

The use of higher order finite difference schemes is not dangerous

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Abstract

We discuss the issue of choosing a finite difference scheme for numerical differentiation in case the smoothness of the underlying function is unknown. If low order finite difference schemes are used for smooth functions, then the best possible accuracy cannot be obtained. This can be circumvented by using higher order finite difference schemes, but there is discussion that this may cause bad error behavior. Here we show, theoretically and by numerical simulation, that this is not the case. However, by doing so, the step-size should be chosen a posteriori.

Key words: numerical differentiation, finite difference scheme, spline approximation

1 Problem formulation

The objective of this note is to confirm that the use of high order finite difference schemes for numerical differentiation is not problematic if the choice of step-size is done adaptively, complementing the previous study [1]. To this end we shall prove that the use of high order finite difference schemes allows for optimal order reconstruction of the derivative (at any given interior point

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of the domain), i.e., the same order which would be achievable when choosing a scheme which is adjusted to the smoothness. Since often the latter is not known, some authors argue that one should use lower order schemes in case of uncertainty, see e.g. [6, Remark 5.1]. Here the authors establish that the order of a finite difference scheme has a role similar to the *qualification* of regularization, and hence higher order finite difference schemes may be used for low order smoothness.

The error bound which is obtained in Theorem 3 relies on some tools from spline approximation, such that in Section 2 we start our analysis with the discussion on bounds for some K -functionals, related to the numerical differentiation problem. We then use this bound in Section 3 to obtain the main result. In Section 4 we conclude our study with a discussion based on numerical simulation and an a posteriori choice for the step-size.

2 Bounding the K -functional

For any continuous function $y \in C[0, 1]$ we introduce the K -functional with respect to the space $C^s[0, 1]$ as

$$K(y, C^s[0, 1], t) := \inf_{z \in C^s[0, 1]} \left(\|y - z\|_\infty + t \|z^{(s)}\|_\infty \right), \quad 0 < t < 1. \quad (1)$$

We recommend the seminal monograph [2] on the study of these. Here the following bound for the K -functional will prove important.

Proposition 1 *Suppose that $0 \leq r \leq s < \infty$ are naturals. There is a constant $C = C(r, s)$ ¹ for which*

$$K(y, C^s[0, 1], t) \leq C t^{r/s} \|y^{(r)}\|_\infty, \quad 0 < t < 1. \quad (2)$$

The proof of this proposition will use results from spline approximation. To this end we subdivide the interval $[0, 1]$ into n equally sized subintervals, say Δ_h of length $h := 1/n$. A function, say z , belongs to the set $\mathcal{S}_h^{s,d}$ of splines of order s with defect $d < s$ if it is polynomial of degree at most s on each subinterval Δ_h and has overall derivatives of order $s - d$. Therefore the number d is called *defect* of z . The approximation of functions by splines from sets $\mathcal{S}_h^{s,d}$ is classical in approximation theory, we recommend [3]. The following result can be derived from there.

Lemma 1 *Suppose that $0 < r < s$.*

¹ Here and below constants are generic and the same symbol C may represent a different value at different places.

(1) There is a constant $C < \infty$ such that to each function $y \in C^r[0, 1]$ we can assign a spline $z \in \mathcal{S}_h^{s+1,1}$ such that for $i = 0, \dots, r$ it holds

$$\|y^{(i)} - z^{(i)}\|_\infty \leq Ch^{r-i}\|y^{(r)}\|_\infty, \quad \text{as } h \rightarrow 0. \quad (3)$$

(2) There is a constant $C = C(r, s)$ such that for each spline $z \in \mathcal{S}_h^{s+1,1}$ it holds that

$$\|z^{(s)}\|_\infty \leq Ch^{r-s}\|z^{(r)}\|_\infty, \quad \text{as } h \rightarrow 0. \quad (4)$$

