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Development of an improved numerical integration scheme, its algorithm and application in the least square approximation

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Abstract

In this paper, we derived an improved numerical integration for finding the approximation of functions. An algorithm was written for the implementation in the least square approximation via shifted Gegenbauer polynomials and subsequently, the accuracy was tested on some selected examples to show the suitability of the scheme. All the computations were done using Matlab.

1. Introduction

Least square approximation is a procedure to determine the best fit line to data and well-known method of finding polynomial approximation to a function. The method easily generalizes to finding the best fit of the form $y = a_1 f_1(x), \cdots, a_r f_r(x)$ [11]. This method is considered in the situation when the input data for the dependent variable are given in the form of intervals [11, 12]. In 1805, Adrien Marie Legendre proposed the method of least square approximation to fit a line to data, but the method is credited to Carl Friedrich Gauss. Carl Friedrich Gauss claims to have been in possession of the method of least square approximation since 1795 after he published his method for calculating

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the orbits of celestial bodies in 1809. However, Gauss went beyond Legendre and succeeded in connecting the method with the principle of probability and normal distribution. Numerical quadrature was first proposed by David Gibbs in 1915, in his paper titled "A course in interpolation and numerical integration for the mathematical laboratory". The use of numerical techniques in finding an approximate computation of an integral is called "Numerical integration" [2, 4]. Numerical integration is used to compute an approximate value for integrals of the form:

$$\int_a^b f(x)dx, \tag{1}$$

various formula can be deduced by increasing the number of sub-intervals (n), which will be discussed later in this paper. Fadugba [6] develop an improved numerical integration method via transcendental function of exponential form for the solution of initial value problems in ordinary differential equations, Xia [19] proposed an improved numerical integration based on the Lagrange interpolation scheme to predict the milling stability accuracy and efficiency.
Orthogonal polynomials play an important role in numerical analysis, as different researchers have embedded it in different methods such as Tau method [7, 20], Galerkin method [8, 3] to find an approximate solution to differential equations. Chebyshev polynomials of all kinds (first, second, third and fourth kinds) [16, 1, 17], Legendre $P_n(x)$ [15], Gegenbauer $C_n^{\alpha}(x)$ polynomials [10, 9], to mention but few were used by different researchers to solve fractional diffusion equations.

2. Least Square Approximation (LSA)

Given a function $f(x)$ defined on some interval (a, b), least square approximation is used to approximate $f(x)$ by a polynomial of degree m $(\Gamma_m(x))$ (see [2, 4]). In least square approximation, the values of constants c_j are determined so as to minimize the equation

$$E(c_0,\ c_1, \dots,\ c_m) = \int_a^b w(x)\left[f(x) - \Gamma_m(x)\right]^2 dx \tag{2}$$

where,

$$\Gamma_m(x) = \sum_{j=0}^{m} c_j \varphi_j(x) \tag{3}$$

and $w(x)$ is the weight function, $\varphi_j(x)$, $j = 0,\ 1, \dots, m$ are the orthogonal polynomials with respect to the weight function $w(x)$ over $[a,\ b]$. The necessary condition for $(c_0, c_1, \dots, c_m)$ to be minimum are

$$\frac{\partial E}{\partial a_j} = 0,\ j = 0,\ 1, \ldots,\ m \tag{4}$$

$$\frac{\partial E}{\partial a_j} = -2\int_a^b w(x)[f(x) - \sum_{r=0}^{m} a_j\varphi_j(x)]\varphi_j(x)dx = 0 \tag{5}$$

$$a_j = \frac{\int_a^b w(x)f(x)\varphi_j(x)dx}{\int_a^b w(x)\varphi_j^2(x)dx},\ j = 0,\ 1, \ldots, m \tag{6}$$

to find a_j in (6), we apply improved numerical integration (24), to be derive in section 3. The value of $\int_a^b w(x)\varphi_j^2(x)dx$ vary depending on the orthogonal polynomials, for examples

$$\int_{-1}^{1} w(x)\varphi_j^2(x)dx = \begin{cases} \frac{2}{2j+1},\ \text{Legendre polynomials} \\ \\ \dfrac{\pi 2^{1-2\alpha}\Gamma(j+2\alpha)}{j!\,[\Gamma(\alpha)]^2\,(j+\alpha)},\ \text{Gegenbauer polynomials} \\ \\ \pi,\ \text{third and fourth kinds Chebyshev polynomials} \end{cases} \tag{7}$$

