

Second Order Derivatives Approximation

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Introduction

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

A second order 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.

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

Section 1: Input

The following simulation approximates the second derivative of a function using Second Order Derivatives 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 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, number of at least correct significant digits in the solution as a function of step size.

Function $f(x)$:

```
In[1559]:= f[x_] := Exp[2 * x];
```

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

```
In[1560]:= xv = 4.0;
```

Starting step size, h

```
In[1561]:= h = 0.2;
```

Number of times step size is halved

```
In[1562]:= n = 12.0;
```

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 order derivate of an equation at a point xv .

$f(x)$ = function

xv = value at which the solution is desired

h = step size value

n = number of times step size is halved

```
In[1632]:= SOD[f_, xv_, h_] := Module[{deriv},
  deriv = (f[xv + h] - 2 * f[xv] + f[xv - h]) / (h ^ 2);
  deriv]
```

Section 3: Calculation

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

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

```
In[1563]:= f[x_]
```

```
Out[1563]= e2 x
```

```
In[1566]:= f''[x_]
```

```
Out[1566]= 4 e2 x
```

```
In[1568]:= Ev = N[f''[xv]]
```

```
Out[1568]= 11.923.8
```

The next loop calculates the following:

Av: Approximate value of the second derivative using Second Order Derivatives Approximation by calling the procedure "SOD"

Ev: Exact value of the second derivative

Et: True Error

et: Absolute relative true percentage error

Ea: Approximate Error

ea: Absolute relative approximate percentage error

Sig: Least number of correct significant digits in an approximation

```
In[1633]:= Do[
  Nn[i] = 2 ^ i;
  H[i] = h / Nn[i];
  AV[i] = SOD[f, xv, H[i]];
  Et[i] = Ev - AV[i];
  et[i] = Abs[(Et[i] / Ev)] * 100.0;
  If[i > 0,
    Ea[i] = AV[i] - AV[i - 1];
    ea[i] = Abs[Ea[i] / AV[i]] * 100.0;
    Sig[i] = Floor[(2 - Log[10, ea[i] / 0.5])];
    If[Sig[i] < 0, Sig[i] = 0];
  ]
, {i, 0, n - 1, 1}]
```

The loop halves the value of the 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 second 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 is shown as zero.

Section 4: Spreadsheet

The next table shows 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.

```
In[1640]:= Print[" ", "h", " ", "Av", " ", "Et", " ",
  "et", " ", "Ea", " ", "ea", " ", "Sig"];
Print[" "]
Grid[Table[{H[i], AV[i], Et[i], et[i], Ea[i], ea[i], Sig[i]}, {i, 0, n - 1}]]
```

	h	Av	Et	Ea	ea	Sig	
	0.2	12083.7	-159.835	1.34046	Ea[0]	ea[0]	Sig[0]
	0.1	11963.6	-39.7991	0.333778	-120.036	1.00334	1
	0.05	11933.8	-9.93984	0.0833611	-29.8593	0.250208	2
	0.025	11926.3	-2.48434	0.0208351	-7.4555	0.062513	2
	0.0125	11924.5	-0.621046	0.00520844	-1.86329	0.0156258	3
	0.00625	11924.	-0.155259	0.00130209	-0.465787	0.0039063	4
	0.003125	11923.9	-0.0388146	0.000325521	-0.116444	0.000976565	4
	0.0015625	11923.8	-0.009704	0.00008138	-0.0291099	0.000244132	5
			67	88			
Out[1642]=	0.00078125	11923.8	-0.002425	0.00002034	-0.007279	0.00006104	5
			64	27	03	61	
	0.000390625	11923.8	-0.000587	4.92775 × 10 ⁻⁶	-0.001838	0.000015415	6
			577		06		
	0.000195313	11923.8	-0.000146	1.22865 × 10 ⁻⁶	-0.000441	3.6991 × 10 ⁻⁶	7
			502		074		
	0.00009765	11923.8	-0.000325	2.72829 × 10 ⁻⁶	0.000178814	1.49963 × 10 ⁻⁶	7
			63	316			

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.

