2. Numerical Differentiation, Part II

Richardson's Extrapolation

Background.

Numerical differentiation formulas can be derived by first constructing the Lagrange interpolating polynomial $P_3(x)$ through three points, differentiating the Lagrange polynomial, and finally evaluating $P_3'(x)$ at the desired point. The truncation error is be investigated, but round off error from computer arithmetic using computer numbers will be studied in another lab.

Theorem (Three point rule for $f'[x]$). The central difference formula for the first derivative, based on three points is

$$f'[x] \approx D_{three}[x, h] = \frac{f[x+h] - f[x-h]}{2h},$$

and the remainder term is

$$R_{three}[x, h] = \frac{-f^{(3)}[c]}{6} h^2.$$

Together they make the equation $f'[x] = D_{three}[x, h] + R_{three}[x, h]$, and the truncation error bound is

$$EB_{three}[h] = \left| \frac{-f^{(3)}[c]}{6} h^2 \right| \leq \frac{M_3}{6} h^2$$

where $M_3 = \max_{a \leq x \leq b} |f^{(3)}[x]|$. This gives rise to the Big "O" notation for the error term for $f'[x]$:

$$f'[x] = \frac{f[x+h] - f[x-h]}{2h} + O(h^2).$$

Theorem (Five point rule for $f'[x]$). The central difference formula for the first derivative, based on five points is

$$f'[x] \approx D_{five}[x, h] = \frac{f[x-2h] - 8f[x-h] + 8f[x+h] - f[x+2h]}{12h},$$

and the remainder term is

$$R_{five}[x, h] = \frac{f^{(5)}[c]}{30} h^4.$$

Together they make the equation $f'[x] = D_{five}[x, h] + R_{five}[x, h]$, and the truncation error bound is

$$EB_{five}[h] = \left| \frac{f^{(5)}[c]}{30} h^4 \right| \leq \frac{M_5}{30} h^4$$

where $M_5 = max_{a \leq x \leq b} \; | f^{(5)}[x] |$. This gives rise to the Big "O" notation for the error term for $f'[x]$:

$$f'[x] = \frac{f[x-2h] - 8 f[x-h] + 8 f[x+h] - f[x+2h]}{12 h} + O(h^4).$$

Theorem (Richardson's Extrapolation for $f'[x]$). The central difference formula for the first derivative, based on five points is a linear combination of $D_{three}[x, y]$ and $D_{three}[x, 2h]$.

$$f'[x] \approx D_{five}[x, h] = \frac{4 D_{three}[x, y] - D_{three}[x, 2h]}{3},$$

where $D_{three}[x, h] = \dfrac{f[x+h] - f[x-h]}{2h}$ and $D_{three}[x, 2h] = \dfrac{f[x+2h] - f[x-2h]}{4h}$.

Example 1. Consider the function $f[x] = e^{-x} Sin[x]$. Find the formula for the third derivative $f^{(5)}[x]$, it will be used in our explorations for the remainder term and the truncation error bound. Graph $f^{(5)}[x]$. Find the bound $M_5 = max_{0 \leq x \leq \pi} \; | f^{(5)}[x] |$. Look at it's graph and estimate the value M_5, be sure to take the absolute value if necessary.
Solution 1.

Example 2. Consider the function $f[x] = e^{-x} Sin[x]$. Find the approximations $D_{three}[1.0, 0.02]$, $D_{three}[1.0, 0.01]$ and then use the extrapolation formula $\dfrac{4 D_{three}[1.0, 0.01] - D_{three}[1.0, 0.02]}{3}$.
Compute $D_{five}[1.0, 0.01]$ directly. Finally, compare these numerical approximations for the derivative with $f'[1.0]$.
Solution 2.

Various Scenarios fffor Richardson's Extrapolation and higher derivatives.

Example 3. Given $f[x] = e^{-x} Sin[x]$, find numerical approximations to the derivative $f'[1.0]$, using five points and the central difference formula.
Solution 3.

Example 4. Given $f[x] = e^{-x} Sin[x]$, find numerical approximations to the derivative $f''[1.0]$, using five points and the central difference formula.

Solution 4.

Example 5. Given $f[x] = e^{-x} \mathrm{Sin}[x]$, find numerical approximations to the derivative $f'''[1.0]$, using five points and the central difference formula.

