New limit definition of fractional derivatives: Toward improved accuracy and generalization

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Abstract

We computationally study 2 most recently defined fractional derivatives (FDs) with classical properties, both based on 1st principles, also known as delta methods, involving limit approaches. Using the advantages of both the definitions we present a new limit definition of the FD that has always less computational error or, equivalently, more computational accuracy and at the same time satisfies all the classical properties that are observed by the foregoing 2 definitions. Such definitions are desirable so that these provide a smooth transition to/from the most extensively used and the best understood classical derivative (CD). Our study throws more light on the pros and cons of these definitions and possibly encourage further innovative approach to improve the definitions for still better/complete compatibility/generalization, and possibly to understand and to write the physical significance of the FD readily.

Keywords

Classical properties, Computational complexity, Fractional derivatives with classical properties, Improved accuracy, Limit definition of fractional derivatives.

AMS Subject Classification

26A33, 30E25, 34A12, 34A34, 34A37, 37C25, 45J05.

1 Introduction

Isaac Newton (1642-1727), an English physicist and mathematician and Gottfried Wilhelm (von) Leibniz (1646-1716), a German polymath and a philosopher may be considered as the 2 pioneers of modern calculus. Classical (i.e. integer-order) derivatives (CDs) of a function defined in modern calculus have been known and used since later half of the 17\textsuperscript{th} century.

The (non-integer) fractional order derivative or, simply fractional derivative (FD), of a function has been a fascinating research area for over 3 centuries. Guillaume de l’Hôpital (1661-1704), a French mathematician asked, in a letter to Leibniz in 1695, the question

What does it mean by $D^n f(t)$ when $n = \frac{1}{2}$?

where $D^n = \frac{d^n}{dt^n}$. This question has made several mathematicians over 3 centuries to spend countless hours to ponder over and provide an answer that will be convincing and has a physical meaning compatible with that of the CD.

The findings are not unique. Different types of FDs were introduced. None of these FDs is completely compatible with the corresponding CD in terms of satisfying all the classical properties of the CD.

Besides, the physical meaning of an FD is yet to be made
harmonious with that of the CD exactly in the way we understand the precise significance of the CD arising out of a real-world problem.

Consider that a coconut is dropped from an altitude (height) $a$ of 96 meters. Also consider, taking into account the air resistance, that $a$ is a function of time $t$ sec such that $a = 96 - \frac{6}{2}t^2$ meter

The instantaneous velocity at time $t$ is $a'(t) = D^1 a(t) = -12t$ meter per sec

Since the distance (here height) $a$ is decreasing with time $t$ increasing, the derivative CD is negative. When the coconut touches the ground, the height $a$ becomes 0. That is, $t^2 = 16 \text{ sec}^2$. Hence time $t = 4 \text{ sec}$. It takes just 4 sec for the coconut to touch the ground (i.e. height $a = 0$).

After 2 sec the height $a$ will reduce to 72 meter. After 3 sec height $a$ will further reduce to 42 meter. The velocity when it touches the ground is 48 meter per sec or, equivalently, 204 kph. Hence the physical significance of the CD is understood readily.

We are now faced with 3 questions:

(i) In the same way as in the foregoing example, can we readily know the exact physical significance of $D^\frac{1}{2} a(t) =$?

(ii) It is possible to somehow manipulate the frictional forces to determine (not readily though) the value of the fractional order $\alpha$ for fractional differential equations (FDEs) corresponding to a physical problem. At the same time given the (same) physical problem, one can readily set up the mathematical model viz, the classical (i.e. integer-order) differential equations (CDEs) by virtue of the laws of physics globally known/meant for CDEs. Do the solution of the FDEs and that of the corresponding CDEs become numerically identical for the problem?

(iii) How do the computational error (CE) and the computational complexity (CC) of the CDEs and those of the corresponding FDEs compare?

Based on individual perception, the mathematicians over centuries introduced different types of fractional derivatives (FDs). However, the study of FDs appeared in the early 19th century A.D., when Lacroix (1819) defined an FD based on the traditional/classical definition of the $n^{th}$ derivative of the power function.

Since then the fractional differential operators, more generally the fractional calculus, became an interesting area of research to mathematicians. Several different forms of non-integer order derivatives were introduced.

Some of these are the Grünwald–Letnikov, Riemann–Liouville, Hadamard, Caputo, and Riesz operators [2–5].

More recent definitions of FD are due to Kilbas and Saigo (2004), Klimek (2005), and Cresson (2007) [6–8]. Agrawal (2010) attempted to generalize/ unify all the foregoing notions of FDs.

The merits of the generalization were later explored/studied in Malinowska, Odzijewicz, and Torres (2015) [10], Tomovski et al. (2010) [11], and others. The authors concentrated on general fractional differential operators. These operators reduce to the standard fractional operators when appropriate (special) kernels are selected. One may consider other non-standard kernels as particular cases.

Still more recent definitions of a fractional derivative are due to Khalil, Horani, Yousef, and Sababheh (2014) [12] and Katugampola (2014) [13]. These authors have been significantly successful in generalizing more the definitions. Such FD definitions not only allow smooth transition from fractional order to integer order and vice versa but also permit satisfaction of most rules i.e. classical properties obeyed by CDs — a desirable requirement.