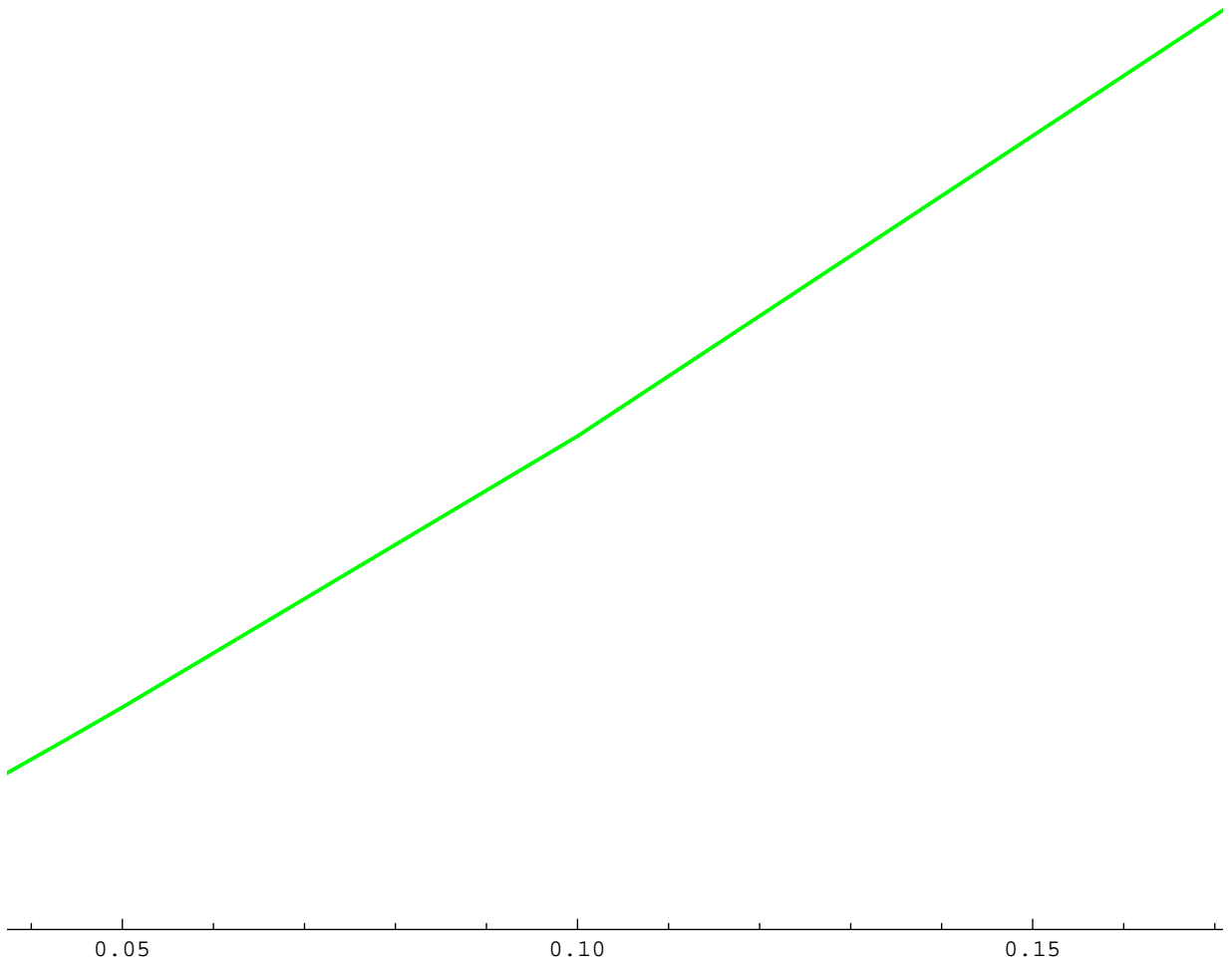
```

In[1691]:= data = Table[{H[i], AV[i]}, {i, 0, n - 1}];
plot = ListPlot[data,
  PlotJoined → True,
  PlotStyle → {Thickness[0.002], RGBColor[0, 1, 0]},
  DisplayFunction → Identity,
  PlotRange → Full];
Show[plot,
  PlotLabel → "Approximate Solution of the Second Derivative of a Function
    using\nSecond Order Derivatives
    Approximation as a Function of Step Size",
  AxesLabel → {"Step Size", "Approximate Value"}]
data = Table[{H[i], et[i]}, {i, 0, n - 1}];
plot = ListPlot[data,
  PlotJoined → True,
  PlotStyle → {Thickness[0.002], RGBColor[0, 1, 0]},
  DisplayFunction → Identity,
  PlotRange → Full];
Show[plot, PlotLabel →
