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Piotr Ostalczyk*, Dariusz Brzeziński**

Numerical Evaluation of Variable – Fractional-Order Derivatives

1. Introduction

Fractional calculus is plying recently a major role in many scientific and technical areas. The fractional-order derivative (FOD) and integral (FOI) are natural extensions of the well known derivatives and integrals. This extension enables better physical phenomena identification [27, 28], analysis [2, 3, 9, 13–16, 24, 29] and control [14, 20, 21, 25].

The innovative field of the science where the FOD/FOI can be applied is modelling of the real dynamical systems and its phenomena as well as systems control. One of the hard point of the simulations accuracy of the dynamics of the automated regulation of a close-loop system with an object described by the differential equation of the non-integer orders and PID (PID stands for Proportional Integral Derivative) regulator of the non-integer orders is the calculations accuracy of FOD/FOI. Obtaining error free values allows to exclude the numerical errors as the cause of the instability in the so called "near steady states". But there are still problems in numerical evaluation of FOD/FOI [4, 6–8, 15, 27, 30, 33].

There are several methods of FOD/FOI calculations which can be used to calculate derivatives and integrals of integer orders as well. One of them is Grünwald–Letnikov – and second one – Riemann–Liouville formula [21, 27, 29]. They differ from each other in one main way. The Grünwald–Letnikov method (it is the reference method in context of calculation accuracy) derives from difference quotient. The Riemann–Liouville formula (it will be evaluated) derives from multiple integrals. It involves numerical integration, which implies that the accuracy of calculations depends not only on amount sample points, shape of the integrand but also on abilities of particular method of numerical integration applied, as well.

The main goal of this paper is to determine the most accurate and effective method of numerical integration in such context.

The paper is organized as follows: firstly basic definitions of Riemann–Liouville and Grünwald–Letnikov FOD/FOI formulas are given. In next section there are shortly

* Computer Engineering Department, Technical University of Lodz, Poland
** Ph.D. student, Computer Engineering Department, Technical University of Lodz, Poland

reviewed fundamentals of numerical methods of integration. Then there are listed methods of numerical integration applied, the function tested and expressions calculated. After that the results are presented and conclusions drawn.

2. The Riemann–Liouville formula of a fractional-order differ-integral

The definite Riemann–Liouville integral of the real function $f(t)$ of the $v > 0$ order is defined as follows:

$$ {}_{t_0}I_t^{\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_{t_0}^{t} (t-\tau)^{\nu-1} f(\tau)\, d\tau \tag{1} $$

where:

t_0, t – integration range, which comply the condition $-\infty < t_0 < t < \infty$,

$\Gamma(\nu)$ – Euler's Gamma Function.

Now, we describe natural number n:

$$ n = [\nu] + 1 \tag{2} $$

The Riemann-Liouville derivative of the real function $f(t)$ of the order $v > 0$ is defined as follows:

$$ {}_{t_0}D_t^{\nu} f(t) = \sum_{i=0}^{n-1} \frac{(t-t_0)^{i-\nu} f^{(i)}(t_0)}{\Gamma(i+1-\nu)} + \frac{1}{\Gamma(n-\nu)} \int_{t_0}^{t} (t-\tau)^{n-\nu-1} f^{(n)}(\tau)\, d\tau \tag{3} $$

where n – also denotes order of classical derivative of the integer order.

3. The Grünwald–Letnikov formula of a fractional-order differ-integral

The derivative of a real order $v > 0$ (for the integral we use order $-v < 0$) of a continuous bounded function $f(t)$ is defined as follows

$$ {}_{t_0}D_t^{\nu} f(t) = \lim_{\substack{h \to 0 \\ t-t_0 = kh}} \frac{\sum_{i=0}^{\frac{t-t_0}{h}} a_i^{(\nu)} f(t-hi)}{h^{\nu}} \tag{4} $$

where:

$$a_i^{(\nu)} = \begin{cases} 1 \quad \text{for} \quad i = 0 \\ a_{i-1}^{(\nu)}\left(1 - \frac{1+\nu}{i}\right) \quad \text{for} \quad i = 1,2,3,\ldots \end{cases} \tag{5}$$