The definitions of FD due to Caputo, Riemann-Liouville, Grünwald-Letnikov, Hadamard, Erdélyi-Kober, Marchaud, and Riesz are just some, which have been studied by several authors [14–16]. Most of the FDs are defined through fractional integrals. These FDs depict non-local behaviors. Such a behavior results in applications such as memory effects and future dependence [14].

The existing FDs have following drawbacks:

(i) Most of the FDs, barring Caputo and Caputo-like derivatives, do not satisfy $D^\alpha h(t) = 0$ where $h(t)$ is a constant and $\alpha$ is not a positive integer.

(ii) All FDs do not satisfy the traditional Product Rule in differentiation for 2 or more differentiable functions. Let $f(t), g(t), h(t)$ be 3 differentiable functions. The Product Rule may be written as

$$\frac{d}{dt} (f \cdot g \cdot h) = \frac{df}{dt} \cdot g \cdot h + f \cdot \frac{dg}{dt} \cdot h + f \cdot g \cdot \frac{dh}{dt}$$

The generalization to n differentiable functions is straightforward.

(iii) All FDs do not satisfy the traditional Quotient Rule in differentiation. Let the functions $f, g, h$ be as defined above and $f'(t) = \frac{df}{dt}, g'(t) = \frac{dg}{dt}, h(t) = \frac{dh}{dt}$, and $f(t) = \frac{g(t)}{h(t)}$. Then the Quotient Rule may be written as

$$f'(t) = \frac{g'(t)h(t) - g(t)h'(t)}{[h(t)]^2}$$

The Quotient Rule is not an independent rule. It can be readily derived from the Product Rule by considering $\frac{1}{h(t)} = [h(t)]^{-1}$.

(iv) All FDs do not satisfy the Chain Rule. The Chain Rule is used to differentiate a composite function. The rule may be written as

$$\frac{d}{dt} [f(g(t))] = f'(g(t)) \cdot g'(t).$$

Let $f(t) = \ln(\cos(t))$. Then $f'(t) = \frac{1}{\cos(t)} - \sin(t) = -\tan(t)$

(v) All FDs do not, in general, satisfy $D^\alpha D^\beta f(t) = D^{\alpha+\beta} f(t)$. 

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(vi) FDs do not have a corresponding Rolle’s Theorem stated below. A real-valued differentiable function \( f(t) \) that has 2 equal values at 2 distinct points has at least 1 stationary point (i.e. a point where the 1st derivative is 0). The functions, for instance, the function \( f(t) = \sin(t), t \in [0, \pi] \) and the function \( g(t) = \sqrt{25 - t^2}, t \in [-5, 5] \) have 1 stationary point at \( t = \pi/2 \) and \( t = 0 \), respectively.

(vii) FDs do not have a corresponding Mean Value Theorem stated as follows. If the function \( f(t) \) is continuous on the closed interval \([a,b]\) and differentiable on the open interval \((a,b)\), \( a < b \), then there exists a point \( c \in (a,b) \) so that \( f'(c) = \frac{f(b) - f(a)}{(b-a)} \). The function, for example, \( f(t) = t^3 + 3t^2 - t + 1 \) has a \( c \) viz. \( c = 1.577350270005475 \) in \([0,2]\). There is yet another \( c = 0.422649729995468 \) in \([0,2]\). The numerical value of \( c \) is computed by solving the equation \( 3t^2 - 6t + 2 = 0 \) using the Matlab command

\[
\Rightarrow t = \text{solve}(t(3t^2 + 2 - 6t + 2),[0,2])
\]

resulting in the solutions \( t = 0.422649729995468 \), 1.577350270005475.

(viii) The Caputo FD assumes that the function \( f(t) \) is differentiable. Khalil et al. [12] extends the usual limit definition of the derivative of a function to circumvent some of these difficulties. They define the FD of the function \( f(t) \) of order \( \alpha \) as

\[
D^\alpha f(t) = \lim_{h \to 0} \frac{f(t + h t^{-\alpha}) - f(t)}{ht}, (f \text{ dkh}) \tag{1.1}
\]

where \( t > 0, \alpha \in (0,1), f : [0,\infty) \to R \). If \( f(t) \) is \( \alpha \)-differentiable in some open interval \((0,\alpha)\) and \( \lim_{h \to 0} D^\alpha f(t) \) exists, then \( D^\alpha (f(t)) = \lim_{h \to 0} D^\alpha (f(t)) \). We call Definition (1.1) as KHYS definition or fdkha.

The foregoing definition satisfies the Product Rule (i.e. obviates Drawback (ii)), the Quotient Rule (i.e. removes Drawback (iii)), and produces the results non-contradictory to the Rolle’s Theorem (i.e. overcomes the Drawback (vii)) and the Mean Value Theorem (i.e. gets rid of the Drawback (viii)) of the classical calculus.

Katugamola [13] also provides yet another distinct limit definition for the FD of \( f(t) \) to further generalize the results derived by Khalil et al. His definition is as follows.

\[
D^\alpha f(t) = \lim_{h \to 0} \frac{f(te^{h\alpha}) - f(t)}{h}, (f \text{ dkat}) \tag{1.2}
\]

where \( \alpha \in [0,1] \). He terms this definition the most natural generalization of the calculus properties based on a limit approach. We term Definition (1.2) as fdkat.

