Differentiation of Continuous Functions

Second Derivative Approximation

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Introduction

This worksheet demonstrates the use of Mathcad to illustrate the approximation of the second derivative of continuous functions.

A second derivative approximation uses a point *h* ahead and a point *h* behind of the given value of *x* at which the second derivative of *f (x)* is to be found.

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + 0(h^2)$$

Section 1: Input

The following simulation approximates the second derivative of a function using second order accurate approximation. The user inputs are

a) function, *f(x)*
b) point at which the derivative is to be found, *xv*
c) starting step size, *h*
d) number of times user wants to halve the starting step size, *n*

The outputs include

a) approximate value of the second derivative at the point and initial step size given
b) exact value
c) true error, absolute relative true error, approximate error and absolute relative approximate error, least number of correct significant digits in the solution as a function of step size.

Function *f(x)*

$f(x) := \exp(2 \cdot x)$

Value of *x* at which *f ''(x)* is desired, *xv*

$xv := 4.0$

Starting step size, *h*

$h := 0.2$

Number of times starting step size is halved

$n := 12$

This is the end of the user section. All the information must be entered before proceeding to the next section.

Section 2: Procedure

The following procedure estimates the solution of second derivate of an equation at a point *xv*.

f (x) = function

xv = value at which the solution is desired

h = starting step size value

n = number of times starting step size is halved

$$\mathrm{SOD}(f, xv, h) := \left| \begin{array}{l} \mathrm{deriv} \leftarrow \dfrac{f(xv + h) - 2 \cdot f(xv) + f(xv - h)}{h^2} \\ \mathrm{deriv} \end{array} \right.$$

Section 3: Calculation

The exact value EV of the second derivative of the equation:

Given the function

$$f(x) \rightarrow e^{2\cdot x}$$

First, using the derivative command the solution is found. In a second step, the exact value of the derivative is shown

The solution of the second derivative is

$$f''(x) := \frac{d^2}{dx^2} f(x) \qquad f''(x) \rightarrow 4\cdot e^{2\cdot x}$$

The exact solution of the second derivative is

$$EV := f''(xv)$$

$$EV = 11923.831948$$

The next loop calculates the following:
Av: Approximate value of the second derivative using second order accurate approximation by calling the procedure "SOD"
Ev: Exact value of the second derivative
Et: True error
ε_t: Absolute relative true percentage error
Ea: Approximate error
ε_a: Absolute relative approximate percentage error
n_{sig}: Least number of correct significant digits in an approximation

$$
\begin{aligned}
\text{table1} := \ & \text{for } i \in 0 .. n-1 \\
& \quad N_i \leftarrow 2^i \\
& \quad H_i \leftarrow \frac{h}{N_i} \\
& \quad AV_i \leftarrow SOD(f, xv, H_i) \\
& \quad E_{t_i} \leftarrow EV - AV_i \\
& \quad \varepsilon_{t_i} \leftarrow \left| \frac{E_{t_i}}{EV} \cdot 100 \right| \\
& \text{augment}(H, AV, E_t, \varepsilon_t)
\end{aligned}
$$

$$
\begin{aligned}
\text{table2} := \; & \text{for } i \in 0..n-1 \\
& \quad N_i \leftarrow 2^i \\
& \quad H_i \leftarrow \frac{h}{N_i} \\
& \quad AV_i \leftarrow \text{SOD}\left(f, xv, H_i\right) \\
& \quad E_{t_i} \leftarrow EV - AV_i \\
& \quad \varepsilon_{t_i} \leftarrow \left| \frac{E_{t_i}}{EV} \cdot 100 \right| \\
& \quad \text{if } i > 0 \\
& \quad \quad E_{a_i} \leftarrow AV_i - AV_{i-1} \\
& \quad \quad \varepsilon_{a_i} \leftarrow \left| \frac{E_{a_i}}{AV_i} \right| \cdot 100 \\
& \quad \quad n_{sig_i} \leftarrow \text{floor}\left(\left(2 - \log\left(\frac{\varepsilon_{a_i}}{0.5}\right)\right)\right) \quad \text{if } 0 < \varepsilon_{a_i} < 5 \\
& \quad \quad n_{sig_i} \leftarrow 0 \quad \text{otherwise} \\
& \quad \text{augment}\left(H, AV, E_a, \varepsilon_a, n_{sig}\right)
\end{aligned}
$$