Remark 2 We comment on both assertions. The first result is classical in spline approximation, see e.g. [3, Eq. (6.50)]. The second result follows from successive application of the Markov inequality, see e.g. [4], on any fixed subinterval Δ_h . There the spline $z^{(i-1)}$ is a polynomial of degree $s - i + 2$, and the Markov inequality asserts that

$$\|z^{(i)}\|_\infty \leq 2(s - i + 2)^2/h\|z^{(i-1)}\|_\infty.$$

Hence this implies that

$$\|z^{(s)}\|_\infty \leq \frac{2 \cdot 4}{h}\|z^{(s-1)}\|_\infty \leq \dots \leq \frac{2^{s-r}[(s-r+1)!]^2}{h^{s-r}}\|z^{(r)}\|_\infty.$$

Proof.(of Proposition 1) Fix any $y \in C^r[0, 1]$. For $h > 0$ we assign a spline $z \in \mathcal{S}_h^{s+1,1}$ according to Lemma 1. This spline obeys

$$\|y - z\|_\infty \leq Ch^r\|y^{(r)}\|_\infty, \quad \text{and} \quad \|z^{(s)}\|_\infty \leq Ch^{r-s}\|z^{(r)}\|_\infty.$$

In addition, applying (3) with $i := r$ provides us with

$$\|z^{(r)}\|_\infty \leq \|y^{(r)}\|_\infty + \|z^{(r)} - y^{(r)}\|_\infty \leq (1 + C)\|y^{(r)}\|_\infty,$$

Therefore, letting $n \asymp t^{-1/s}$, and hence $h \asymp t^{1/s}$, we obtain that

$$\begin{aligned} K(y, C^s[0, 1], t) &\leq Ch^r\|y^{(r)}\|_\infty + t\|z^{(s)}\|_\infty \\ &\leq \tilde{C} \left(h^r + th^{r-s} \right) \|y^{(r)}\|_\infty \\ &\leq Ct^{r/s}\|y^{(r)}\|_\infty, \end{aligned}$$

and the proof is complete. \square

3 The residual error of high order finite difference schemes

We restrict to linear finite difference schemes of the form

$$D_h^l y(t) = h^{-1} \sum_{j=-l}^l a_j^l y(t + jh), \quad (5)$$

where a_j^l are some fixed real numbers (independent of t), and a step-size h is so small that $t + jh \in [0, 1]$ for $j = 0, \pm 1, \pm 2, \dots, \pm l$. We shall abbreviate by a^l the corresponding vector of weights, i.e., $a^l := (a_{-l}^l, \dots, a_l^l)$.

Both the forward finite difference schemes D_h^f and the central difference D_h^1 are obtained in this way with $l := 1$ and $a^1 = (0, -1, 1)$, and $a^1 = 1/2(-1, 0, 1)$, respectively. As we can see, all such finite difference schemes involve the step-size h as a parameter to be chosen.

Given a continuously differentiable function y and a finite difference scheme D_h^l its *residual error* (at $t \in (0, 1)$) is given by

$$e(D_h^l, y) := |y'(t) - D_h^l y(t)|,$$

which is well-defined for $h > 0$ small enough. Of course, we expect this to converge to zero as $h \rightarrow 0$ for every continuously differentiable function y . This is comprised in the concept of consistency.

Definition 1 A finite difference scheme D_h^l is called consistent if $e(D_h^l, y) \rightarrow 0$ as $h \rightarrow 0$, for every continuously differentiable function y .

This may further be strengthened by assuming decay rates.

Definition 2 The finite difference scheme D_h^l is of order $s \leq 2l + 1$ if there is a constant $C < \infty$ such that for every $y \in C^{s+1}[0, 1]$ it holds

$$e(D_h^l, y) \leq Ch^s \|y^{(s+1)}\|_\infty. \quad (6)$$

Checking convergence to zero for schemes as in (5) on the functions $y_0 \equiv 1$, and $y_1(t) = t$ we must necessarily have that

$$\sum_{j=-l}^l a_j^l = 0 \quad \text{and} \quad \sum_{j=-l}^l j a_j^l = 1. \quad (7)$$

We further restrict to *central* finite difference schemes, i.e., we assume that $a_j^l = -a_{-j}^l$, $j = 0, \dots, l$. In particular this means that $a_0^l = 0$, and the first equality in (7) is automatically fulfilled. We list a few examples which are discussed more recently.