The author perhaps implies by using the term “the most natural generalization” that there is a smooth transition from fractional order to integer order and vice versa. The term may not imply anything connected with the precise physical significance of the fraction \( \alpha \) when the term \( t + h \) of the classical derivative (limit definition) \( \text{CD viz} D^\alpha f(t) = \lim_{h \to 0} \frac{f(t+h) - f(t)}{h} \) is replaced by \( te^{h\alpha} \), although terms such as one representing a friction force in mechanics may be interpreted as one corresponding to an \( \alpha \).

For \( \alpha = 1 \), the definition is equivalent to the classical definition of \( \text{Df(t)} \) i.e. \( f'(t) \). There are \( \alpha \)-differentiable functions which are not differentiable.

Let \( \alpha \in (0,0.5] \) be a real fraction. Then a function \( f(t) \) could be \( \alpha \)-differentiable at a point but may not be differentiable at that point. Consider, for instance, the function \( f(t) = 5\sqrt{t} \) is not differentiable at \( t = 0 \). But it is \( \alpha \)-differentiable at \( t = 0 \).

The CD of the function \( f(t) \) is defined according to the 1st principle as

\[
Df(t) = \lim_{h \to 0} \frac{f(t+h) - f(t)}{h} \tag{CD} \tag{1.3}
\]

In the FD definitions of \( f(t) \), Khalil et al. and Katugamola have replaced ‘\( t + h \)’ in the CD of \( f(t) \) in the numerator as follows.

\[
t + h \leftarrow t + h t^{-\alpha} (in \text{ fdkha}) \tag{1.4}
\]

\[
t + h \leftarrow te^{h\alpha} (in \text{ fdkat}) \tag{1.5}
\]

It can be seen that in both the definitions the parameter \( h \) (arbitrarily small negative/positive) is not stand alone. It occurs along with the variable \( t > 0 \) — an undesirable restriction (toward better generalization) for both the definitions (1.1) and (1.2) unlike CDs. Consequently the numerical value of \( h \) must be relative to that of the value of \( t(\geq 0) \).

The value of \(|h|\) should thus be small relative to the order of the value of \( t \) if \( t \) is of the order of \( 10^{-6} \), then taking \(|h| = 10^{-8} \) will be considered too large when we work with Matlab standard precision (word-length) of 15 decimal digits — the most widely used precision of scientific and engineering computation globally. The optimal value of \(|h|\) will be \( t \times 10^{-8} \) in 15 digit precision context.

If, on the other hand, \( t > 0 \) is of the order of \( 10^0 \) or, equivalently, 1, then taking \(|h| = 10^{-8} \) will be considered computationally optimally small (but not too small) for the foregoing 15 digit precision. In fact, it (i.e.\(|h| = 10^{-8} \) is the optimal \( h \), that needs to be used in CD, fdkh, and fdkat. Taking \(|h| = 10^{-9} \) or less (subject, of course, to precision of 15 digits), the CE will start increasing or, equivalently, the accuracy will start decreasing.

We call \( h \) as the optimal base \( h \) i.e. \(|h| = 10^{-8} \) (fixed) when (i) the precision is 15 digits and (ii) the value of \( t \) is of the order of 1.

Therefore, considering the value of \(|h|\) independent of that of FD/CD of \( f(t) \) is untenable in practical numerical computation. Hence, both KHYS and Katu FD definitions
are reasonable from a generalization point of view. But from a real-world problem point of view, we do not know readily what \( \alpha \) should be in the foregoing definitions and also what the ideal replacements in (1.4) and (1.5) viz. in KHYS and Katu definitions should be.

As a matter of fact, the exact physical significance of the value of the non-integer fractional order \( \alpha \) (unlike the exact physical significance of the value of the integer-order) is yet a problem to be fully sorted out.

The question arises: What was it that prompted Khalil et al. and Katugampola to introduce such replacements? Was it all due to the indomitable requirement for generalizing the FD definitions so that these obviate all the known drawbacks of various FD definitions given by several mathematicians over the past centuries? Or, have these something to do (in terms of compatibility) with the requirements by the physical/natural environment (as is the case with the CD definition)? It appears that “indomitable requirement for generalizing the FD definitions” is the sole motivation rather than the physical (real-world) considerations.

In section 2, we demonstrate that the definition fdkha viz. Definition (1.1) due to Khalil et al. and the definition fdkat viz. Definition (1.2) due to Katugampola, when used in numerical computation, produce distinct FDs for a function. The Matlab programs along with numerical examples illustrate this fact. This is preceded by the mathematical simplification of both the equations (1.1) and (1.2) to illustrate the equivalence of both the definitions for a function.

It may be seen that many texts use \( \Delta t \) (for change in the independent variable \( t \)). This viz. the use of 2 symbols \( \Delta, t \) makes the algebra appear more unwieldy, so here we use \( h \) for \( \Delta t \) instead. We still may call it a “delta method”.

The limit approach in KHYS definition and that in Katu definition are not identical since we do not neglect the 2nd and higher order terms; for if we neglect them, then both the definitions become identical. Consequently, the Katu definition of FD, which refers KHYS definition becomes redundant.