The loop halves the value of the starting step size *n* times. Each time, the approximate value of the second derivative is calculated and saved in a vector. The approximate error is calculated after at least two approximate values of the derivative have been saved. The number of significant digits is calculated and written as the lowest real number. If the number of significant digits calculated is less than zero, then it is shown as zero.

Section 4: Table of Values

The next tables show the step size value, approximate value, true error, the absolute relative true percentage error, the approximate error, the absolute relative approximate percentage error and the least number of correct significant digits in an approximation as a function of the step size value.

table1 =

	H	AV	E_t	ε_t
	0	1	2	3
0	0.2	$1.21\cdot10^{4}$	-159.83	1.34
1	0.1	$1.2\cdot10^{4}$	-39.8	0.33
2	0.05	$1.19\cdot10^{4}$	-9.94	0.08
3	0.03	$1.19\cdot10^{4}$	-2.48	0.02
4	0.01	$1.19\cdot10^{4}$	-0.62	0.01
5	0.01	$1.19\cdot10^{4}$	-0.16	0
6	0	$1.19\cdot10^{4}$	-0.04	$3.26\cdot10^{-4}$
7	0	$1.19\cdot10^{4}$	-0.01	$8.14\cdot10^{-5}$
8	$7.81\cdot10^{-4}$	$1.19\cdot10^{4}$	-0	$2.03\cdot10^{-5}$
9	$3.91\cdot10^{-4}$	$1.19\cdot10^{4}$	$-5.88\cdot10^{-4}$	$4.93\cdot10^{-6}$
10	$1.95\cdot10^{-4}$	$1.19\cdot10^{4}$	$-1.47\cdot10^{-4}$	$1.23\cdot10^{-6}$
11	$9.77\cdot10^{-5}$	$1.19\cdot10^{4}$	$-3.25\cdot10^{-4}$	$2.73\cdot10^{-6}$