Example 1 The central difference D_h^1 has order 2, and is obtained as $a^1 = 1/2(-1, 0, 1)$. The fourth-order central scheme D_h^2 with coefficients

$$a^2 = \frac{1}{12}(1, -8, 0, 8, -1) \quad (8)$$

is often presented, and we refer to [5], while the seventh-order central scheme D_h^4

with coefficients

$$a^4 = \frac{1}{8760}(-3, -128, 1272, -6528, 0, 6528, -1272, 128, 3) \quad (9)$$

was analyzed in [6].

For central finite difference schemes, the second equality in (7) is also sufficient for consistency. To this end we recall the notion of the *modulus of continuity* of a function $f \in C[0, 1]$ as

$$\omega(f, h) := \sup_{|t-\tau| \leq h} |f(t) - f(\tau)|, \quad h \text{ small enough.}$$

It is easy to check that it is a non-decreasing function in h , and converges to zero for any continuous function f . Moreover, it holds $\omega(f, lh) \leq l\omega(f, h)$, where we refer to [3] for details.

Proposition 2 *A central finite difference scheme D_h^l is consistent if and only if it obeys $\sum_{j=1}^l ja_j^l = 1/2$.*

In this case there is a constant $C < \infty$ such that for any $y \in C^1[0, 1]$ it holds

$$e(D_h^l, y) \leq C\omega(y', h), \quad \text{as } h \rightarrow 0.$$

Proof. The necessity was discussed above. To prove the sufficiency we observe that for a continuously differentiable function y we have $y(t) - y(0) = \int_0^t y'(\tau) d\tau$, and we can rewrite $D_h^l y(t)$, using also the first equality in (7), as

$$\begin{aligned} D_h^l y(t) &= \frac{1}{h} \sum_{j=-l}^l a_j^l \left(y(0) + \int_0^{t+jh} y'(\tau) d\tau \right) \\ &= 0 + 2 \sum_{j=1}^l ja_j^l \frac{1}{2jh} \int_{t-jh}^{t+jh} y'(\tau) d\tau. \end{aligned}$$

Since $2 \sum_{j=1}^l ja_j^l = 1$, we conclude from here that

$$y'(t) - D_h^l y(t) = 2 \sum_{j=1}^l ja_j^l \frac{1}{2jh} \int_{t-jh}^{t+jh} (y'(t) - y'(\tau)) d\tau,$$

such that we can bound

$$\begin{aligned} e(D_h^l, y) &\leq 2 \left(\sum_{j=1}^l j |a_j^l| \right) \max_{1 \leq j \leq l} \frac{1}{2jh} \int_{t-jh}^{t+jh} |y'(t) - y'(\tau)| d\tau \\ &\leq 2 \left(\sum_{j=1}^l j |a_j^l| \right) \omega(y', lh) \rightarrow 0, \quad \text{as } h \rightarrow 0. \end{aligned}$$

□

We are going to apply Proposition 1 to bound the residual error of finite difference schemes D_h^l when the order of D_h^l is larger than the smoothness of the function to be differentiated.