However the purpose of Katu definition based on limit approach is distinctly different from that of KHYS definition. Hence both the definitions deserve to be studied (at least computationally) using the very 1st principles they have adopted in their definitions (and not from neglecting 2nd and higher order terms of \( h \) — a quantity tending to 0 in the limit from both the positive as well as from the negative sides). This study, we will show, depicts that the accuracy and generality of the 2 definitions using Matlab with standard 15 decimal digit precision do differ and the computational pros and cons of both the definitions become more pronounced and visible.

Section 3 comprises new limit definition fdnew — an improvement over fdkha and fdkat while section 4 includes conclusions.

2. KHYS and Katu Definitions with best \( h \): Equivalent but Distinct with Pros and Cons

**Equivalence** The Taylor series of a real- or a complex-valued function \( f(t) \) that is infinitely differentiable at a real or a complex number \( t_0 \) may be written as, substituting \( t - t_0 = h \) (the value of \( t \) is such that \( h \) is sufficiently small and its 2nd and higher order terms can be neglected)

\[
f(t) = f(t_0) + h f'(t_0) + \frac{h^2}{2!} f''(t_0) + \cdots + \frac{h^n}{n!} f^n(t_0) + \cdots \quad (2.1)
\]

Expanding the 1st function in the numerator of the KHYS definition (Definition (1.1)) using the Taylor series (2.1) and neglecting 2nd and higher order terms involving \( h \neq 0 \), we have

\[
D^\alpha f(t) = t^{1-\alpha} f'(t) \quad (2.2)
\]

Similarly, expanding the 1st function in the numerator of the Katu definition (Definition (1.2)) using the Taylor series (2.1) and neglecting 2nd and higher order terms involving \( h \neq 0 \), we have

\[
D^\alpha f(t) = t^{1-\alpha} f'(t) \quad (2.3)
\]

Thus both the distinct limit definitions viz. Definitions (1.1) and (1.2) produce the same (identical) FD of a function when terms \( O(h^2) \) are neglected.

**Distinctiveness** However, we use directly, in numerical computation, Definitions (1.1) and (1.2) and not the identical Equations (2.2) and (2.3). Consequently we obtain distinct numerical values of the FDs of a given function.

This implies that the neglected terms \( O(h^2) \) in Definition (1.1) and those in Definition (1.2) for a function \( f(t) \) do not contribute identical numerical values, these values are relatively small though. Consider the well-behaved functions (i) \( \sin(t) \) and (ii) \( 4t^3 - 5 \).

The Matlab program fdhkhatatsin (omitted to conserve space) demonstrates the distinctiveness (Figure 1) of fdkha and fdkat for the FD of \( \sin(t) \), \( t > 0 \) besides the improved accuracy of fdkha over fdkat. We have taken \( t = 5 \) and \( h = 10^{-5} \).

Similarly the Matlab program fdhkhatatubpoly (also omitted to conserve space) for the cubic polynomial \( 4t^3 - 5 \) for \( t = 2 \) and \( h = 10^{-5} \), we obtain the fdkha, fdkat and their differences (deviations) to highlight the better accuracy in fdkha over fdkat (Figure 2).

The differences viz. diffkha and diffkat are printed to demonstrate how, for the increasing values of \( \alpha \) (between 0 and 1), the values of FD go on changing and then merging with the value of the CD. These differences show that fdkha performs better than fdkat always in terms of both accuracy (CE) and computational complexity (CC).

When we talk about the existence of a limit, we must show that the left-hand limit = the right-hand limit in the foregoing computations. Observe that in fdkha, \( \alpha \in [0, 1) \)
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We will now experiment how these 2 definitions viz. fdkha, fdkat with the standard 15 decimal digit precision while that in fdkat $\alpha$ (also working value here) $t$ value of $\alpha$ in the context of 15 digit precision computer (that understands and executes Matlab commands) Matlab machine that we use here is the has to be performed using a finite precision machine. The derivatives of the traditional/classical calculus.

Definitions fdkha, fdkat with best $h$

We will now experiment how these 2 definitions viz. fdkha and fdkat compare in terms of obeying classical properties of derivatives of the traditional/classical calculus.

**Determination of optimal $h$** Any numerical computation has to be performed using a finite precision machine. The machine that we use here is the Matlab machine — a virtual computer (that understands and executes Matlab commands) with the standard 15 decimal digit precision. To obtain the best value of $h$ subject to (i) 15 digit precision and (ii) given $t > 0$, we carry out the simple computation executing the Matlab programs on the Matlab machine.

Our numerical experiment demonstrates that the best value (also working value here) of $h$ is $\pm 10^{-8}$, i.e., $|h| = 10^{-8}$ in the context of 15 digit precision for computing the derivative of $f(t)$ — both FDs and CD$s$ — with positive $t$ having the order of value 1. Precisely the optimal (best) value of $|h| = 10^{-8} \times t$.

Any value sufficiently greater than or less than the best value of $h$ will result in the inferior FD/CD value of $f(t)$.

However, in the foregoing experiment, even if we take the value of $|h|$ 100 times larger than the optimal value of $h$ i.e., $|h| = \pm 10^{-6}$, the computation of our new FD viz. fdkha will still be sufficiently accurate (from engineering application point of view). Hence a value close to that of optimal $|h|$ is usually good enough.