4. Short review of fundamentals of numerical integration

The essence of the numerical integration is to approximate the definite integral over the range $\langle a,b \rangle$ of the function *f*(*t*) by the following formula

$$\int_a^b f(x)\,dx = \sum_{k=1}^{N} A_k f(x_k) + R \tag{6}$$

where:

x_k – quadrature nodes,
A_k – quadrature coefficients (weights),
R – the rest of the approximation.

The right side of the equation is often called quadrature. The formula (6) is shared by all quadratures. The difference lies in algorithms of calculating their nodes and coefficients [1, 5, 11–13, 32].

The interpretation of quadrature coefficients A_k (so called weights) is the width of the subintervals the range of integration is divided into. In case of Newton–Cotes Quadratures (Rectangular, Trapezoidal and Simpson Rule) the integration range is divided into subintervals, which are of equal width. In case of Newton–Cotes' Midpoint Rule the sample point is taken from the middle of the subinterval. The Gaussian quadratures feature is that the sample points are not placed in the middle of each subintervals, but in the places which definitely guarantee superior accuracy of the calculated interval [13]. The nodes of Gauss Quadratures are determined by abscissas of the applied in approximation polynomials.

The composition of Gauss–Kronrod quadrature, which is very popular modification of Gauss–Legendre Quadrature was enhanced by additional sample points and all new weights [8].

The Newton-Cotes quadratures may be applied to almost all types of functions. Trapezoidal and Simpson Rule are the most often used. They are so called "closed formulas", which implies that the values of *f*(*a*) and *f*(*b*) must be determinable. Therefore they can't be applied to integrands which have singularities, asymptotes, etc. In such cases the Newton–Cotes' Midpoint Rule should be applied.

The Gauss Quadratures others than the Gauss–Legendre quadrature (weights equal (1)) may be applied only to selected kinds of integrands. This is due to relationship with their weight functions [1, 5, 11–13, 32].

5. Methods of numerical integration used, formulas applied and function tested

We used following formulas to calculate differ-integrals:

– Riemann–Liouville (RL),
– Grünwald–Letnikov (GrLET).

Our C++ programs which were developed especially for the purpose of this experiment used following methods of numerical integration while applying RL formula:

– Newton–Cotes Midpoint Rule (NCM),
– Newton–Cotes Trapezoidal Rule (NCT),
– Newton–Cotes–Simpson Rule (NCS),
– Gauss–Legendre Quadrature (GaLEG),
– Gauss–Kronrod Quadrature (GaKRO).

There was tested very well known function used in technical applications

$$f(t) = e^{-ta} \tag{7}$$

This function is not only a “real-life” function applied in voltage regulators, but also states a typical member in solutions of linear, stationary differential equations of the integer orders.

For function (7) we calculated derivatives of the orders which were designated by a function of time $\nu(t) \in (0,(0.1),2)$

$$ {}_0D_2^{\nu(t)}\left[e^{-ta}\right] = \begin{cases} {}_0D_1^{(1)} e^{-ta} \\ {}_1D_2^{(2)} e^{-ta} \end{cases}, \quad a = 2 \tag{8}$$

Our goal was to determine applying which of the methods of numerical integration it is possible to obtain the values of selected expressions charged with the smallest possible absolute error using the smallest possible number of sample points (L).

For GrLET and NCM, NCT, NCS we used 4,32 and 600 sample points.

For GaLEG – L = 4,32 and for GaKRO – L = 7/15 and 30/61 (so called pairs).

Remark: it is known that number of L grater that 30–40 for Gauss methods often causes the error rise rapidly. Even 100% and more! That is why you will encounter empty fields in all tables with results for these methods.