Theorem 3 *Suppose that some finite difference scheme D_h^l is of order s . There is a constant $C < \infty$ such that for any $y \in C^{k+1}[0, 1]$ and $k \leq s$ it holds*

$$e(D_h^l, y) \leq Ch^k \|y^{(k+1)}\|_\infty, \quad \text{as } h \rightarrow 0. \quad (10)$$

Proof. For any $z \in C^{s+1}[0, 1]$ we can bound the residual error as

$$e(D_h^l, y) \leq e(D_h^l, z) + e(D_h^l, y - z). \quad (11)$$

Since D_h^l is assumed to have order s we can bound the first summand on the right as

$$e(D_h^l, z) \leq Ch^s \|z^{(s+1)}\|_\infty. \quad (12)$$

If the finite difference scheme D_h^l is consistent then Proposition 2 allows us to estimate the second term in (11) by

$$e(D_h^l, y - z) \leq C\omega(y' - z', h) \leq 2C\|y' - z'\|_\infty.$$

Thus, there is a constant $C < \infty$ such that for any $z \in C^{s+1}$ the bound

$$e(D_h^l, y) \leq C \left(\|y' - z'\|_\infty + h^s \|z^{(s+1)}\|_\infty \right)$$

holds true. Hence, taking the infimum over such functions z we see that the bound from (11) can be expressed in terms of the K -functional from (1) as

$$e(D_h^l, y) \leq CK(y', C^s[0, 1], h^s), \quad \text{as } h \rightarrow 0. \quad (13)$$

Therefore, Proposition 1, applied with $r := k$ and $t := h^s$ yields that $e(D_h^l, y) \leq Ch^k \|y^{(k+1)}\|_\infty$, and the proof is complete. □

Actually, the result just proved provides more than stated. The bounds apply *uniformly* for points $t \in (0, 1)$ where the derivative shall be approximated. However, in order to construct finite difference schemes it is necessary that the point t is bounded away from the boundary. Thus, the asymptotics would read, that for every $0 < a < b < 1$ the bound from Theorem 3 holds true uniformly for $t \in [a, b] \subset [0, 1]$.

4 A posteriori choice of the step-size

The above bounds for the residual error provide us with bounds for the error of finite difference schemes when the step-size is chosen a posteriori, in particular according to rule described in [1]. To this end we first summarize our findings to the following form, where $k \wedge s$ denotes the minimum of both values.

Corollary 4 *Suppose that some finite difference scheme D_h^l is of order s . There is a constant $C < \infty$ such that for any $y \in C^{k+1}[0, 1]$ it holds that*

$$e(D_h^l, y) \leq Ch^{k \wedge s} \|y^{((k \wedge s)+1)}\|_\infty, \quad \text{as } h \rightarrow 0.$$

Proof. If $k \leq s$ then this was proved in Theorem 3. In case that $k \geq s + 1$ then the order bound from (6) yields the corresponding bound. \square

This allows us to continue the discussion started in [1], in which the authors presented a principle for the choice of the step-size h when only noisy data $y_\delta(s)$ with

$$\sup_{s \in [0, 1]} |y(s) - y_\delta(s)| \leq \delta,$$

are available. In this case the step-size should be adjusted to δ , as this exhibits the overall error bound, see e.g. [1, Eq (2.5)],

$$|y'(t) - D_h^l y_\delta(t)| \leq e(D_h^l, y) + C \frac{\delta}{h}, \quad \text{as } h \rightarrow 0. \quad (14)$$

Notice, that in order to have the overall error converge to zero along with $\delta \rightarrow 0$, the step-size h necessarily must converge to zero, which is exactly the framework in which the theoretical results from above. In [1] a rule for choosing the step-size h was presented which is capable to balance both terms above without information on $e(D_h^l, y)$. To apply this, one has to choose a finite difference scheme D_h^l , and apply this along a sequence of step-sizes $\delta = h_1 < h_2 < \dots < h_N < 1$, such that $0 \leq t \pm lh_N \leq 1$. Corollary 4 asserts that for a finite difference scheme of order s one should choose $h_N \sim \delta^{1/(s+1)}$, at least, in order to capture the best possible order. This restricts the possible choice of order s , unless $\delta > 0$ is small. But, if so, then the rule from [1] chooses some step-size, say h_+ , dependent on the data $y_\delta(t \pm jh_k)$, $k = 1, \dots, N$. Precisely, we let (with constant C from (14))

$$h_+ := \max \left\{ h_i : \left| D_{h_j}^l y_\delta(t) - D_{h_i}^l y_\delta(t) \right| \leq \frac{4C\delta}{h_j}, \quad j = 1, \dots, i-1 \right\}.$$

In general, when choosing the spacing between consecutive step-sizes small, many comparisons must be carried out. However, within the present context, the evaluation of a finite difference scheme at given step-size is quick. In practice, the step-sizes are along some geometric progression.