We will discuss later in detail the computation of optimal base $h$ (i.e., the optimal value of $h$ for $t$ having the order of value 1 for 15 digit precision). This value will be the working $h$ for all $t$'s having the foregoing order. Using this optimal value of $h$ viz. $h = \pm 10^{-8}$ we obtain the working $h$ for any $f(t)$ whose argument $t > 0$ has the order of value different from 1 (as long the precision remains fixed at 15 digits) just by taking $|h| = 10^{-3} \times t$ as stated earlier.

The foregoing numerical values, as observed earlier, demonstrate that fdkha performed better than fdkat both in CE and in CC for well-conditioned functions such as $\sin(t)$ and $\sin^2(t)$ — both FDs and CDs — with positive $t$ having the foregoing order. Using this optimal value of $h$ viz. $h = \pm 10^{-8}$ we obtain the working $h$ for any $f(t)$ whose argument $t > 0$ has the order of value different from 1 (as long the precision remains fixed at 15 digits) just by taking $|h| = 10^{-3} \times t$ as stated earlier.

It may be observed that the CC (implying amount of computation or, equivalently, time spent for computation) is more in fdkat due to 2 exponentiations than that in fdkha having only 1 exponentiation. However, the complexity issue is not a dominant issue in most real-world problems in the current 2019 (exa-flops computation) context.

There are other ways such as the bisection way and the linear interpolation way to compute an optimal $h$ for a given function with the specified interval(s). In essence, when mathematically $|h| \to 0$ in the limit i.e., when $h$ becomes increasingly small from both positive as well as negative sides, the value of the limit will be increasingly accurate (when the limit exists).

The mathematical optimal value of $|h| = 0$ in the limit (i.e., $h \neq 0$). In other words, the smaller the value of $|h|$ is, the better should be the value of the numerical limit (when it exists) under the assumption of infinite precision of computation. We leave these ways to the reader to explore for different functions with varying precision.

Although an engineer in a real-world situation cannot does not implement any numerical data with an accuracy (relative) greater than 0.5 $\times 10^{-4}$ or, equivalently, 4 significant decimal digits (due to the limitation of any measuring device — electronic or otherwise), in an intensive computational environment with specially ill-conditioned functions (with respect to numerical differentiation) the foregoing 2 definitions do matter for engineers since the number of significant digits accuracy could/would depend depending on the nature of the $f(t)$.

It is necessary to explicitly know the numerical quality (CE) of solutions by everybody including the engineers and
scientists. This will enable one to have confidence in the solutions meant for physical-world implementation.

3. New Limit Definition fdnew: Improvement over fdka & fdkat

**Derivation of fdnew** We have, for example, our function $f(t) = \sin(t) = \sin(5)$ for $t = 5$ and $alp = \alpha = 0.9999999 \approx 1$. We also have classical derivative $CD$ $f$, $FD$s $fdka$, $fdkat$ (for $h = +10^{-6}$, say), $fdkham$, $fdkatm$ (for $h = -10^{-6}$) as follows (in stands for minus).

$$fd = 0.283662185463226, \quad fdka = 0.283662710542920, \quad fdkham = 0.283662738964630, \quad fdkatm = 0.283661751643294, \quad fdkat = 0.283661723443629$$

Solving the equation $A\kappa = b$ where the following left-hand side $2 \times 2$ matrix is A, the left-hand side $2 \times 1$ vector is $k$ and the following right-hand side $2 \times 1$ vector is $b$.  

$$A = \begin{bmatrix} f_{dkha} & f_{dkat} \\ f_{dkham} & f_{dkatm} \end{bmatrix}, \quad b = \begin{bmatrix} f_d \\ f_d \end{bmatrix}$$

we obtain $k = \begin{bmatrix} k_1 \\ k_2 \end{bmatrix} = [17.9352911338374 \quad -16.9352912880691]$

Our $fdnew = k(1) * f_{dkha} + k(2) * f_{dkat} = \n$ $k(1) * f_{dkham} + k(2) * f_{dkatm}$ (numerically), where $k_1 = k(1), k_2 = k(2)$. We can easily verify using the following command

$$r1 = k(1) * f_{dkha} + k(2) * f_{dkat} - f_d$$

that the residues are $r1 = 3.88578058618050 - 016$ and $r2 = -4.996036108132 - 016$. Both the residues are 0 up to 15 digits.

We have used the Matlab `linsolve` command to get the solution as follows.

$$A = \begin{bmatrix} f_{dkha} & f_{dkat}; f_{dkham} & f_{dkatm} \end{bmatrix}, \quad b = \begin{bmatrix} f_d; f_d \end{bmatrix}$$

$$k = linsolve(A,b)$$

$$r1 = k(1) * f_{dkha} + k(2) * f_{dkat} - f_d$$

$$r2 = k(1) * f_{dkham} + k(2) * f_{dkatm} - f_d$$

The Matlab program `fdlcnr1(f, t, h)` along with its output (omitted here to conserve space) permits $h$ to be chosen by the user according to the given function primarily to perform numerical experiment varying the value of $h$ and gain a deeper insight into the character (robustness) of $fdnew$. To execute the program, we enter the commands in the Matlab command window as

$$\gg clear all; format long; close all; syms t; double t; fdlcnr1(4*r^3 - 5, 2, 10^6 - 6)$$

where $f(t) = 4r^3 - 5, t = 2$, and $h = 10^{-6}$. We have another version of the foregoing Matlab program `fdlcnr2(f, t, h)`. We call this version `fdlcnr2(f, t, h)` for which the command in the Matlab command window is

$$\gg clear all; close all; format long g; syms t; double t; fdlcnr2(4*r^3 - 5, t, 2, 10^6 - 6)$$

or the following line without 2 quotes. The method is evidently valid for any other continuous function $f(t)$.