The classical derivative of the integer order of the function (7) necessary for formula (3) were calculated using analytical formula

$$f^{(n)}(t) = (a)^n e^{-ax}, a = 1,2,3,\ldots \tag{9}$$

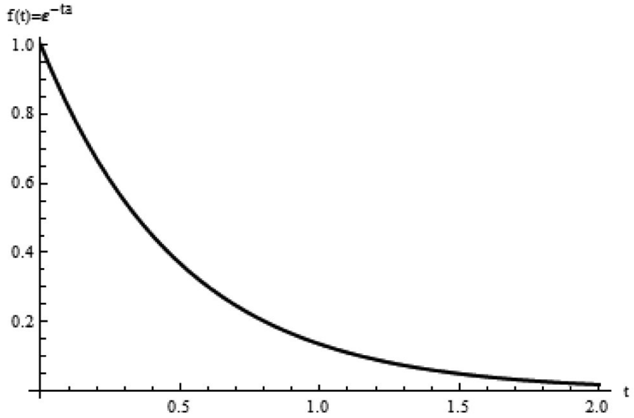

Fig. 1. Graph of the function tested (7)

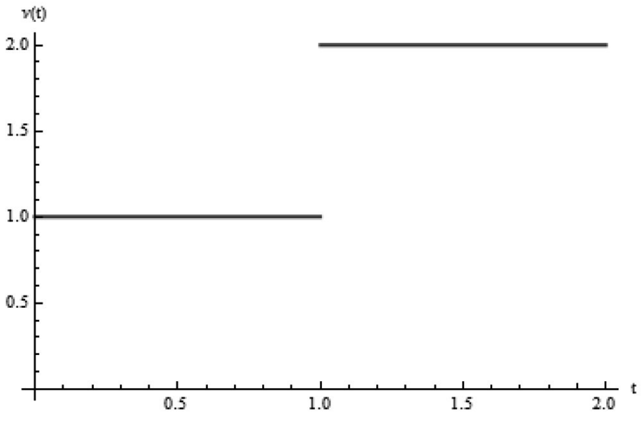

Fig. 2. Graph of the order of derivative of the function (7) – as a function of time (8)

Test procedure: firstly, the values of derivatives designated by function (8) using formula (9) were obtained. Then the similar procedure was done to obtain the values of derivatives applying GrLET and RL formulas. In case of the last one – we used methods of numerical integration mentioned in section 5. Finally the absolute error as the difference between exact value and obtained one was calculated on the basis of which the conclusions were drawn.

6. Test results

Table 1a
The values of absolute error for L = 4, range $\langle 0,1 \rangle$

t	GrLET	NCM	NCT	NCS	GaLEG	GaKRO
0.0	2.663 e-04	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**
0.1	4.163 e-02	3.775 e-05	7.553 e-05	1.258 e-08	4.441 e-16	**0.0**
0.2	6.932 e-02	2.747 e-04	5.494 e-04	3.659 e-07	2.414 e-13	**0.0**
0.3	8.660 e-02	8.454 e-04	1.691 e-03	2.531 e-06	8.416 e-12	**0.0**
0.4	9.617 e-02	1.833 e-03	3.669 e-03	9.743 e-06	1.016 e-10	**2.220 e-16**
0.5	1.001 e-01	3.286 e-03	6.578 e-03	2.723 e-05	6.864 e-10	**0.0**
0.6	1.001 e-01	5.227 e-03	1.047 e-02	6.222 e-05	3.214 e-09	**3.331 e-16**
0.7	9.732 e-02	7.664 e-03	1.535 e-02	1.238 e-04	1.168 e-09	**5.551 e-17**
0.8	9.270 e-02	1.056 e-02	2.123 e-02	2.228 e-04	3.528 e-08	**1.665 e-16**
0.9	8.692 e-02	1.400 e-02	2.808 e-02	3.713 e-04	9.524 e-08	**2.220 e-16**
1.0	8.051 e-02	1.788 e-02	3.588 e-02	5.830 e-04	2.171 e-07	**4.996 e-16**