  "Absolute Relative True Percentage\nError as a Function of Step Size",
  AxesLabel → {"Step Size", "Absolute Relative
  True Error"}]
data = Table[{H[i], ea[i]}, {i, 0, n - 1}];
plot = ListPlot[data,
  PlotJoined → True,
  PlotStyle → {Thickness[0.002], RGBColor[0, 1, 0]},
  DisplayFunction → Identity,
  PlotRange → Full];
Show[plot,
  PlotLabel → "Absolute Relative Approximate Percentage\n Error as a
    Function of Step Size", AxesLabel → {"Step Size", "Absolute Relative
  Approximate Error"}]
sigdigplot = Table[{H[i], Sig[i]}, {i, 0, n - 1}];
BarChart[sigdigplot, BarStyle → Green,
  PlotLabel → "Least Significant Digits Correct\nas a Function of Step Size"]

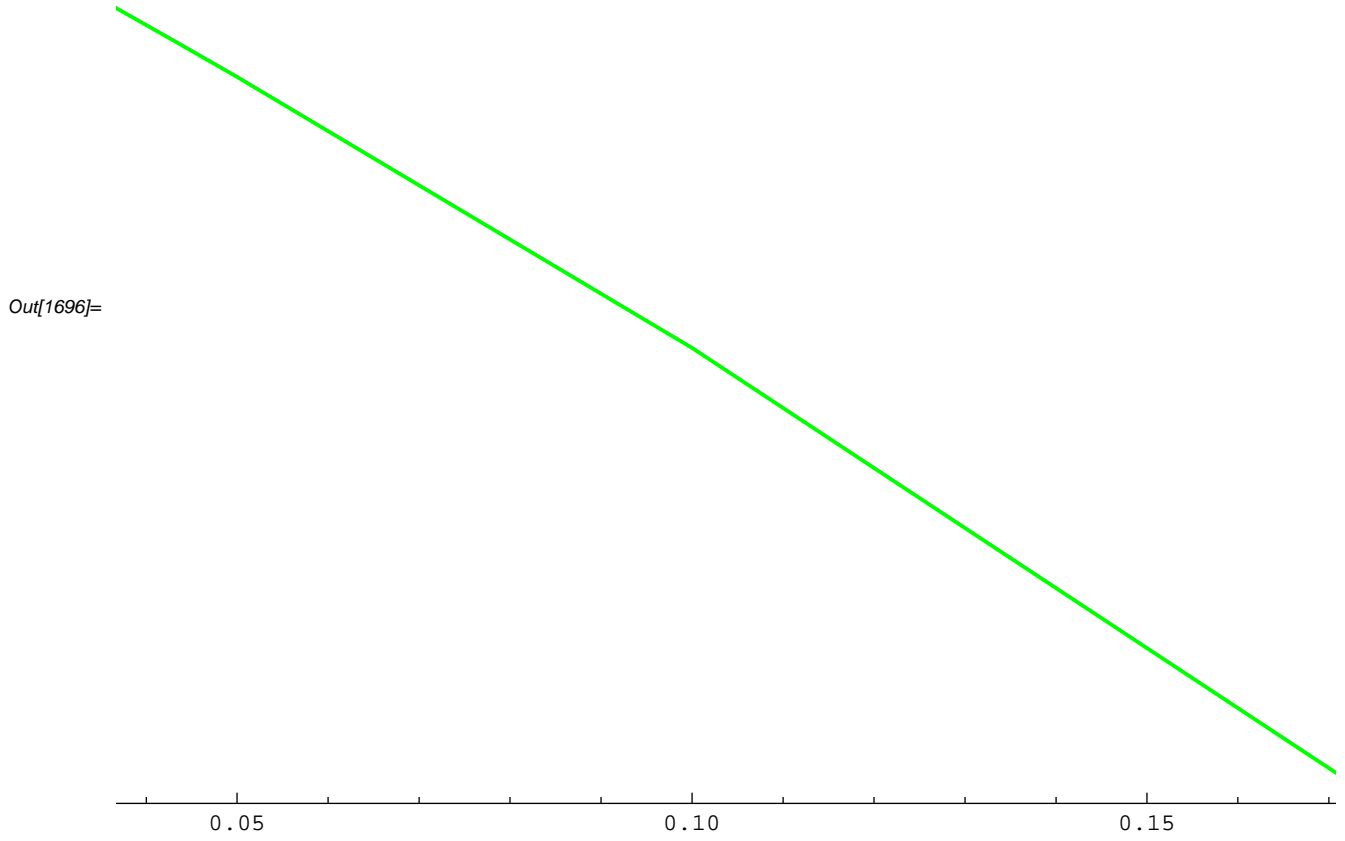
```