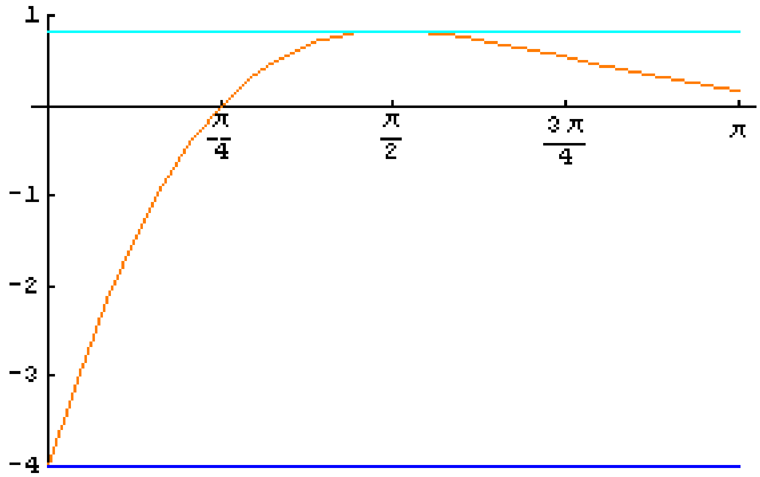
Solution 5.

Example 1. Consider the function $f[x] = e^{-x}\,\mathrm{Sin}[x]$. Find the formula for the third derivative $f^{(5)}[x]$, it will be used in our explorations for the remainder term and the truncation error bound. Graph $f^{(5)}[x]$. Find the bound $M_5 = \max_{0\le x\le\pi} |f^{(5)}[x]|$. Look at it's graph and estimate the value M_5, be sure to take the absolute value if necessary.

Solution 1.

$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f^{(3)}[x] = 2\,e^{-x}\,\mathrm{Cos}[x] + 2\,e^{-x}\,\mathrm{Sin}[x]$$
$$f^{(4)}[x] = -4\,e^{-x}\,\mathrm{Sin}[x]$$

$$f^{(5)}[x] = -4\,e^{-x}\,\mathrm{Cos}[x] + 4\,e^{-x}\,\mathrm{Sin}[x]$$



$y = f^{(5)}[x] = -4\,e^{-x}\,\mathrm{Cos}[x] + 4\,e^{-x}\,\mathrm{Sin}[x]$

The minimum occurs at $x = 0$, and the maximum occurs at $x = \frac{\pi}{2}$.

Extrema of $f^{(5)}[x]$: $\{-4,\ 4\,e^{-\pi/2}\}$

$$|f^{(5)}[c]| \le 4$$

The absolute value of the remainder term:

$$|R[x,h]| = \left|\frac{f^{(5)}[c]}{30}h^4\right| \le \frac{2\,h^4}{15}$$

The error bound is:

$$EB_{five}[h] \le \frac{2\,h^4}{15}$$

Example 2. Consider the function $f[x] = e^{-x} \text{Sin}[x]$. Find the approximations $D_{three}[1.0, 0.02]$, $D_{three}[1.0, 0.01]$ and then use the extrapolation formula $\frac{4 D_{three}[1.0, 0.01] - D_{three}[1.0, 0.02]}{3}$.
Compute $D_{five}[1.0, 0.01]$ directly. Finally, compare these numerical approximations for the derivative with $f'[1.0]$.

Solution 2.

$$f[x] = e^{-x} \text{Sin}[x]$$

$$D_{three}[1.0, 0.02] = -0.110726$$
$$D_{three}[1.0, 0.01] = -0.110777$$

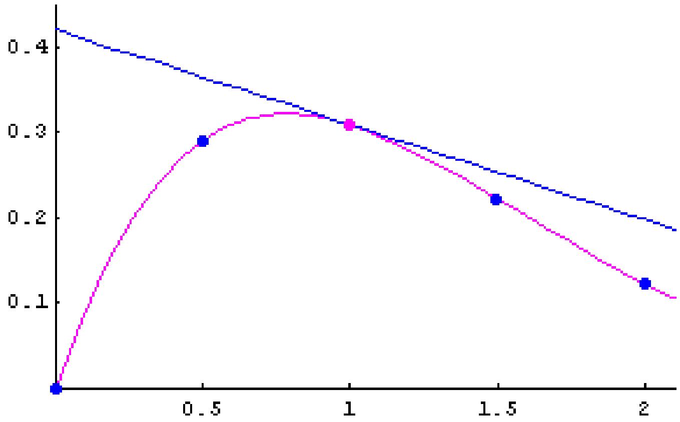
$$\frac{4 D_{three}[1.0, 0.01] - D_{three}[1.0, 0.02]}{3} = (4(-0.110777) - (-0.110726))/3$$
$$\frac{4 D_{three}[1.0, 0.01] - D_{three}[1.0, 0.02]}{3} = ((-0.443107) - (-0.110726))/3$$
$$\frac{4 D_{three}[1.0, 0.01] - D_{three}[1.0, 0.02]}{3} = (-0.332381)/3$$
$$\frac{4 D_{three}[1.0, 0.01] - D_{three}[1.0, 0.02]}{3} = -0.110794$$

