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Comparison of Numerical Differentiation of a Known Function using Interpolating Polynomial and Least Squares Approximation with Orthogonal Polynomials

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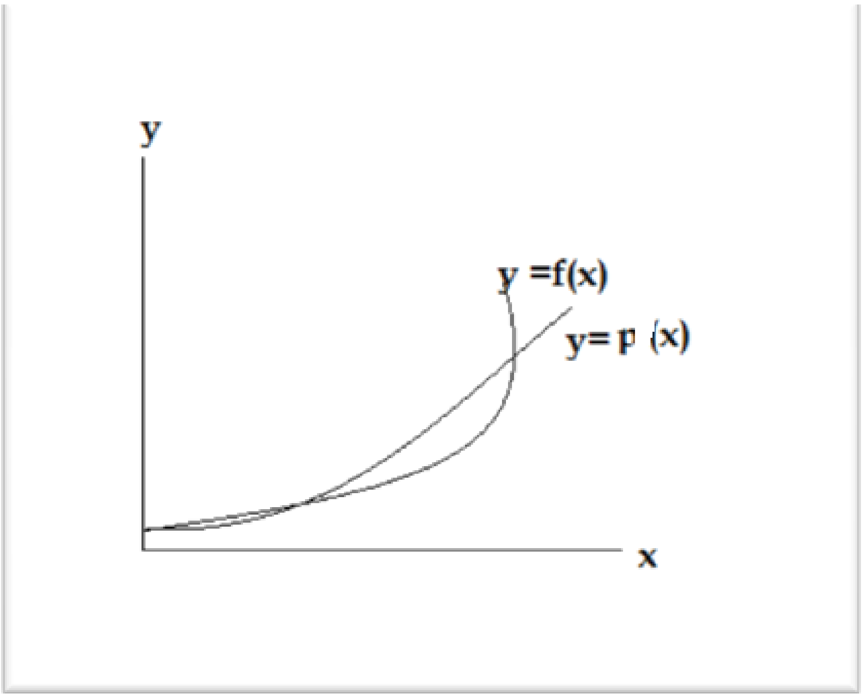
Abstract: In this paper, numerical differentiation of a known function is accomplished by using interpolating polynomial and then by using least squares orthogonal polynomial approximation. A numerical example is illustrated to support the fact that numerical differentiation using least squares polynomial fit gives better result.

Keywords: numerical differentiation, interpolating polynomial, least squares polynomial approximation.

1. INTRODUCTION

Numerical differentiation is a process of calculating the derivatives of a function by means of a set of given values of that function [1]. One can obtain the derivative of a function by the methods of elementary calculus. But if the function is very complicated or the function is given in the form of table of values and explicit form of function is not known then it may be necessary to resort to numerical differentiation.

The general approach the numerical differentiation is that one first obtain polynomial $P_n(x)$ and then differentiate this polynomial r times (n>r) to get $P_n^r(x)$. The value of $P_n^r(x)$ gives an approximate value of $f_n^r(x)$ at the point $X=X_k$ [2]. In numerical differentiation based on interpolating polynomial a considerable amount of error occur. The basic difficulty in numerical differentiation is that while $(f(x)- P_n(x))$ may be small, the differences $(f_n^r(x) - P_n^r(x))$, r = 1,2,3,… may be very large. It is clear from the following figure that although the curves y=f(x) and the interpolating curve $y=P_n(x)$ are close yet these two curves differ considerably in slope, variation is slope etc.



These comments will be made more clear and precise in the following discussion.

2. NUMERICAL DIFFERENTIATION USING INTERPOLATING POLYNOMIAL

Let the function f(x) be continuously differentiable on some interval (a,b). if …., X_{-2}, X_{-1}, X_0, X_1 X_2, … are district point in (a,b) then we can approximate f(x) by using stirling's formula: [3], [6].

$$F(x) \sim Y_0 + p\,\frac{(\Delta Yo + \Delta Y-1)}{2} + \frac{p2}{2!}\Delta^2 Y_{-1} + - - \qquad (1)$$

Where $p = \frac{(X-Xo)}{h}$ So

$$f'(x) = \frac{df}{dp}\frac{dp}{dx} = \frac{1}{h}\left[\frac{\Delta Yo + \Delta Y1}{2} + p\Delta^2 Y_{-1} + - - - - -\right] \quad (2)$$

And $f''(x) = \frac{1}{h^2}\,[\Delta^2 Y_{-1} + p(\Delta^3 Y_{-1} + \Delta^3 Y_{-2})/2 + - -]$

In particular, if $X=X_0$ then

$$f'(X_0) = \frac{1}{h}\left[\frac{\Delta Yo + \Delta Y_{-1}}{2} - \frac{1}{6}\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} + - - - - - - - -\right] \quad (3)$$

$$\text{And } f''(X_0) = \frac{1}{h^2}\left[\Delta^2 Y_{-1} - \frac{1}{12}\Delta^4 Y_{-2} + - - - - - -\right] \quad (4)$$

3. NUMERICAL DIFFERENTIATION USING LEAST SQUARES APPROXIMATION BY ORTHOGONAL POLYNOMIALS

Let f(x) be a function whose explicit form is known. Let it be defined on some interval (a,b) and one wish to find $F^1(x)$ at some point between a and b. For this, we first give the following definitions.

Definition 1: the scalar product of two functions U (n) and V (x) which are both defined on (a, b) is defined as

$$<U,V> = \int_a^b U(x)\,V(x)\,W(x)\,dx \qquad (5)$$

Where w(x) is a known function and is positive on (a, b) usually called a weight function ; provided the integral exists.