**Ill-conditioned problems with respect to differentiation** For an ill-posed problem such as $DF(t) = D\sin(\frac{1}{t})$ near $t = 0$, we execute the program `fdlcnr1` entering the commands in Matlab command window as follows (where $t = 10^{-4}$ and $h = 10^{-8}$).

$$\gg clear all; format long; close all; syms t; double t; fdlcnr1(sin(1/t), 10^{-4} - 4)$$

where the Matlab program `fdnew1(f(t), t)` (omitted to conserve space) having 2 parameters viz. $f(t)$ and $t$ is used. The output that we obtain as is follows (Figure 3)

$$cd = 9.521553682590148e+007; \quad h = 1.000000000000000e-012 \quad (h \quad is \quad positive);$$

$$A = 1.0e+007*$$

$$9.521697573294796 9.521697746495139$$

$$9.521392132666451 9.521392132666451$$

$$b = 1.0e+007*$$

$$9.521553682590147$$

$$k = 1.0e+003*$$

$$1.764540520660579$$

$$-1.763540503695607$$

$$t = 1.0e+007*0.00000000010000;$$

$$CD = 1.0e+007+9.521553682590147$$

**Optimal base h with graph in Matlab (std. precision=15 digits)** We consider a sine function with precision 15 digit and with argument 5. Just by executing the function program

$$\gg h_optimal_base_with_graph$$

omitted to conserve space in the command window, we get the output (Figure 4) including the graph (Figure 5) as follows.

We obtain the fractional derivative of $\sin(t), t = \pi/2$ executing the program `fdnew1` (omitted to conserve space) as follows. Here $|h|= |optimal \ base \ h|$.  

$$\gg clear all; format long; close all; syms t; double t; fdlcnr1(sin(t), \pi/2);$$

$$CD = 6.123233995736766e-017;$$

$$h = 1.570796326794897e-008 \quad (h \quad is \quad positive);$$

$$A = 1.0e-008*$$

$$-0.706789929214115 \quad -0.706789929214115$$

$$0.706789929214115 \quad 0.706789929214115$$

$$b = 1.0e-016*$$

$$0.612323399573677$$

$$0.612323399573677$$

$$k = 0$$

$$0$$

$$t= 1.570796311086933; \quad CD = 0.000000000000000$$

The following Figure (Figure 6) depicts the accuracy of $fdnew$ against that of $fdka$ & $fdkat$.

The Matlab programs `fdlcnr1(f, t, h)` and `fdlcnr2(f, t, h)` are identical except that in Line 1, `fdlcnr1` is replaced by `fdlcnr2`. With the foregoing line the print format will be slightly changed due to “format long g” instead of “format long”.

It can be seen that the numerical computation of the column vector $k = [k_1 \quad k_2]^T$ provides us our desired new FD `fdnew` by executing the Matlab command `fdnew = k(1) * f_{dkha} + k(2) * f_{dkat};`
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Figure 3. fdnew versus fdkha & fdkat; fdnew is more accurate.

Figure 4. Computation of best $h$.

We have chosen $h = 10^{-6}$ in the foregoing example. Our precision of computation is 15 decimal digits. It is advisable to vary the value of $h$ such as $h = 10^{-3}, 10^{-6}, 10^{-7}, 10^{-8}, 10^{-9}$ and so on and choose that value of $h$ which corresponds to the best (optimal) CD for the given problem.

Figure 5. The optimal base $h$ is $10^{-8}$ for the function $f(t) = \sin(t)$ for $t = 5$. The optimal base $h$ remains fixed as long as (i) the precision is 15 digits and (ii) the value of $t$ is of order 1.

Figure 6. Accuracy of fdnew versus fdkha & fdkat; fdnew is more accurate than both within 15 digit precision.

Assuming the existence of the FD, our new FD fdnew is always better from numerical quality (CE) of solution than both fdkha as well as fdkat without exception (i.e. for all FD problems). According to the computational logic followed through the linear combination at $\alpha = 0.9999999 \approx 1$, we have chosen parameters $k_1, k_2$ such that fdnew satisfies CD exactly subject to, however, the finite precision (viz. 15 digits) used here.

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It is to be noted that the very philosophy of replacements viz. \( t + h = t + h t^{1-\alpha} \) (KHYS definition) and \( t + h = te^{h\alpha} \) (Katu definition) raises the question regarding the parameter \( \alpha \) not so much from satisfying the classical properties but from its physical significance.