$$D_{five}[1.0, 0.01] = -0.110794$$

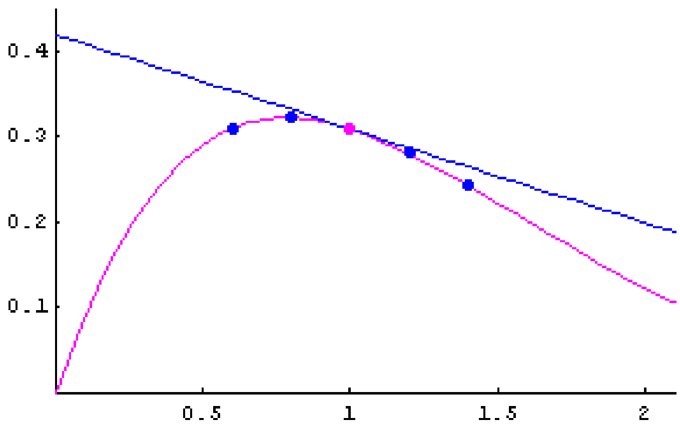
$$f'[1.0] = -0.110794$$

Example 3. Given $f[x] = e^{-x} \text{Sin}[x]$, find numerical approximations to the derivative $f'[1.0]$, using five points and the central difference formula.

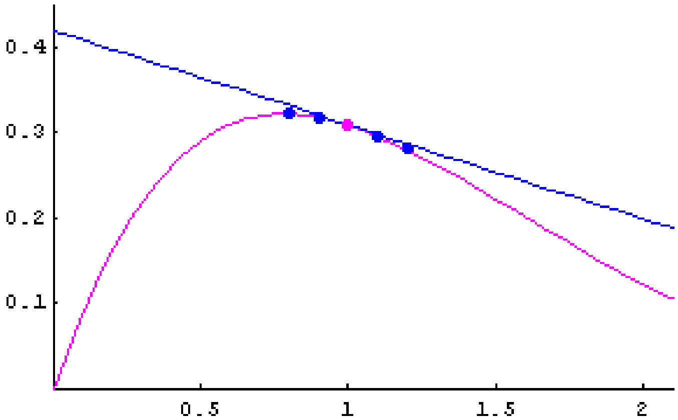
Solution 3.



$$f[x] = e^{-x} \text{Sin}[x]$$
$$f'[x] = e^{-x} \text{Cos}[x] - e^{-x} \text{Sin}[x]$$
$$f'[1.] = -0.110793765$$
$$h = 0.5$$
$$f'[1.] \approx (f[1.-1.] - 8f[1.-0.5] + 8f[1.+0.5] - f[1.+1.])/(6.) = -0.111463434$$



$$f[x] = e^{-x} \text{Sin}[x]$$
$$f'[x] = e^{-x} \text{Cos}[x] - e^{-x} \text{Sin}[x]$$
$$f'[1.] = -0.110793765$$
$$h = 0.2$$
$$f'[1.] \approx (f[1.-0.4] - 8f[1.-0.2] + 8f[1.+0.2] - f[1.+0.4])/(2.4) = -0.110816367$$