The main result from [1, Thm. 2.1] asserts that such choice of the parameter is (up to a constant) the *best possible* for any function $y \in C^1[0, 1]$ in the sense of an oracle inequality. The result from Corollary 4 provides us with the additional information about the *order* of the error, if the smoothness, say $k + 1$, of the function y , was known. Specifically, it provides the order

$$\left| y'(t) - D_h^l y_\delta(t) \right| \leq C \delta^{\frac{k \wedge s}{(k \wedge s) + 1}}, \quad \text{as } \delta \rightarrow 0. \quad (15)$$

We finally report some numerical simulations ², extending the ones from [1,6] for the following functions

$$f_k(t) := |t|^k + |t - 0.25|^k + |t - 0.5|^k + |t - 0.75|^k + |t - 0.85|^k, \quad k = 3, 5, 7.$$

These functions are defined everywhere, and we may choose nodes at any location. They exhibit different smoothness at the point $t := 0.5$ of interest. The finite difference schemes used in the simulation are the central difference D_h^1 , which has the order 2, and the finite difference schemes from example 1, which are known to have orders 4 and 7, respectively. The noise level δ varies from 10^{-10} to 10^{-1} . The plots in Figure 1 exhibit the observed rates of convergence, by using the balancing principle for the choice of the step size. Below, in Table 1, the convergence rates are estimated from regression ³

$$|error| \sim \text{constant} \times \delta^{\text{exponent}}.$$

We comment on this. The author in [6, § 5] observes that for fixed step-size ($h = 0.1$ in his case) the results deteriorate if high-order finite difference schemes are used for functions of a low order smoothness. In that study the data were assumed to be noise-free (computer accuracy). In contrast, the numerical studies in [1, § 2.2] reveal, that this is not the case if the step-size is chosen *a posteriori*. As could be seen from the numerical simulations, the chosen step size is almost constant, if the order of the finite difference scheme is close to the smoothness, while it varies significantly if high order finite difference schemes are used for functions of low smoothness. For example, at the function f_3 , and using the finite difference scheme of order 7, the step size varies from 0.08 to 0.20. This also holds true in the opposite case, i.e., when smoothness is higher than the order of the finite difference scheme.

Furthermore, as one can see, in case of functions f_5, f_7 with high order smoothness the low order scheme D_h^1 exhibits a saturation, while high order schemes produce better results. However, the estimated rates differ from the theoretical bound (15), probably due to small sample size.

² The numerical simulations were carried out in MATLAB, and they are reproduced here with kind permission by Shuai Lu, RICAM Linz.

³ Regression and production of the pictures in Figure 1 were carried out in the package **R**, see [7].