Table 1b
The values of absolute error for L = 4, range $(1,2)$

1.0	4.477 e-04	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**
1.1	2.282 e-02	3.338 e-06	1.022 e-05	3.406 e-09	1.110 e-16	**0.0**
1.2	3.850 e-02	2.428 e-05	7.437 e-05	9.903 e-08	6.545 e-15	**5.551 e-17**
1.3	4.873 e-02	7.475 e-05	2.288 e-04	6.851 e-07	2.278 e-12	**5.551 e-17**
1.4	5.485 e-02	1.622 e-05	4.963 e-04	2.637 e-06	2.750 e-11	**2.776 e-17**
1.5	5.790 e-02	2.908 e-04	8.895 e-04	7.371 e-06	1.858 e-10	**1.110 e-16**
1.6	5.870 e-02	4.628 e-04	1.415 e-03	1.684 e-05	8.698 e-10	**2.776 e-17**
1.7	5.788 e-02	6.790 e-04	2.074 e-03	3.351 e-05	3.162 e-09	**0.0**
1.8	5.594 e-02	9.391 e-04	2.867 e-03	6.030 e-05	9.550 e-09	**9.714 e-17**
1.9	5.324 e-02	1.243 e-03	3.790 e-03	1.005 e-04	2.505 e-08	**2.776 e-17**
2.0	5.006 e-02	1.588 e-03	4.840 e-03	1.578 e-04	5.877 e-08	**6.938 e-17**

Table 2a
The values of absolute error for L = 32, range $\langle 0,1 \rangle$

t	GrLET	NCM	NCT	NCS	GaLEG	GaKRO
0.0	3.937 e-04	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**
0.1	5.128 e-03	6.714 e-07	1.180 e-06	3.037 e-012	2.093 e-09	**0.0**
0.2	8.414 e-03	4.844 e-06	8.585 e-06	8.943 e-11	3.920 e-09	**0.0**
0.3	1.035 e-02	1.504 e-05	2.644 e-05	6.196 e-10	5.624 e-09	**2.220 e-16**
0.4	1.133 e-02	3.263 e-05	5.736 e-05	2.390 e-09	7.306 e-09	**6.661 e-16**
0.5	1.162 e-02	5.853 e-05	1.029 e-04	6.697 e-09	9.034 e-09	**0.0**
0.6	1.144 e-02	9.317 e-05	1.638 e-04	1.535 e-08	1.086 e-08	**1.110 e-16**
0.7	1.1095 e-02	1.367 e-05	2.403 e-04	3.066 e-08	1.280 e-08	**1.665 e-16**
0.8	1.027 e-02	1.892 e-04	3.325 e-04	5.541 e-08	1.490 e-08	**1.665 e-16**
0.9	9.475 e-03	2.504 e-04	4.402 e-04	9.281 e-08	1.714 e-08	**0.0**
1.0	8.637 e-03	3.202 e-04	5.692 e-04	1.465 e-07	1.955 e-08	**7.216 e-16**

Table 2b
The values of absolute error for L = 32, range $(1,2)$

1.0	9.243 e-05	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**
1.1	2.780 e-03	1.597 e-07	3.194 e-07	8.317 e-13	5.665 e-10	**0.0**
1.2	4.569 e-03	1.162 e-06	2.324 e-06	2.421 e-11	1.061 e-09	**5.551 e-17**
1.3	5.632 e-03	3.578 e-06	7.156 e-06	1.677 e-10	1.522 e-09	**5.551 e-17**
1.4	6.171 e-03	7.763 e-05	1.553 e-05	6.469 e-10	1.977 e-09	**8.327 e-17**
1.5	6.388 e-03	1.392 e-05	2.785 e-05	1.813 e-09	2.455 e-09	**3.866 e-16**
1.6	6.250 e-03	2.216 e-05	4.433 e-05	4.155 e-09	2.939 e-09	**2.776 e-17**
1.7	5.992 e-03	3.253 e-05	6.505 e-05	8.299 e-09	3.466 e-09	**5.551 e-17**
1.8	5.628 e-03	4.500 e-05	9.001 e-04	1.500 e-08	4.032 e-09	**1.388 e-17**
1.9	5.203 e-03	5.957 e-05	1.910 e-04	2.512 e-08	4.640 e-08	**2.776 e-17**
2.0	4.7500 e-03	7.618 e-05	1.524 e-04	3.966 e-08	5.292 e-08	**1.249 e-17**