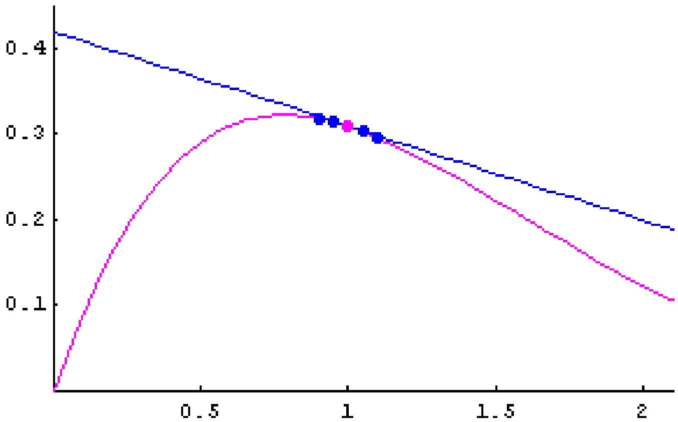
$$f[x] = e^{-x} \mathrm{Sin}[x]$$

$$f'[x] = e^{-x} \mathrm{Cos}[x] - e^{-x} \mathrm{Sin}[x]$$

$$f'[1.] = -0.110793765$$

$$h = 0.1$$

$$f'[1.] \approx (f[1.-0.2] - 8f[1.-0.1] + 8f[1.+0.1] - f[1.+0.2])/(1.2) = -0.110795226$$



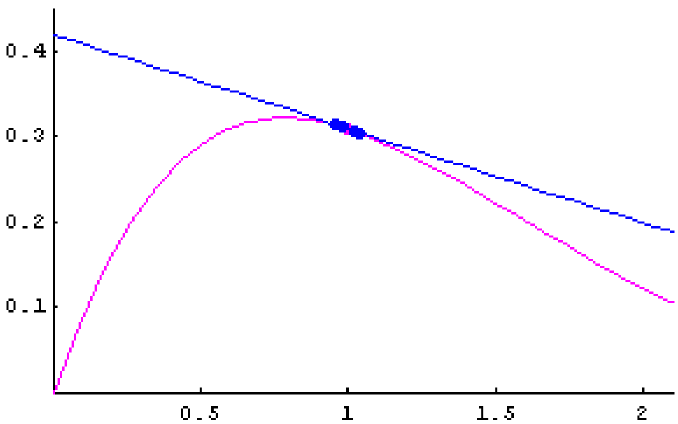
$$f[x] = e^{-x} \mathrm{Sin}[x]$$

$$f'[x] = e^{-x} \mathrm{Cos}[x] - e^{-x} \mathrm{Sin}[x]$$

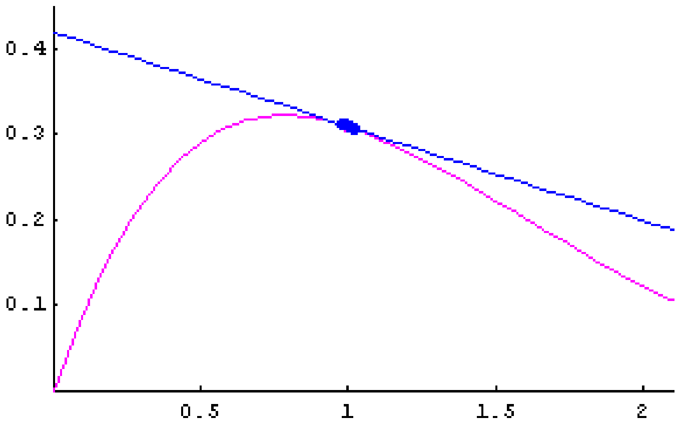
$$f'[1.] = -0.110793765$$

$$h = 0.05$$

$$f'[1.] \approx (f[1.-0.1] - 8f[1.-0.05] + 8f[1.+0.05] - f[1.+0.1])/(0.6) = -0.110793857$$



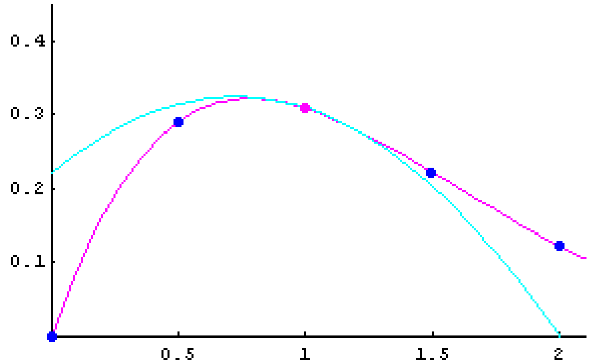
$$f[x] = e^{-x} \mathrm{Sin}[x]$$
$$f'[x] = e^{-x} \mathrm{Cos}[x] - e^{-x} \mathrm{Sin}[x]$$
$$f'[1.] = -0.110793765$$
$$h = 0.02$$
$$f'[1.] \approx (f[1.-0.04] - 8f[1.-0.02] + 8f[1.+0.02] - f[1.+0.04])/(0.24) = -0.110793768$$