Approximate Solution of the Second Derivative of a Function using
Second Order Derivatives Approximation as a Function of Step Size

Out[1693]=

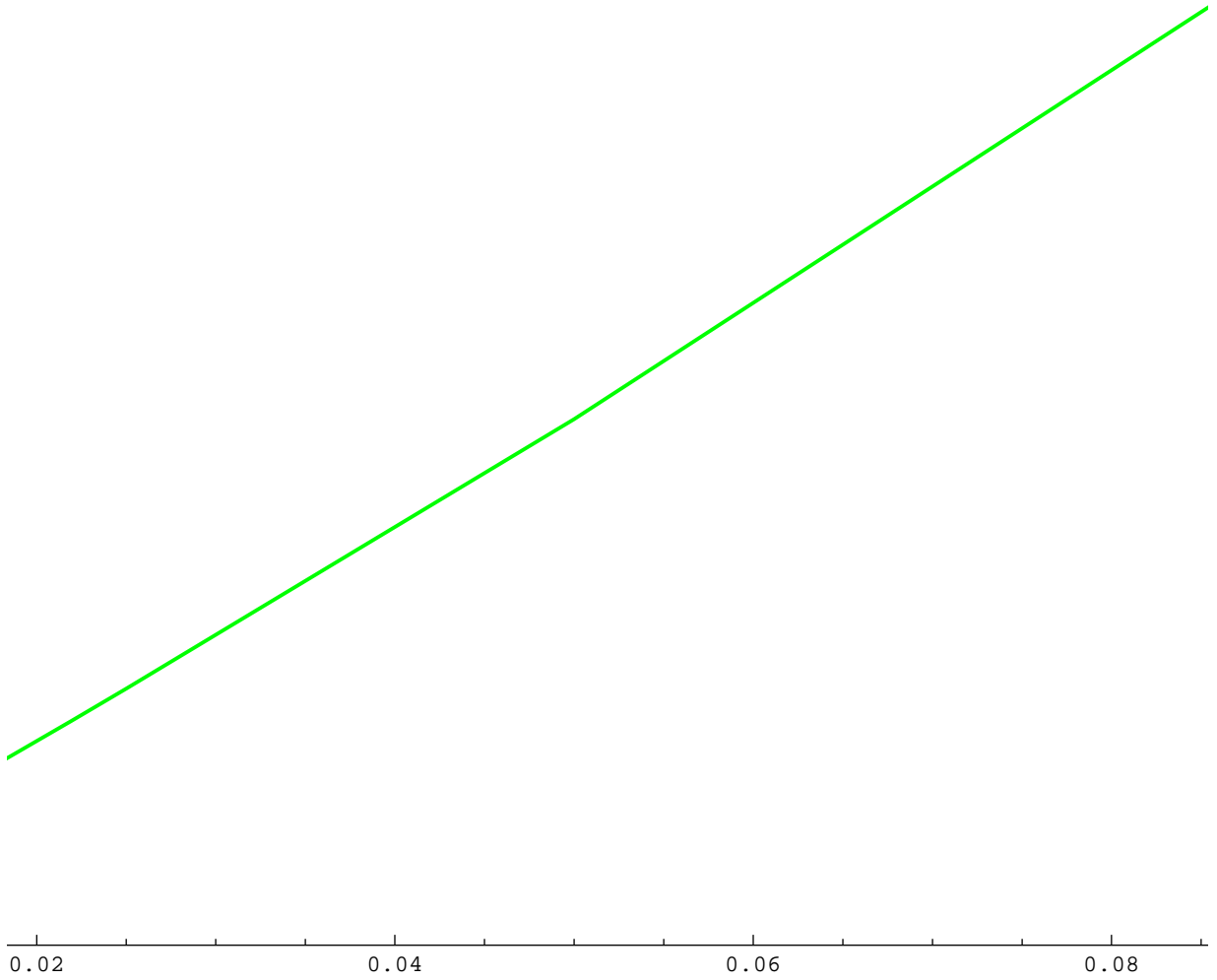


Absolute Relative True Percentage
Error as a Function of Step Size

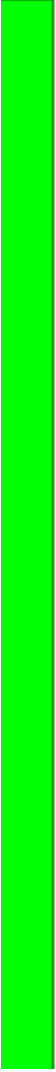


Absolute Relative Approximate Percentage
Error as a Function of Step Size

Out[1699]=



Lea

Out[1701]=


References

Numerical Differentiation of Continuous Functions.

See <http://numericalmethods.eng.usf.edu/mws/gen/0.2def/>

Questions

1. The velocity of a rocket is given by

$$v(t) = 2000 \ln \frac{140\,000}{140\,000 - 2100t} - 9.8t$$

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 coincidental?

Conclusions

To obtain more accurate values of the second derivative using Second Order Derivative Approximation, the step size needs to be small. 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.

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