Table 3a

The values of absolute error for L = 600, range $\left(0,1\right\rangle$

t	GrLET	NCM	NCT	NCS	GaLEG	GaKRO
0.0	3.997 e-05	**4.000 e-12**	**4.000 e-12**	**4.000 e-12**	–	–
0.1	2.729 e-04	1.678 e-09	3.357 e-09	**2.220 e-16**	–	–
0.2	4.470 e-04	1.221 e-08	2.442 e-08	**1.110 e-15**	–	–
0.3	5.490 e-04	3.760 e-08	7.520 e-08	**5.107 e-15**	–	–
0.4	5.994 e-04	8.158 e-08	1.632 e-07	**1.799 e-14**	–	–
0.5	6.135 e-04	1.463 e-07	2.926 e-07	**5.240 e-14**	–	–
0.6	6.028 e-04	2.329 e-07	4.659 e-07	**2.501 e-13**	–	–
0.7	5.758 e-04	3.418 e-07	6.836 e-07	**4.489 e-13**	–	–
0.8	5.398 e-04	4.730 e-07	9.459 e-07	**7.561 e-13**	–	–
0.9	4.964 e-04	6.260 e-07	1.252 e-06	**1.185 e-12**	–	–
1.0	4.516 e-04	8.006 e-07	1.601 e-06	**1.185 e-12**	–	–

Table 3b

The values of absolute error for L = 600, range $\left(1,2\right)$

1.0	4.174 e-04	**1.083 e-12**	**1.083 e-12**	**1.083 e-12**	–	–
1.1	1.478 e-04	4.543 e-10	9.086 e-10	**1.110 e-15**	–	–
1.2	2.420 e-04	3.305 e-09	6.610 e-09	**3.941 e-15**	–	–
1.3	2.973 e-04	1.018 e-08	2.035 e-08	**8.549 e-15**	–	–
1.4	3.246 e-04	2.208 e-08	4.416 e-08	**1.663 e-14**	–	–
1.5	3.265 e-04	3.961 e-08	7.921 e-08	**3.048 e-14**	–	–
1.6	3.119 e-04	6.305 e-08	1.261 e-07	**5.343 e-14**	–	–
1.7	2.919 e-04	9.252 e-08	1.850 e-07	**4.996 e-14**	–	–
1.8	5.594 e-02	1.280 e-07	2.560 e-07	**1.071 e-13**	–	–
1.9	5.324 e-02	1.694 e-07	3.387 e-07	**1.927 e-13**	–	–
2.0	5.006 e-02	2.167 e-07	4.344 e-07	**3.142 e-13**	–	–

7. Conclusions

Comparison analysis of the Tables 1–3 allows the following conclusions.

The Riemann–Liouville formula is perfectly suited for calculations of all kinds of derivatives and integrals. If we apply the right tool – the proper method of numerical integration – we may obtain almost error free values.

The method used to calculate particular derivative using formula (3) should depend on the characteristics of the function subjected integration.

Proper choice always awards with almost error-free results. Tracking the results for method GaKRO in Tables (1, 2), shows almost no errors at all! It is 15–16 times better – in almost all cases – than the values obtained by reference method – GrLET! The perfect results were scored with only 4 sample points which is not even 1% of points the method GrLET needed!