Definition 2:
The two functions U(x) and V(x) are said to be orthogonal w.r.t. weight function w(x) if
$<U,V>=0$

Definition 3: F_o, F_1,- - - f_m is a sequence of orthogonal polynomials if each f_i is a polynomial of degree exactly i and $<fi, fj> = 0$ for $i \neq j$

If one wish to approximate some function f(x) on (a, b) by a polynomial g(x) of degree < m then by principle of least squares,

$$<f(x)-g(x), f(x)-g(x)> = \int_a^b [f(x) - g(x)]^2 w(x)dx \quad (6)$$

should be minimum. (6) is called a weighted sum of squares of errors [5]. The Polynomial g(x) is called least square approximation to f(x).

To find such polynomial g(x), we find a sequence of orthogonal polynomial $g_0(x)$, $g_1(x)$, - - - g_m (x) such that

$$g(x) = a_o\,g_0(x) + a_1\,g_1(x) + - - - - - - + a_m\,g_m(x) \qquad (7)$$

Where a_0, a_1 - - a_m are unknowns.
From (6), it follows that
$<f(x) - a_0 g_0(x) - a_1g_1(x) - - - - a_m g_m(x),\ f(x) - a_0 g_0(x) - a_1g_1(x) - - - - a_m g_m(x)>$
should be minimum
Let us denote it by $E(a_0\,a_1,- -, a_m)$
So, from (6), $E(a_0\,a_1,- -, a_m)$ will be minimum if partial derivatives of E w.r.t. $a_0\,a_1$,- -, a_m are all zero, which on Simplification gives
$a_0<g_0, g_i> + a_1 <g_1, g_i> + - + a_m <g_m, g_i> = <f, g_i>$, i= 0, 1, 2- - - - m
Since g_0, g_1, - - - g_m is a sequence of orthogonal polynomials so
$a_i <g_i, g_i> = <f, g_i>$; i = 0, 1, 2, - -, m

$$\text{So } a_i = \frac{<f,gi>}{<gi,gi>} ;\ i = 0, 1, - - - m \qquad (8)$$

These coefficient when substituted in (7) gives best least square fit to the given function f(x) on (a, b).
So $f(x) \approx a_0\,g_0(x) + a_1\,g_1(x) + - - - + a_m g_m(x)$
Differentiating both sides w.r.t.x, we get
$F^1(x) \approx a_0\,g_0'(x) + a_1\,g_1'(x) + - - - + a_m g_m'(x)$
For a particular point say X_0 in (a, b),

$$F^1(x_0) \approx a_0\,g_0'(x_0) + a_1\,g_1'(x_0) + - - - + a_m g_m'(x_0) \qquad (9)$$

Formula (9) can be used as required formula for numerical differentiation.

4. NUMERICAL EXAMPLE

Let us consider a simple example to illustrate how to use numerical differentiation using least square fit and to check whether it is better that numerical differentiation using interpolating polynomial, let $f(x) = e^x$ and one wish to f'(0) and f'' (0) by approximating it by a polynomial of degree <3 on the interval [-1, 1] using results obtained in section (2), we have,

X	$Y=e^x$	Δy	$\Delta^2 y$
-1	0.36787944	0.63212056	
0	1	1.71828183	1.08616325
1	2.71828183		

Using (3), $f'(0) = \frac{1}{1}\left[\frac{1.71828183 + 0.63212056}{2}\right]$
$= 1.175201195$

And using (4), $f''(0) = \frac{1}{(1)}\,[1.08616325]$
$= 1.08616325$

Now, let us use the result obtained in section 3 to find f'(0) and f'' (0).
Here $F(x) = a_0\,g_0(x) + a_1\,g_1(x) + a_2\,g_2(x) + a_3\,g_3(x)$
Where $a_i = \frac{<f,gi>}{<gi,gi>}$

For the scalar product < f, gi>, the orthogonal polynomials are Legendre's polynomial [4]

i.e. $g_0(x) = 1$, $g_1(x) = x$, $g_2(x) = \frac{3}{2}(x^2 - \frac{1}{3})$, $g_3(x) = \frac{5}{2}(x^3 - \frac{3x}{5})$
and for Legendre's polynomial, $<gi, gi> = \frac{2}{2i+1}$ for all i
So $<a_0, g_0> = 2$, $< g_1, g_1> = \frac{2}{3}$, $< g_2, g_2> = \frac{2}{5}$, $<g_3, g_3> = \frac{2}{7}$
So f(x) = 0.99629402+0.99795487x
+ $0.53672153x^2 + 0.17613908x^2$

Differentiating both sides w.r.t x, and setting x=0,
f'(0) = 0.99795487
And f''(0) = 2(0.53672153)
= 1.07344306
Obviously, f'(0) = 1 and f''(0)=1 (analytically)

5. RESULT AND DISCUSSION

In above section 4, we have calculated f'(0) and f'''(0) by using two different techniques. First, we have used numerical differentiation by using interpolating polynomial and we got

f'(0) = 1.175201195 and f''(0) = 1.08616325

But exact values of f'(0) and f''(0) is 1 analytically . So the calculated values are too far from exact values. This difference is due to the truncation error which can be reduced by reducing the value of h. but reducing the value of h too much will introduce round off errors in computations there by increasing the total error. So we are in a 'cleft Stick' and must compromise with some optimum choice of h. [6]
In brief, we can say that in numerical differentiation based on interpolating polynomial, there may occur large amount of errors.
Now by using numerical differentiation based on least squares approximately, we see that
f'(0) = 0.99795487 and f''(0) = 1.07344306
Which is quite close to the exact values f'(0) = 1 and f''(0)=1

6. CONCLUSION

The comparison of results obtained by using interpolating polynomial and using least squares polynomial indicates that it is more advantages to estimate f' and f'' by estimating f by least squares orthogonal polynomials.

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