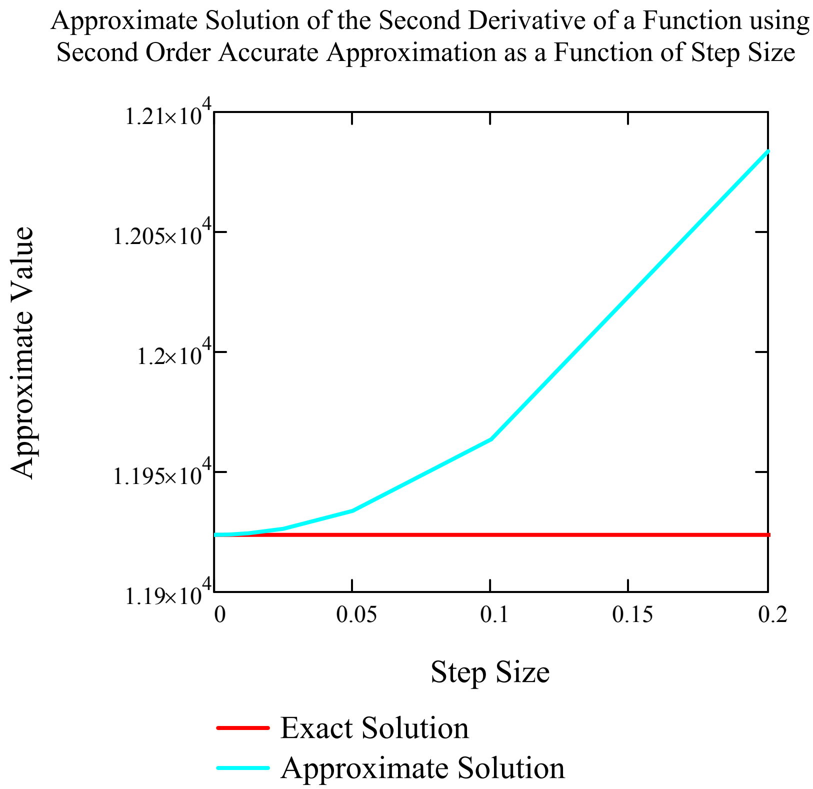
table2 =

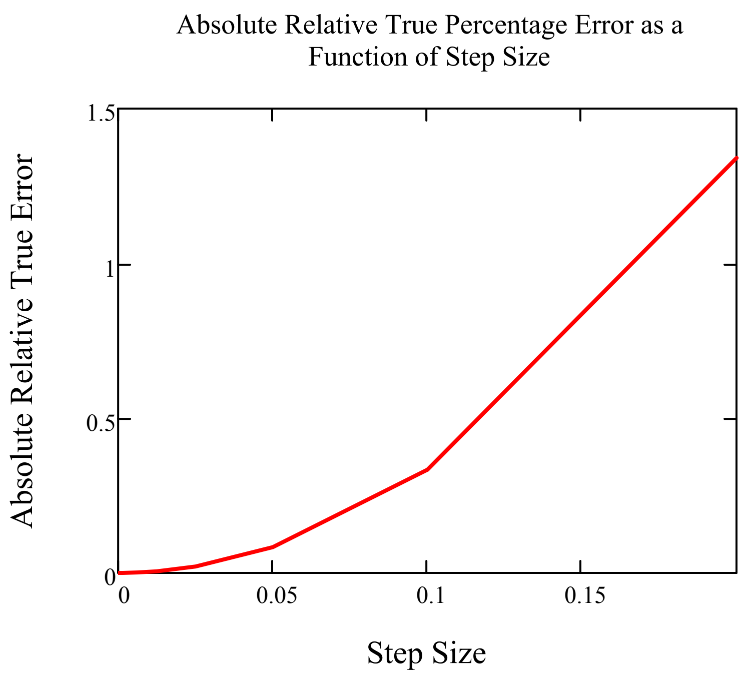
	H	AV	E_a	ε_a	n_{sig}
	0	1	2	3	4
0	0.2	$1.21\cdot10^{4}$	0	0	0
1	0.1	$1.2\cdot10^{4}$	-120.04	1	1
2	0.05	$1.19\cdot10^{4}$	-29.86	0.25	2
3	0.03	$1.19\cdot10^{4}$	-7.46	0.06	2
4	0.01	$1.19\cdot10^{4}$	-1.86	0.02	3
5	0.01	$1.19\cdot10^{4}$	-0.47	0	4
6	0	$1.19\cdot10^{4}$	-0.12	$9.77\cdot10^{-4}$	4
7	0	$1.19\cdot10^{4}$	-0.03	$2.44\cdot10^{-4}$	5
8	$7.81\cdot10^{-4}$	$1.19\cdot10^{4}$	-0.01	$6.1\cdot10^{-5}$	5
9	$3.91\cdot10^{-4}$	$1.19\cdot10^{4}$	-0	$1.54\cdot10^{-5}$	6
10	$1.95\cdot10^{-4}$	$1.19\cdot10^{4}$	$-4.41\cdot10^{-4}$	$3.7\cdot10^{-6}$	7
11	$9.77\cdot10^{-5}$	$1.19\cdot10^{4}$	$1.79\cdot10^{-4}$	$1.5\cdot10^{-6}$	7

