( f(x) \in AC[a, b] \cap H^{2,p}(a, b) \), then (4.5) holds. Moreover, since \( f' \in H^{1,p}(a, b) \), and as \( C^1[a, b] \) is dense in \( H^{1,p}(a, b) \), there exists a sequence \( \Phi_k(x) \in C^1[a, b] \) such that
Lemma 4.3. Letting $k \parallel \delta \rightarrow 0$, By Proposition 4.1 and (4.5),

From Lemma 3.3, for the first term on the right side of (4.6), we get

hence, then, the error between

Proof. Theorem 4.1. Suppose $f(x) \in AC[a, b]$. If $h = h(\delta) \rightarrow 0$ and $\frac{\delta}{h(\delta)} \rightarrow 0$ as $\delta \rightarrow 0$, then

(1) If $f(x) \in AC[a, b]$ and $h < \frac{1}{2}(b - a)$, then

(2) If $f(x) \in AC[a, b] \cap H^3, p(a, b)$ and $h < \frac{1}{2}(b - a)$, then

If $h = h(\delta)$ is chosen a priori by $h \sim \delta^{\frac{1}{2}}$, then

(3) If $f(x) \in AC[a, b] \cap H^3, p(a, b)$ and $h < \frac{1}{2}(b - a)$, then

If $h = h(\delta)$ is chosen a priori by $h \sim \delta^{\frac{1}{3}}$, then

Proof. The error between $D_h f_\delta$ and $f'$ can be bounded as

From Lemma 3.3 for the first term on the right side of (4.6), we get

\[ ||\Phi_k - f'||_{H^1, p} \rightarrow 0, \text{ as } k \rightarrow +\infty. \]

This implies

\[ ||\Phi'_k||_p \rightarrow ||f'||_p \text{ and } ||\Phi_k - f'||_p \rightarrow 0, \text{ as } k \rightarrow +\infty. \]

By Proposition 4.1 and (4.5),

\[
\|D_h f - f'\|_p \leq \|\rho_h f' - \rho_h \Phi_k\|_p + \|\rho_h \Phi_k - \Phi_k\|_p + \|\Phi_k - f'\|_p \\
\leq (2^\frac{1}{p} + 1) ||\Phi_k - f'||_p + \|\rho_h \Phi_k - \Phi_k\|_p \\
\leq (2^\frac{1}{p} + 1) ||\Phi_k - f'||_p + 2 ||\Phi'_k||_p h.
\]

Letting $k \rightarrow +\infty$, we have

\[ ||D_h f - f'||_p \leq 2 ||f'||_p h. \]

By the same reasoning used in the proof of Lemma 4.2 we have:

Lemma 4.3. Assume $f(x) \in C[a, b] \cap H^3, p(a, b)$. If $h < \frac{1}{2}(b - a)$, then

\[ ||D_h f - f'||_{p, [a+h, b-h]} \leq \left( \frac{1}{p+1} \right)^{\frac{1}{p}} ||f''||_p h^2. \]

Theorem 4.1. (1) Suppose $f(x) \in AC[a, b]$. If $h = h(\delta) \rightarrow 0$ and $\frac{\delta}{h(\delta)} \rightarrow 0$ as $\delta \rightarrow 0$, then

\[ ||D_{h(\delta)} f_\delta - f'||_p \rightarrow 0, \delta \rightarrow 0. \]

(2) If $f(x) \in AC[a, b] \cap H^2, p(a, b)$ and $h < \frac{1}{2}(b - a)$, then

\[
||D_h f_\delta - f'||_p \leq (b - a)^{\frac{1}{2}} (\frac{2\delta}{b-a} + \frac{4M}{h}) + 2 ||f''||_p h.
\]

If $h = h(\delta)$ is chosen a priori by $h \sim \delta^{\frac{1}{2}}$, then

\[ ||D_{h(\delta)} f_\delta - f'||_p = O(\delta^{\frac{1}{2}}). \]

(3) If $f(x) \in AC[a, b] \cap H^3, p(a, b)$ and $h < \frac{1}{2}(b - a)$, then

\[
||D_h f_\delta - f'||_{p, [a+h, b-h]} \leq (b-a)^{\frac{1}{2}} (\frac{2\delta}{b-a} + \frac{4M}{h}) + \left( \frac{1}{p+1} \right)^{\frac{1}{p}} ||f''||_p h^2.
\]

If $h = h(\delta)$ is chosen a priori by $h \sim \delta^{\frac{1}{3}}$, then

\[ ||D_{h(\delta)} f_\delta - f'||_{p, [a+h, b-h]} = O(\delta^{\frac{1}{3}}). \]