TABLE 1. **some commonly Used orthogonal polynomials**

n	Orthogonal polynomials ($\varphi_j(x)$)	$w(x)$
1	Legendre	1
2	Chebyshev of first kind ($T_j(x)$)	$(1-x^2)^{-\frac{1}{2}}$
3	Chebyshev of second kind ($U_j(x)$)	$(1-x^2)^{\frac{1}{2}}$
4	Chebyshev of third kind ($V_j(x)$)	$\sqrt{\frac{1+x}{1-x}}$
5	Chebyshev of fourth kind ($W_j(x)$)	$\sqrt{\frac{1-x}{1+x}}$
6	Gegenbauer $C_j^{\alpha}(x)$)	$(1-x^2)^{\alpha-\frac{1}{2}}$
7	Hermite $H_j(x)$)	e^{-x^2}

2.1. **Overview of numerical integration.** The general form of the problem of numerical integration may be written as:
Given a set of data points $(x_j,\ y_j)\,,\ i = 0,\ 1, \cdots,\ n$ of a function $y = f(x)$, where $f(x)$ is not explicitly known. then evaluating the definite integral

$$I = \int_a^b f(x)dx \tag{8}$$

by replacing $y = f(x)$ by an interpolating polynomial $\theta(x)$ to obtain approximate value for the definite integral of (8). Then it was derived by different researchers, a general formula for numerical integration by using Newton's forward difference formula with an assumption that the interval $(a,\ b)$ is divided into n-equal subintervals such that

$$h = \frac{b-a}{n},\ a = x_0 < x_2 < \cdots < x_n = b \tag{9}$$

with $x_n = x_0 + nh$, where h is the step-length, n is the number of subintervals a and b is the limits of integration with $b > a$.
Hence, the integral in (8) can be written as

$$I = \int_{x_0}^{x_n} f(x)dx \tag{10}$$

Using Newton's forward interpolation formula, that is

$$I = \int_{x_0}^{x_n} \left[f_0 + \binom{p}{1} \triangle f_0 + \binom{p}{2} \triangle^2 f_0 + \cdots \right] dx \tag{11}$$

where $x = x_0 + ph$

$$I = h \int_0^n \left[f_0 + \binom{p}{1} \triangle f_0 + \binom{p}{2} \triangle^2 f_0 + \cdots \right] dp \tag{12}$$

Hence, after simplification, we get
(13)

$$I = \int_{x_0}^{x_n} f(x)dx = nh \left[f_0 + \frac{n}{2} \triangle f_0 + \frac{n(2n-3)}{12} \triangle^2 f_0 + \frac{n(n-2)^2}{24} \triangle^3 f_0 + \cdots \right]$$

Equation (13) has been established to be **Newton-Cotes closed quadrature formula**. From the general formula (13), a lot researchers had work on (13) to derive different integration formulae by substituting $n = 1,\ 2, \cdots$
Substituting $n = 1$ in (13) gives Trapezoidal's rule(see (14)) , for $n = 2$ and $n = 3$ give Simspson $\frac{1}{3}$ (see (15)) and Simspon $\frac{3}{8}$ (16)) respectively, for $n = 4$ and $n = 6$ give Boole's rule (see (17)) and Weddle's rule (see (18)) see [4, 2, 5, 18]. Convergence of the trapezoidal rule was reported in [14, 13].

$$I = \sum_{r=1}^{n} I_r = \int_{x_0}^{x_n} f(x)dx = \frac{h}{2}\left[f_0 + 2(f_1 + f_2 + \cdots + f_{n-1}) + f_n\right] \tag{14}$$

$$I = \int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\left[f_0 + 4(f_1 + f_3 + f_5 + \cdots + f_{2n-1}) + 2(f_2 + f_4 + f_6 + \cdots + f_{2n-2}) + f_{2n}\right] \tag{15}$$

$$\begin{aligned} I = \int_{x_0}^{x_n} f(x)dx =& \frac{3h}{8}\left[f_0 + 3(f_1 + f_2 + f_4 + f_5 + f_7 + \cdots + f_{3n-2} + f_{3n-1})\right. \\ &\left. +2(f_3 + f_6 + f_9 + \cdots + f_{3n-3}) + f_{3n}\right] \end{aligned} \tag{16}$$

$$\begin{aligned} I = \int_{x_0}^{x_n} f(x)dx =& \frac{2h}{45}\left[7f_0 + 32(f_1 + f_3 + f_5 + f_7 + \cdots) + 12(f_2 + f_6 + f_{10} + \cdots)\right. \\ &\left. +14(f_4 + f_8 + f_{12} + \cdots) + 7f_n\right] \end{aligned} \tag{17}$$

$$\begin{aligned} I = \int_{x_0}^{x_n} f(x)dx =& \frac{3h}{10}\left[f_0 + 5(f_1 + f_5 + f_7 + f_{11} + \cdots) + (f_2 + f_4 + f_8 + f_{10} + \cdots)\right. \\ &\left. +6(f_3 + f_9 + f_{15} + \cdots) + 2(f_6 + f_{12} + f_{18} + \cdots) + f_n\right] \end{aligned} \tag{18}$$

3. Methodology

Here, an improved numerical integration is propose to solve (6), by increasing the number of sub-intervals to $n = 8$, then substitute the resulting equation in (3) to give the least square approximation to the function $f(x)$.