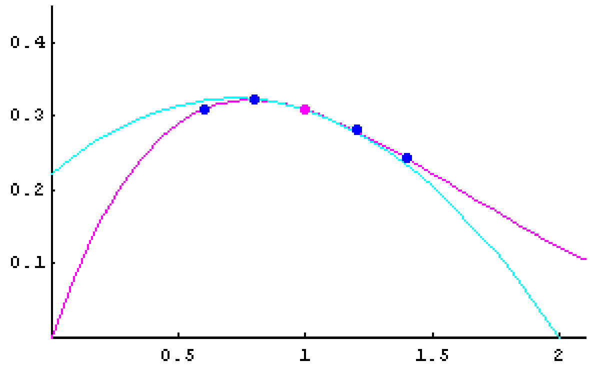
$$f[x] = e^{-x} \mathrm{Sin}[x]$$
$$f'[x] = e^{-x} \mathrm{Cos}[x] - e^{-x} \mathrm{Sin}[x]$$
$$f'[1.] = -0.110793765$$
$$h = 0.01$$
$$f'[1.] \approx (f[1.-0.02] - 8f[1.-0.01] + 8f[1.+0.01] - f[1.+0.02])/(0.12) = -0.110793765$$

Example 4. Given $f[x] = e^{-x} \mathrm{Sin}[x]$, find numerical approximations to the derivative $f''[1.0]$, using five points and the central difference formula.

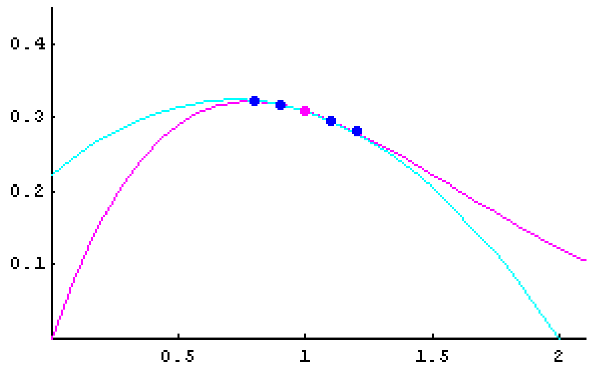
Solution 4.



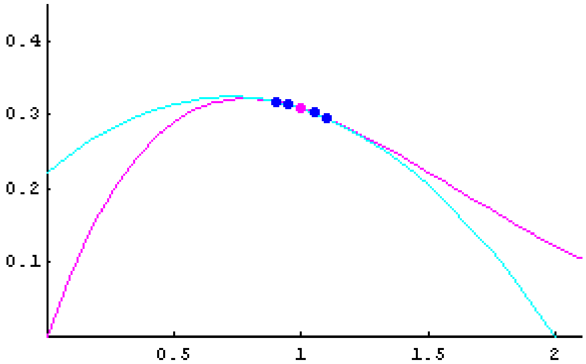
$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f''[1.] = -0.397532221$$
$$h = 0.5$$
$$f''[1.] \approx (-f[1.-1.] + 16f[1.-0.5] - 30f[1.] + 16f[1.+0.5] - f[1.+1.])/(3.) = -0.398712075$$



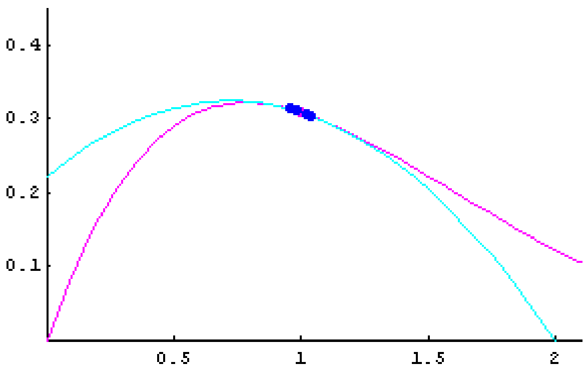
$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f''[1.] = -0.397532221$$
$$h = 0.2$$
$$f''[1.] \approx (-f[1.-0.4] + 16f[1.-0.2] - 30f[1.] + 16f[1.+0.2] - f[1.+0.4])/(0.48) = -0.397560803$$