Proof. The error between $D_h f_\delta$ and $f'$ can be bounded as

(4.6) \[ ||D_h f_\delta - f'||_p \leq ||D_h f_\delta - D_h f||_p + ||D_h f - f'||_p. \]

From Lemma 3.3 for the first term on the right side of (4.6), we get

\[
||D_h f_\delta - D_h f||_p = \left( \int_a^b |D_h f(x) \delta - D_h f(x)|^p dx \right)^{\frac{1}{p}} \\
\leq \left( \int_a^b (||D_h f \delta - D_h f||_{\infty})^p dx \right)^{\frac{1}{p}} \\
= (b-a)^{\frac{1}{p}} (\frac{2\delta}{b-a} + \frac{4M}{h}).
\]
The second term on the right side of (4.6) can be estimated by Lemma 4.1, Lemma 4.2 and Lemma 4.3. Then, the convergence rates results are obvious by the appropriate choice of parameter $h$. □

Remark 4.1. In Lemma 4.1, Lemma 4.2, and Theorem 4.1, the condition $f(x)$ is absolutely continuous ($f(x) \in AC[a, b]$) guarantees that (4.5) holds.

An a posteriori choice of the regularization parameter is key to effective methods. In [14] an a posteriori rule is suggested for the choice of the stepsize $h$ in the finite-difference methods, but there is little study on the a posteriori choice of regularization parameter in integral methods. The same approach as in [14] can be used to address this issue for our proposed method. To do this one may also use a general argument from [16]. Here, if the error bound $\delta$ in (2.1) is known, we simply choose the regularization parameter $h = \delta^{\frac{1}{2}}$.

5. Numerical examples

In order to test our method, we consider the derivative of several functions $y = f(x)$, $x \in [a, b]$. Suppose we only know the value \{y_{\delta}^i\}_{i=1}^n at points \{x_{i}\}_{i=1}^n, where $x_{i} = a + \frac{(i-1)}{n-1}(b - a)$, $y_{\delta}^i = f(x_{i}) + (2 \times \text{rand} - 1)\delta$, and rand is a random number between 0 and 1. We choose $f(x) = f_k(x)$, $(k = 1, 2, 3, 4)$ given by

$$f_1(x) = \sin x, \quad x \in [-\pi, \pi],$$
$$f_2(x) = \sin(x^2), \quad x \in [0, \pi],$$
$$f_3(x) = \begin{cases} -x, & x \in [-1, 0], \\ x^2, & x \in (0, 1], \end{cases}$$
$$f_4(x) = \begin{cases} -x - 1, & x \in [-2, -1], \\ x + 1, & x \in (-1, 0), \\ -x + 1, & x \in (0, 1], \\ x - 1, & x \in (1, 2]. \end{cases}$$

We only calculate the approximate derivative at the points $x_j = a + \frac{(j-1)}{m-1}(b - a)$, $j = 1, \ldots, m$.

Let $n = 1000$, $\delta = 0.001$, $m = 100$, and we choose

$$j(x) = \begin{cases} \frac{1}{\int_{-1}^{1} (1-x^2)^2 \text{d}x} (1 - x^2)^2, & x \in [-1, 1], \\ 0, & x \notin [-1, 1]. \end{cases}$$

A program to test the numerical viability of our method with regularization parameter $h = \delta^{\frac{1}{2}}$ was written in MATLAB. The numerical results are shown in Figures 1–4. In the figures, “·” denotes the approximate derivative calculated by using our method. Numerical examples show that the method is simple and applicable. We can obtain stable approximations for derivatives of approximately specified functions, and the method is available for any point in a finite closed interval.

Our proposed method is a generalized “Lanczos method”, and the numerical realization is simple. The method allows us to compute a “pseudo-derivative” at points where the function is not differentiable, and is applicable for any point in a finite closed interval. The significance is not in the ability of the derivative to compute a pseudo-derivative, but rather in the properties the derivative shares with
other mathematical subjects. Generalizations of the Lanczos derivative provide a basis for certain grid-free Finite Interpolation Methods (FIMs) which appear to have advantages over alternatives such as the standard Finite Difference Methods (FDMs) or Finite Element Methods (FEMs) for certain problems, e.g., hypervelocity impact problems in computational material dynamics \[17\].

\begin{figure}
\centering
\includegraphics[width=\textwidth]{f1}
\caption{Numerical example for $f_1$}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{f2}
\caption{Numerical example for $f_2$}
\end{figure}
Figure 3. Numerical example for $f_3$

Figure 4. Numerical example for $f_4$
NUMERICAL DIFFERENTIATION BY INTEGRATION

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