Section 5: Graphs

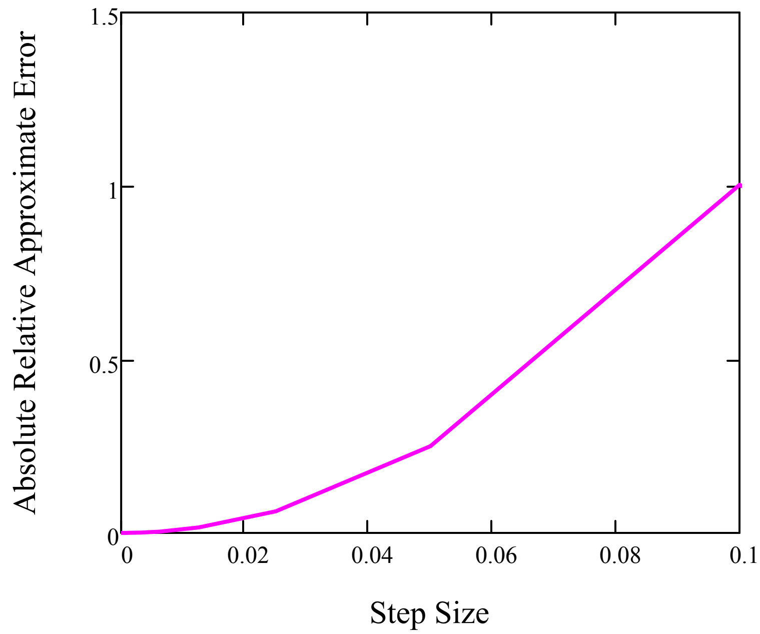
The following graphs show the approximate solution, absolute relative true error, absolute relative approximate error and least number of significant digits as a function of step size.

$x := 0 .. h + 1$

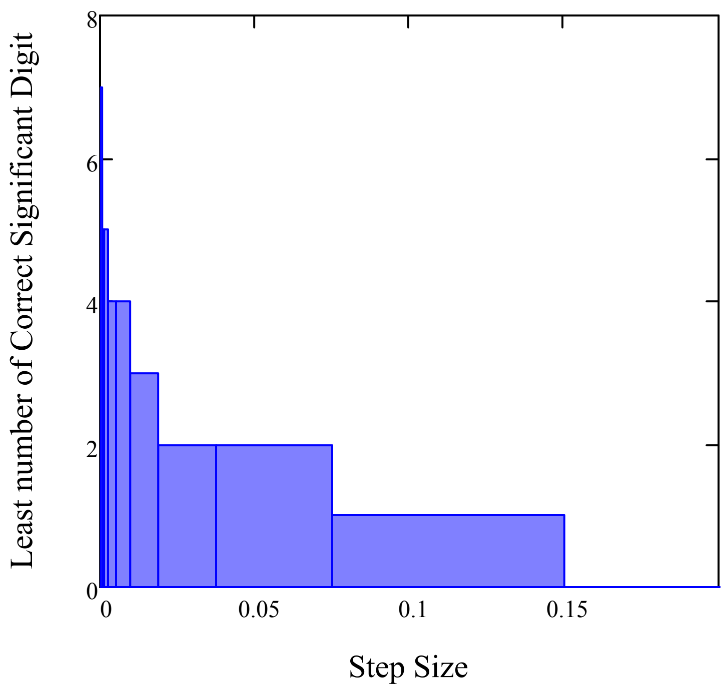




Absolute Relative Approximate Percentage Error as a Function of Step Size



Least Significant Digits Correct as a Function of Step Size



References

Numerical Differentiation of Continuous Functions. See
http://numericalmethods.eng.usf.edu/mws/gen/02dif/mws_gen_dif_txt_continuous.pdf

Questions

1. The velocity of a rocket is given by

$$v(t) = 2000 \cdot ln \frac{140000}{140000 - 2100 \cdot t} - 9.8 \cdot t$$

Use second order derivative approximation method with a step size of 0.25 to find the jerk at $t=5s$. Compare with the exact answer and study the effect of the step size.

2. Look at the true error vs. step size data for problem # 1. Do you see a relationship between the value of the true error and step size ? Is this concidential?

Conclusions

To obtain more accurate values of the second derivative using second order accurate approximation, the step size needs to be smaller. As the spreadsheet shows, the smaller the step size value is, the approximation is closest to the exact value. By decreasing the step size, the least number of significant digits that can be trusted increases. However, a too small step size can result in noticeable round-off errors, and hence giving highly inaccurate results.