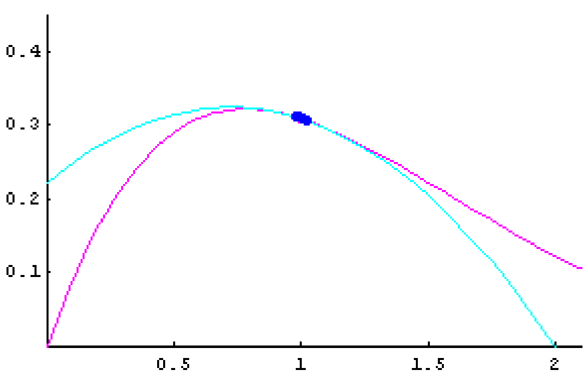
$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f''[1.] = -0.397532221$$
$$h = 0.1$$
$$f''[1.] \approx (-f[1.-0.2] + 16f[1.-0.1] - 30f[1.] + 16f[1.+0.1] - f[1.+0.2])/(0.12) = -0.397533992$$



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f''[1.] = -0.397532221$$
$$h = 0.05$$
$$f''[1.] \approx (-f[1.-0.1] + 16f[1.-0.05] - 30f[1.] + 16f[1.+0.05] - f[1.+0.1])/(0.03) = -0.397532331$$



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f''[1.] = -0.397532221$$
$$h = 0.02$$
$$f''[1.] \approx (-f[1.-0.04] + 16f[1.-0.02] - 30f[1.] + 16f[1.+0.02] - f[1.+0.04])/(0.0048) = -0.397532224$$



$$f[x] = e^{-x}\,\text{Sin}[x]$$

$$f'[x] = e^{-x}\,\text{Cos}[x] - e^{-x}\,\text{Sin}[x]$$

$$f''[x] = -2\,e^{-x}\,\text{Cos}[x]$$

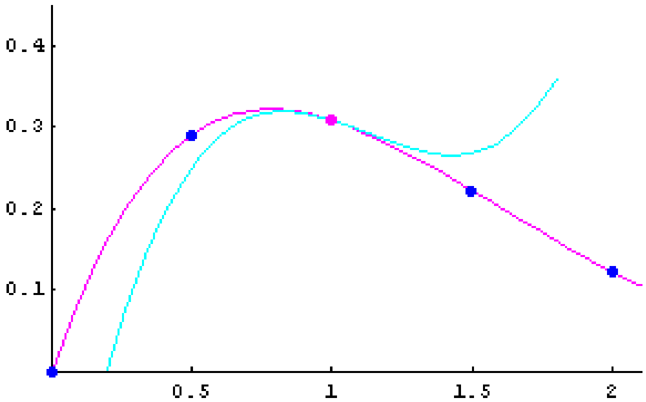
$$f''[1.] = -0.397532221$$

$$h = 0.01$$

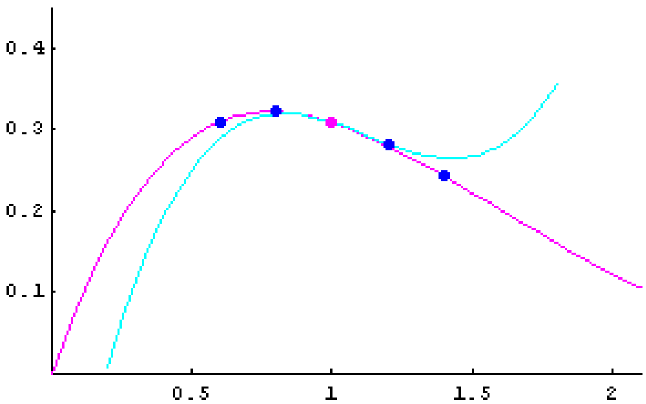
$$f''[1.] \approx (-f[1.-0.02] + 16f[1.-0.01] - 30f[1.] + 16f[1.+0.01] - f[1.+0.02])/(0.0012) = -0.397532221$$

Example 5. Given $f[x] = e^{-x} \mathrm{Sin}[x]$, find numerical approximations to the derivative $f'''[1.0]$, using five points and the central difference formula.