The Newton–Cotes Quadratures are universal tools. Not only they do not depend so strongly as the Gauss Quadratures on shape and changeability of the integrand, but also can be applied (Midpoint Rule) to integrands which have singularities at the both and/or ends of the integration.

In case of the tested function and calculated expressions the shape of the integrand does not influence accuracy of the calculations when applying GrLET method. The number of coefficients used, does. Using maximum number of 600 of coefficients we were able to obtain values with maximum 10e-04 accuracy.

The logic of our tools needed only the grade of the desired polynomial as a input data (GaLEG, GaKRO). All other data were calculated "on the fly" (the polynomial itself, its derivative, abscissas and weights). In practical applications we can and should use tabulated values (of abscissas and weights) which were the subject of standardization by US Department of Commerce. This can yet reduce the complexity of calculations which then can make the method become perfect suitable in practical applications.

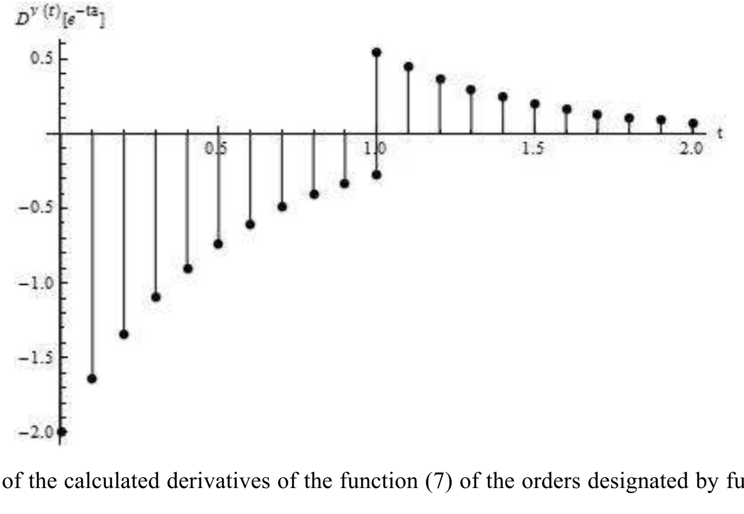

Fig. 3. Plot of the calculated derivatives of the function (7) of the orders designated by function (8)

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References

[1] Burden R.L., Faires J.D., *Numerical Analysis*. 5th ed., Brooks/Cole Cengage Learning, Boston, 2003.

[2] Carpinteri F., Mainardi A. (editors), *Fractals and Fractional Calculus in Continuum Mechanics*. Springer Verlag, Wien and New York 1997.

[3] Chen Y.Q, Vinagre B.M., Podlubny I., *Continued Fraction Expansion Approaches to Discretizing Fractional Order Derivatives – an Expository Review*. Nonlinear Dynamics 38. Kluwer Academic Publishers, 2004, 155–170.

[4] Deng W., *Short memory principle and a predictor-corrector approach for fractional differential equations.* Journal of Computational and Applied Mathematics 206, 2007, 174–188.

[5] Desmarais R.N., *Programs For Computing Abscissas and Weights For Classicaland Nonclassical Gaussian Quadrature Formulas*. NASA Technical Note, NASA TN D-7924, NASA, Washington D.C., 05.October 1975.

[6] Diethelm K., *An algorithm for the numerical solution of differential equations of fractional order*. Electronic Transactions on Numerical Analysis, vol. 5, March 1997, 1–6.

[7] Gorenflo R., *Fractional Calculus: Some Numerical Methods, CISM Courses and Lectures*. Vol. 378, 2001, 277–290.

[8] Kahaner D., Moler C., Nash S., *Numerical Methods And Software*. Prentice Hall, 1989.

[9] Kilbas A.A., Srivastava H.M., Trujillo J.J., *Theory and Applications of Fractional Differential Equations.* North-Holland Mathematics Studies 204, Elsevier, 2006.

[10] Krommer R.A., Ueberhuber Ch.W., *Computational Integration*. SIAM, Philadelphia, 1986.