3.1. Derivation of an improve numerical integration. From (13) put $n = 8$

$$\begin{aligned} I &= h\left[8f_r + 32\Delta f_r + \frac{208}{3}\Delta^2 f_r + 96\Delta^3 f_r + \frac{3928}{45}\Delta^4 f_r\right. \\ &\left. + \frac{2336}{45}\Delta^5 f_r + \frac{18128}{945}\Delta^6 f_r + \frac{736}{189}\Delta^7 f_r + \frac{3956}{14175}\Delta^8 f_r\right] \end{aligned} \tag{19}$$

when $r = 0$,

$$\begin{aligned} I_0 &= \frac{h}{14175}\left[3956f_0 + 23552f_1 - 3712f_2 + 41984f_3\right. \\ &\left. -18160f_4 + 41984f_5 - 3712f_6 + 23552f_7 + 3956f_8\right] \end{aligned} \tag{20}$$

when $r = 8$,

$$I_1 = \frac{h}{14175}\left[3956f_8 + 23552f_9 - 3712f_{10} + 41984f_{11} - 18160f_{12} + 41984f_{13} - 3712f_{14} + 23552f_{15} + 3956f_{16}\right] \tag{21}$$

when $r = 16$,

$$I_2 = \frac{h}{14175}\left[3956f_{16} + 23552f_{17} - 3712f_{18} + 41984f_{19} - 18160f_{20} + 41984f_{21} - 3712f_{22} + 23552f_{23} + 3956f_{24}\right], \tag{22}$$

in general,

$$I_n = \frac{h}{14175}\left[3956f_{8n-8} + 23552f_{2n-7} - 3712f_{2n-6} + 41984f_{2n-5} - 18160f_{2n-4} + 41984f_{2n-3} - 3712f_{2n-2} + 23552f_{2n-1} + 3956f_{2n}\right] \tag{23}$$

therefore,

(24)

$$\begin{aligned} I = \int_{x_0}^{x_n} f(x)dx = \sum_{i=0}^{n} I_i \\ = \frac{h}{14175}\left[3956(f_0 + f_{8n}) + 23552\left(f_1 + f_9 + f_{17} + \cdots + f_{8n-7}\right)\right. \\ -3712\left(f_2 + f_{10} + f_{18} + \cdots + f_{8n-6}\right) + 41984\left(f_3 + f_{11} + f_{19} + \cdots + f_{8n-5}\right) \\ -18160\left(f_4 + f_{12} + f_{20} + \cdots + f_{8n-4}\right) + 41984\left(f_5 + f_{13} + f_{21} + \cdots + f_{8n-3}\right) \\ \left. -3712(f_6 + f_{14} + f_{22} + \cdots + f_{8n-2}) + 23552\left(f_7 + f_{15} + f_{23} + \cdots + f_{8n-1}\right)\right] \end{aligned}$$

```
 function num_integral = issastev(f,a,b,N)
%integral of f(x) over [a,b] using improved numerical integration with N segments
if nargin < 4, N = 100; end
if abs(b - a)<1e-12 | N <= 0, stevissa = 0; return; end
if mod(N,2) ~= 0, N = N + 1; end %make N even
h = (b - a)/N; x = a + [0:N]*h;
num_integral=(h/14175)*((3956*f(1))+(3956*f(N+1))+(7912*sum(f(9:8:N-7)))+...
    (23552*sum(f(2:8:N-6)))+(23552*sum(f(8:8:N)))-(3712*sum(f(3:8:N-5)))-...
    -(3712*sum(f(7:8:N-1)))+(41984*sum(f(4:8:N-4)))+...
    (41984*sum(f(6:8:N-2)))-(18160*sum(f(5:8:N-3))));%(24)
```

3.2. **Algorithm for the interpolant.** To use an improved numerical integration to approximate functions with no close form solution, an algorithm is written to enhances the clarification effectively and to reduce the computational difficulties. The algorithm goes thus:

Data: f: The function to be approximated/interpolated

Ω: set of data

θ: set of evaluation point
n: degree of approximation
Define ε_i in an interval $[a, b]$
$\varphi(x)$: The orthogonal polynomial to be adopted
$w(x)$: The weight function to be used, subject to $\varphi(x)$

for $j = 1, \cdots, m$ do
$a_j = \dfrac{\text{issastev}(w(x)f(x)\varphi_j(x), a, b, N)}{\int_a^b w(x)\varphi_j^2(x)dx}$
$\Gamma_m(x) = \sum_{j=0}^{m} a_j\varphi_j(x)$
end
for $i = 1, \cdots, N$ do
$\varepsilon_i = a + (i-1)(\frac{b-a}{N})$
$error = E_i = |f(\varepsilon_i) - \Gamma_m(\varepsilon_i)|$
end
plot the ε_i versus E_i
Find the maximum of E_i
plot the interpolant $\Gamma_m(\varepsilon_i)$

4. Illustrative Examples

Here,the least square approximation to functions with closed form solution and no closed form solution will be illustrated, and their graphs will be shown to see the accuracy of the improved method. We compute the maximum error E_m and compare with the existing methods, which are written as below:

$$E_m = \max|f(x_n) - \Gamma(x_n)|, \text{ where } x_n = x_0 + nh, \ h = \frac{b-a}{n} \tag{25}$$

Example 4.1. Consider the function $f(x) = e^x$ over the interval $[-1, 1]$ by means of Gegenbauer polynomial $C_j^{\alpha}(x))$.
Using (3) and (6) for degree 4 (that is $m = 4$), taking $\alpha = \frac{1}{2}$ we have: $\Gamma_j(x) = \sum_{j=0}^{m} a_j\varphi_j(x)$,

$$a_j = \frac{j!\,[\Gamma(\alpha)]^2\,(j+\alpha)}{\pi 2^{1-2\alpha}\Gamma(j+2\alpha)} \int_{-1}^{1} (1-x^2)^{\alpha-\frac{1}{2}} f(x) C_j^{\alpha}(x))dx, \ j = 0, \ldots, n$$

$a_0 = 1.1752, a_1 = 1.1036, a_2 = 0.3578, a_3 = 0.0705, a_4 = 0.0100$. Hence

$$\Gamma_4(x) = \frac{7x^4}{160} + \frac{141x^3}{800} + \frac{312x^2}{625} + \frac{19957x}{20000} + \frac{20001}{20000}. \tag{26}$$

For degree 8, we obtain

$$\begin{aligned} \Gamma_8(x) = {} & \frac{307846934225233315275}{1208925819614629174706176}x^8 + \frac{385958363319544715 7}{188894659314785808547 84}x^7 + \\ & \frac{419598019973237337309}{302231454903657293676544}x^6 + \frac{9837205413036188924097 9}{1180591620717411303424000 0}x^5 + \\ & \frac{1263914496112966565550 13}{3022314549036572936765440}x^4 + \frac{3937864026053758500404 23}{2361183241434822606848000}x^3 + \\ & \frac{944185573775435784138598 53}{188894659314785808547840000}x^2 + \frac{11804686386727486114252629}{11805916207174113034240000}x + \\ & \frac{755593037928018677480316443}{755578637259143234191360000} \end{aligned} \tag{27}$$

Figure 1 correspond to (27)

Table 2. Maximum errors at degree 4 (E_4) with $\alpha = \frac{1}{2}$

$f(x)$	E_4
e^{x^2}	0.0192
$\sin(e^{x^2})$	0.0808
$e^{x^2}\cos\left(x^2\right)$	0.0196
$x^2e^{x^2}$	0.0718

Table 3. Maximum errors: LSA of functions via Gegenbauer polynomials with $m = 8$

$f(x)$	$\alpha = \frac{1}{2}$	$\alpha = 1$	$\alpha = \frac{3}{2}$	$\alpha = 2$
e^{x^2}	9.22×10^{-5}	0.015	1.6×10^{-4}	9×10^{-3}
$\sin(e^{x^2})$	3.44×10^{-3}	2.8×10^{-3}	8.0×10^{-3}	8.8×10^{-3}
$e^{x^2}\cos(x^2)$	4.14×10^{-5}	3.0×10^{-3}	9.21×10^{-4}	8.5×10^{-3}
$x^2e^{x^2}$	9.81×10^{-5}	0.015	5.3×10^{-4}	7.0×10^{-3}