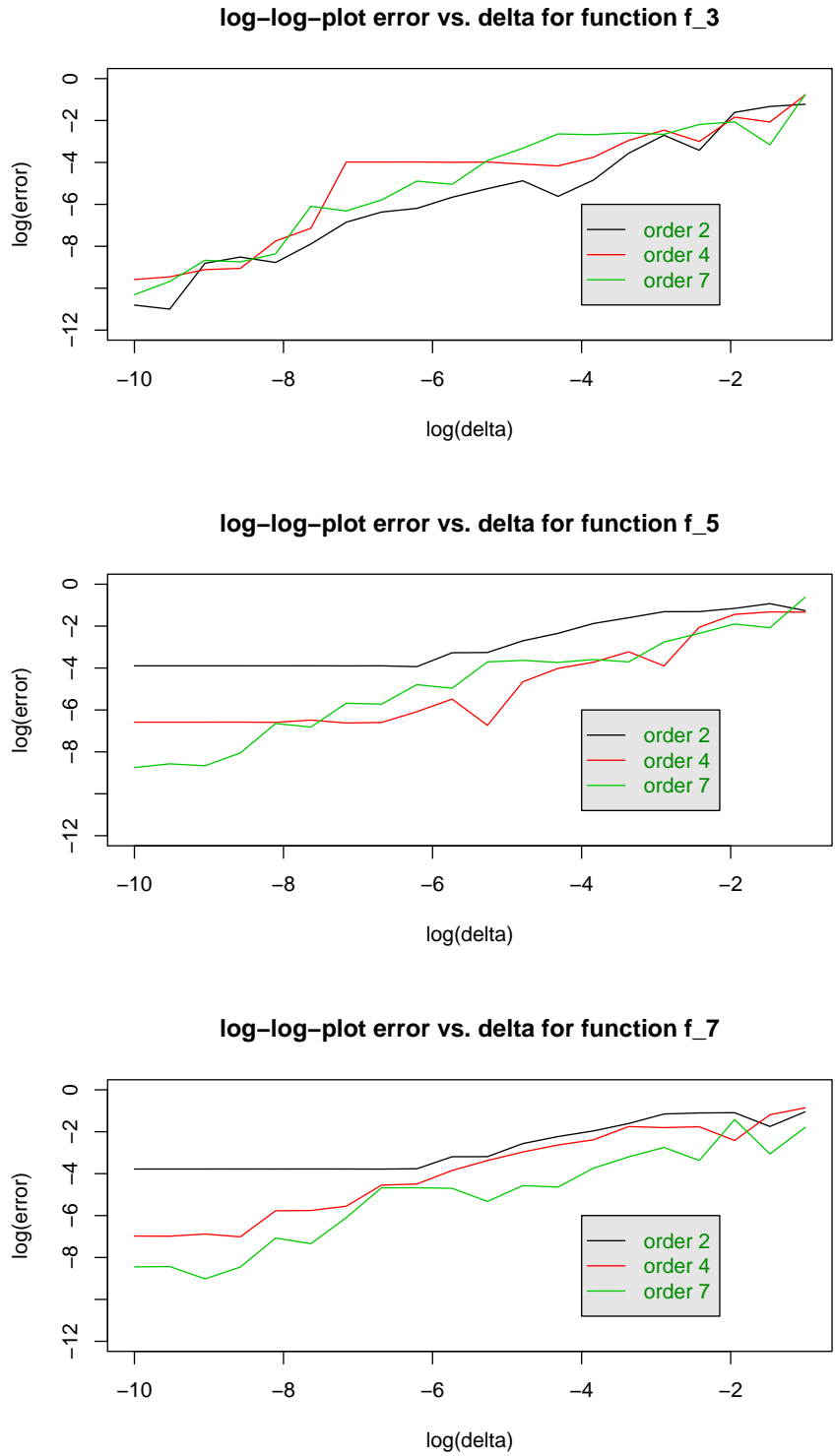


Fig. 1. log-log plots (in base 10) for the convergence at the functions f_3 , f_5 and f_7 , respectively, with parameter choice according to the balancing principle. As can be seen, higher order finite difference schemes capture the best rates, while low order finite difference schemes exhibit saturation for functions with high smoothness, at least if δ is small.

f_3	2	4	7
constant	0.7869	1.515	2.512
exponent	1.0295	0.9159	0.9808
f_5	2	4	7
constant	0.2377	0.06916	0.763
exponent	0.3967	0.6673	0.8581
f_7	2	4	7
constant	0.1983	1.327	0.1652
exponent	0.3713	0.7405	0.7923

Table 1

Estimating convergence rates for finite difference schemes of different order 2, 4, 7 applied to the functions f_3 , f_5 and f_7 , respectively.

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