[11] Krylov V.I., *Priblizhennoe vychislenie integralov*. 2e izd. Nauka, 1967.

[12] Kythe P.K., Schäferkotter M.R., *Handbook of Computational Methods For Integration*. Chapman & Hall/CRC, 2005.

[13] Love C.H., *Abscissas and Weights for Gaussian Quadrature For N=2 to 100, and N=125, 150, 175, 200*. United States Department Of Commerce, National Bureau of Standards Monograph 98 (issued December 28, 1966).

[14] Lubich C.H., *Discretized fractional calculus*. SIAM Journal of Mathematical Analysis, vol. 17, 1986, 704–719.

[15] Machado J.A.T., *Discrete-time fractional-order controllers*. FCAA Journal, vol. 1, 2001, 47–66.

[16] Mayoral L., *Testing for fractional integration versus short memory with trends and structural breaks*. Dept. of Economics and Business, Universidad Pompeu Fabra, 2006.

[17] Michalski M.W., *Derivatives of noninteger order and their applications*. Dissertationes Mathematicae, CCCXXVIII, Inst. Math. Polish Acad. Sci., Warsaw 1993.

[18] Miller K.S.,Ross B., *An Introduction to the Fractional Calculus and Fractional Differential Equations*. John Wiley & Sons Inc., New York, USA, 1993.

[19] Nishimoto K., *Fractional Calculus. Integration and Differentiation of Arbitrary Order*. Tom I – IV, 1984, 1989, 1991, 1996, Descartes Press, Koriyama.

[20] Oldham K.B., Spanier J., *The Fractional Calculus*. Academic Press, New York 1974.

[21] Ostalczyk P., *The time-varying fractional order difference equations*. Proceedings of DETC'03, ASME 2003 Design Engineering Technical Conference & Computers and Information in Engineering Conference, Chicago, USA, 2003, 1–9.

[22] Ostalczyk P., *The linear fractional-order discrete-time system description*. Proceedings of the 9th IEEE International Conference on Methods and Models in Automation and Robotics, MMAR 2002, Międzyzdroje, T.I, 2003, 429–434.

[23] Ostalczyk P., *Discrete-Variable Functions*. A Series of Monographs No 1018, Technical University of Łódź, Poland, 2001.

[24] Ostalczyk P., *The non-integer difference of the discrete-time function and its application to the control system synthesis*. International Journal of System Science, vol. 31, No. 12, 2000, 1551–1561.

[25] Oustaloup A., *La dèrivation non entière, Éditions Hermès*. Paris, France, 1995.

[26] Oustaloup A., *Systèmes Asservis Linéaries d'Ordre Fractionnaire*. Masson, Paris 1984.

[27] Oustaloup A., Cois O., Lelay L., *Représentation et identification par modèle non entire*. Hermes, 2005.

[28] Podlubny I., *Fractional differential equations*. Academic Press, San Diego, USA, 1999.

[29] Sabatier J., Agrawal O.P., Machado T.J.A. (Eds.), *Advances in Fractional Calculus. Theoretical Developments and Applications in Physics and Engineering*. Springer Verlag, 2007.

[30] Samko S., Kilbas A., Marichev O., *Fractional Integrals and derivatives: Theory and Applications*. Gordon and Breach, London, 1993.

[31] Schmidt P., Amsler C., *Test of short memory with trick tailed errors*. Michigan State University, 1999.

[32] Stroud A.H., Secrest D., *Gaussian Quadrature Formulas*. Prentice-Hall, Englewood Cliffs, NJ., 1966.

[33] Taylor J.R., *An Introduction to Error Analysis. The Study of Uncertainties in Physical Measurements*. 2nd ed., University Science Books (1996).

[34] Tuan V.K., Gorenflo R., *Extrapolation to the limit for numerical fractional differentiation*. Zeitschrift Angew. Math. Mech., 75, No. 8, 1995, 646–648.