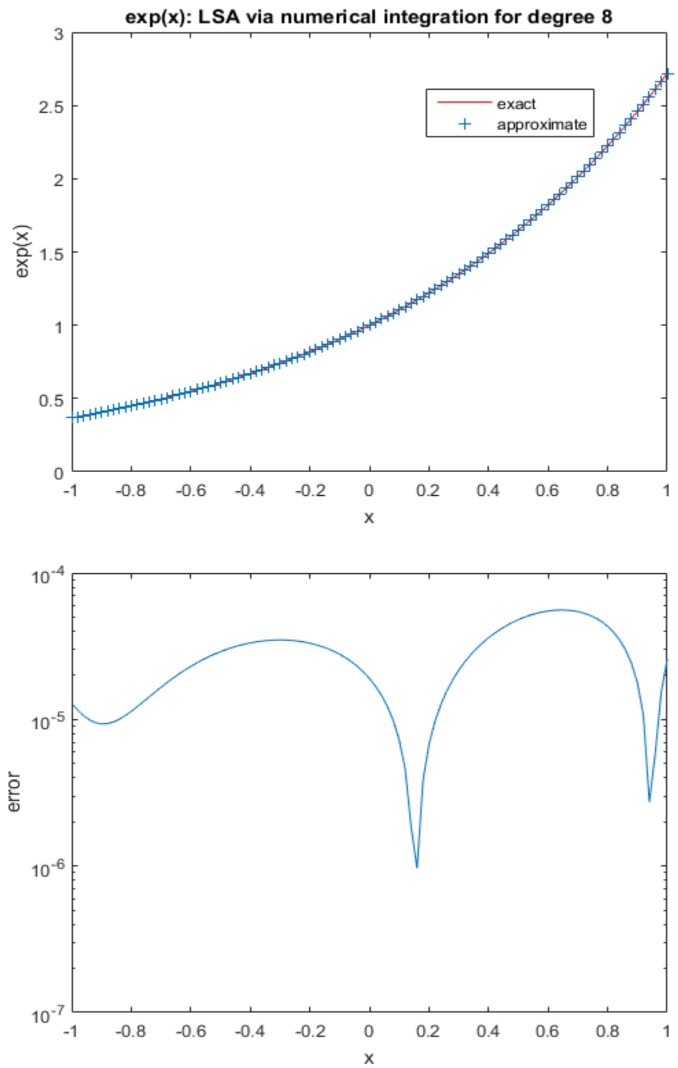

Figure 1: Approximant and the exact for $\exp(x)$ and its corresponding error for degree 8 with $\alpha = \frac{1}{2}$

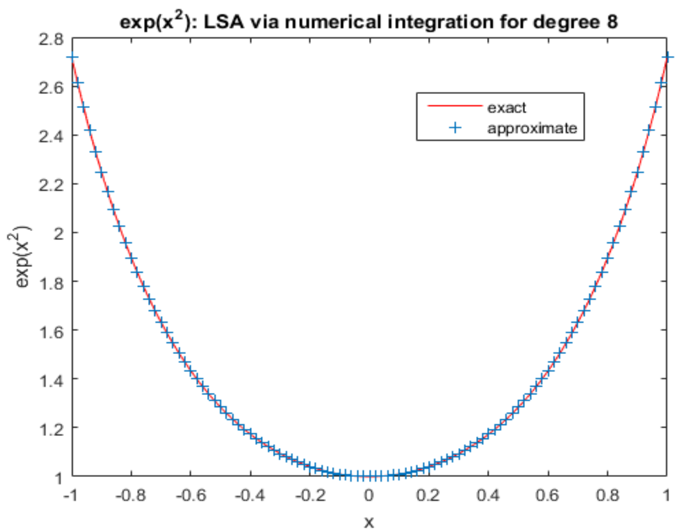

Figure 2: $\exp(x^2)$: Comparision of the approximate solution and the exact for degree 8 with $\alpha = \frac{1}{2}$

Discussion of Results: We take $N = 96$ in the numerical integration for all the examples considered, to have enough sub-intervals. Table 3 is the product of the errors obtained from interpolating examples which summarizes all the maximum errors obtained for the examples considered via Gegenbauer polynomials. For $\alpha = \frac{1}{2}$ perform better irrespective of the functions considered while the accuracy of the errors at $\alpha = 1$ is low compare to other values of the α considered. It is visually obvious that, as the degree of approximation m increases the errors improves (that's the errors decline as m increases) as shown in Tables 2-3.

Conclusions: In this research work, least square approximation couple with derived numerical integration are presented to solved some selected functions and the tables of results shows the effectiveness and efficiency of the propose scheme.

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