What is it that prompted the authors to choose the specific form \( ht^{1-\alpha} \) for \( h \) in KHYS definition besides the satisfaction of several (not all) classical properties of CDs? Did they have anything in mind for the form from any other consideration such as the satisfaction of physical (real-world) properties? We have the same questions for Katu definition too when the author replaces \( t + h \) (observe: not just \( h \)) by \( te^{h\alpha} \).

Both KHYS and Katu definitions seem to have only consideration of satisfying the classical properties to the maximum extent so that the FDs become compatible with CD. Or in other words, the FDs have smooth transition to CD implying improved generalization and the foregoing 2 expressions (in 2 definitions) involving \( \alpha \) perhaps have no immediately/readily known physical significance (unlike that in CD).

The assumption \( t > 0 \) in both KHYS and Katu definitions unlike that in CD is a vital impediment to generalization. If this is removed by an appropriate replacement of \( t + h \) and at the same time the classical properties are satisfied/preserved, then such a definition is more desirable. The physical significance aspect, however, still continues to remain unresolved.

### 4. Conclusions

**Computing FDs for \( \alpha \in (n, n + 1) \) where \( n \) is a positive integer**

To compute the FD of the function \( g(t) \) when \( \alpha \in (n, n + 1) \), \( n \) being a positive integer, we consider the \( n \)th CD of \( g(t) \) as the function \( f(t) \) and then compute the FD \( (\alpha - n) \) of \( f(t) \), i.e. \( D^{\alpha-n} f(t) \).

**Working \( h \) should be significantly (i.e. relatively and not absolutely) optimal**
The best value of \( h \) for a given precision and for a given \( t \) is desirable and is advisable to be computed and used for the computation of all derivatives including FDs.

This optimal value is obtained by simply computing the CD of \( f(t) \) by taking \( h = 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}, 10^{-9}, 10^{-10} \)...

We see that, for \( h = 10^{-8} \), the value of the CD of \( f(t) \) is the most accurate (least CE) one.

The value of the optimal \( h \) should be significant (not absolute) i.e. its value should be relatively small compared to that of the CD of \( f(t) \) but not too small. For too small an \( h \), the accuracy of the value of the CD will drop.

**Better quality (less CE) of new FD definition with classical properties**

Combining the advantages of KHYS and Katu definitions of FD, both based on limit approaches, we have presented a new definition of FD called here fdnew. This new definition provides a quality of solution better than that produced by both the KHYS and the Katu definitions always.

At the same time fdnew satisfies the classical properties that are obeyed by Katu definition. However, the vital issue viz. the assumption (unlike CDs) that \( t > 0 \) in \( f(t) \) poses a major hurdle in the process of generalization of FDs.

**An ill-posed problem**

Consider the function \( f(t) = \sin\left(\frac{1}{t}\right) \), where \( t = 10^{-5} \) (say). The function \( f(t) \) is continuous but is violently fluctuating near the origin i.e. near \( t = 0 \) (on both negative and positive sides). The computation of FD/CD of \( f(t) \) could involve more pronounced CE than that when the \( f(t) \) is not vigorously fluctuating.

**Ranking**

Suppose we have at our disposal 2 or more algorithms to solve our computational problem at hand. What should we do i.e. which algorithm should we use? Evidently we should use the best one for the problem? Isn’t it? In this context, since CE is most often not a big issue specifically with the advent of exa-flops (i.e. \( 10^{18} \) floating-point operations/sec) computers, the only parameter which decides the ranking is the accuracy (CE).

Everybody desires to use the best algorithm for solving his/her computational problem subject, however, to the environmental constraints. Nobody wants to use the second best or the third best algorithm for computation, nor should one do use. In this context the new definition of FD viz. fdnew, and the definitions fdkha and fdkat are ranked as (i) fdnew, (ii) fd kha, and (iii) fdkat form CE point of view.

From CC point of view, the ranking is (i) fdkha, (ii) fdkat, and (iii) fdnew. We have pointed out that CC for FDs and CDs for most real-world problems is not an important issue since all the 3 definitions have CCs \( O(k) \) — linear in the size \( k \) of the function \( f(t) \). We compute the time complexity which is proportional to CC for each of the 3 definitions to get a feel of the relative cost of computation. Since the current (2019) computing speed is around exa-flops and the number of laptop, desktop, and main-frame computers availability is so huge, most physical FD computation problems have near-trivial CC.

**Dealing with \( f(t) \) specified as a table**
The function \( f(t) \) may be known/given in a symbolic form such as \( 2\sin(t) - 5, t^5 - t^3 + 7t - 1 \), and \( e^{\sin(t)} - \tan(t) + 9 \). Or, it may be specified as numerical table such as \( t, f(t_i) \cdot i = 0(n) \), where \( t_i, f(t_i) \cdot i \) are all numerically given.

Suppose we need to compute CD/FD of \( f(t) \) at \( t = \gamma \), where \( \gamma \) is numerically given a value within the range of the values of \( t \). Take 4 consecutive values of \( t \) which enclose \( \gamma \). These 4 values constitute a cubic polynomial. This polynomial will be treated as \( f(t) \). Observe that \( f(t) \) will/could be changing depending on the value of \( \gamma \) given. Follow the foregoing procedure to obtain CD/FD of \( f(t) \). A 2nd or a 4th degree polynomial may not improve the result since the effect of the points farther away may not have either much effect or have too much of effect in terms of unacceptable distortion of the result (here the FD/CD).

We do not usually anticipate a rapidly fluctuating function. The cubic (and sometimes even a quadratic) function would solve the CD/FD problem acceptably.

**Matlab linsolve versus pinv commands**

Both the commands linsolve and pinv may be used to solve a linear system \( Ax = b \). In our context, we have the matrix \( A \times 2 \times 2 \) (square) matrix and the system is consistent. The matrix \( A \) could be categorized as non-singular, near-singular, very near-singular,
or singular. **Assume** that the \(|\text{determinant}|\) of the matrix \(A\) viz. \(|A|\) has the **magnitude of the order of 1**.

With respect to the 15 digit precision of computation, \(A\) may be considered singular if its \(|\text{determinant}|\) viz. \(|A|\) is 0 or less than or equal to \(10^{-15}\). In such a case, only the command \(pinv\) will work. It may be viewed very near-singular if \(|A|\in (10^{-15},10^{-8})\) — an arbitrary interval (one may modify the interval depending on the precision of computation and other local factors such as the CE). In this case, the command \(linsolve\) since \(linsolve\) may involve more error or sometimes a failure.

The matrix \(A\) may be seen as near-singular, if \(|A|\in (10^{-15},10^{-8})\), and non-singular if \(|A|\ge 10^{-5}\). In both the cases, any of the 2 commands may be used. However, choose that command which produces less CE.

However, the Matlab \(linsolve\) is an excellent command from CE point of view. Even for a reasonably (not too) near-singular matrix, \(linsolve\) produces acceptably good solution. The **true ill-conditioned problem** is a **very near-singular** linear system \(Ax = b\). Neither the singular nor the non-singular system is ill-conditioned with respect to the computation of the solution vector \(x\). As a matter of fact, both the singular and the non-singular may be termed as well-conditioned and it is certainly so when the system is consistent.

Both the commands \(linsolve\) and \(pinv\) have pros and cons. The command \(linsolve\) computes the solution vector \(x\) without computing the true inverse/ pseudo-inverse \((pinv)\) of the matrix \(A\) while \(pinv\) obtains the solution via true/pseudo-inverse of \(A\). Observe that the true inverse and the pseudo-inverse of \(A\) would be numerically the same if \(A\) is non-singular.

For a singular \(A\), the true inverse of \(A\) does not exist while \(pinv\) always exists and unique. Without the knowledge of the true/pseudo-inverse, CE computation of the solution vector \(x\) is more involved or not possible. However, in our computation of CD/FD of the function \(f(t)\), the use of \(pinv\) command almost always should solve all the problems in an acceptable way.

**Plotting closely located points: Difficulty** The problem is that our maximum difference is less than 1% of the vertical axis scale, so you can’t exaggerate the differences without distorting the underlying values.

The best we can do is to plot the values, then in another plot, show either the differences or the ratios between the values. The use of a secondary axis shows these things, but not as clearly as separate charts. So we desist from trying to plot the graph using closely spaced values depicting \(fdnew\), \(fdkha\), and \(fdkat\).

However, the tables produced by Matlab readily and clearly depict the accuracy (CE) of \(fdnew\), \(fdkha\), and \(fdkat\). These, we believe, just by looking at the concerned numerical tables, the reader can verify quickly the truth of the foregoing statements.

**Improvement on generalization: How** The improved **computational accuracy** combined with the satisfaction of all the 7 rules observed by CD and also fdkat may be termed as an improvement on generalization. The FD fdkha (used in deriving \(fdnew\)) which does not claim to follow “the most natural generalization” like fdkat and is distinctly different from fdkat has contributed toward not only improved (i.e. reduced) CE but also a better observation of the foregoing 7 rules.

Observe that the real hurdle is the severe restriction viz. \(f(t), t > 0\) on the function \(f(t)\). If the **foregoing generalization** is kept unchanged (valid) for any continuous/analytic function \(f(t)\) for any negative, positive, and complex variable \(t\) then we will truly achieve a significant milestone in fractional calculus.

**Obviating the restriction “\(t > 0\)” for FD of \(f(t)\)** Mathematically, a fraction (fractional order/degree) such as (i) \(1/3\) in the equation \(x^{\frac{1}{3}} - 2 = 0\) would give rise to 3 distinct roots of the equation and (ii) \(0.9\) in the equation \(x^{0.9} - 2 = 0\) should give rise to 9 roots of the equation. On the other hand, the equation \(x^{1/3} = 2\) produces only one root. If the order/degree “1” is slightly reduced making it, say, 0.99, the problem changes drastically. Hence one does need to impose certain (practically meaningful) restriction(s) on the fractional order to achieve really smooth transition from/to an integer order. This is a research problem which needs to be intensely probed to achieve meaningful and widely useful generalization.

**Acknowledgement**

The authors thank the Science and Engineering Research Board (SERB) of the Department of Science and Technology (DST), Government of India for their support of the reported work under the project DST SERB EMR/2016/003572 dated February 06, 2017.

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ISSN(P):2319 – 3786
Malaya Journal of Matematik
ISSN(O):2321 – 5666
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