Solution 5.



$$f[x] = e^{-x} \mathrm{Sin}[x]$$
$$f'[x] = e^{-x} \mathrm{Cos}[x] - e^{-x} \mathrm{Sin}[x]$$
$$f''[x] = -2 e^{-x} \mathrm{Cos}[x]$$
$$f'''[x] = 2 e^{-x} \mathrm{Cos}[x] + 2 e^{-x} \mathrm{Sin}[x]$$
$$f'''[1.] = 1.01665197$$
$$h = 0.5$$
$$f'''[1.] \approx (-f[1.-1.] + 2f[1.-0.5] - 2f[1.+0.5] + f[1.+1.])/(0.25) = 1.03796068$$



$$f[x] = e^{-x} \mathrm{Sin}[x]$$
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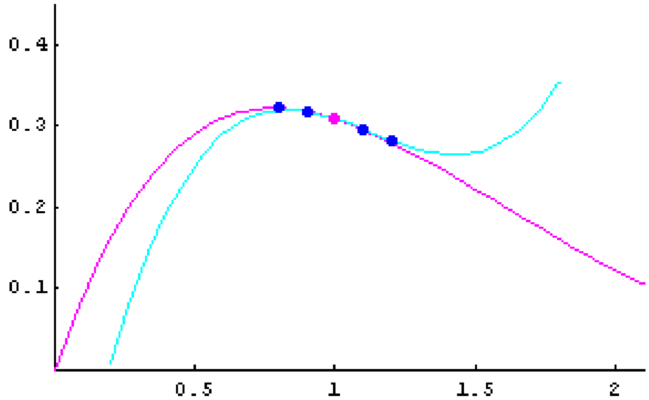
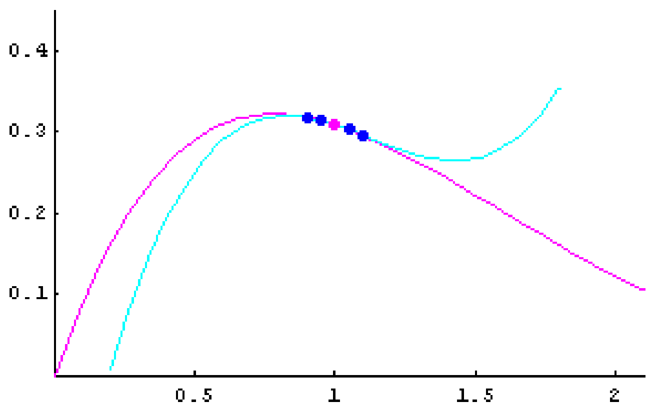
$$f''[x] = -2 e^{-x} \mathrm{Cos}[x]$$
$$f'''[x] = 2 e^{-x} \mathrm{Cos}[x] + 2 e^{-x} \mathrm{Sin}[x]$$
$$f'''[1.] = 1.01665197$$
$$h = 0.2$$
$$f'''[1.] \approx (-f[1.-0.4] + 2f[1.-0.2] - 2f[1.+0.2] + f[1.+0.4])/(0.016) = 1.0209209$$



$$f[x] = e^{-x}\,Sin[x]$$
$$f'[x] = e^{-x}\,Cos[x] - e^{-x}\,Sin[x]$$
$$f''[x] = -2\,e^{-x}\,Cos[x]$$
$$f'''[x] = 2\,e^{-x}\,Cos[x] + 2\,e^{-x}\,Sin[x]$$
$$f'''[1.] = 1.01665197$$
$$h = 0.1$$
$$f'''[1.] \approx (-f[1.-0.2] + 2f[1.-0.1] - 2f[1.+0.1] + f[1.+0.2])/(0.002) = 1.01774974$$



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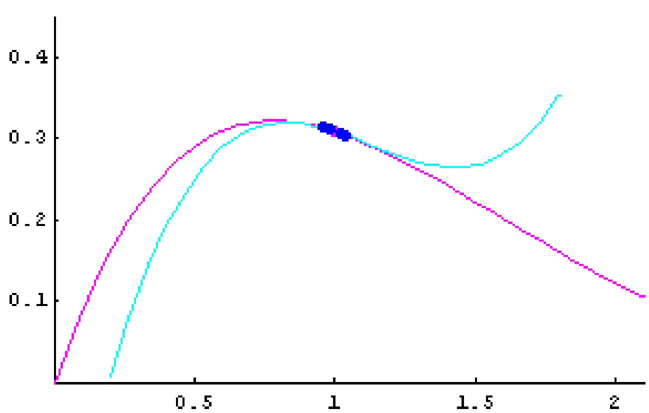
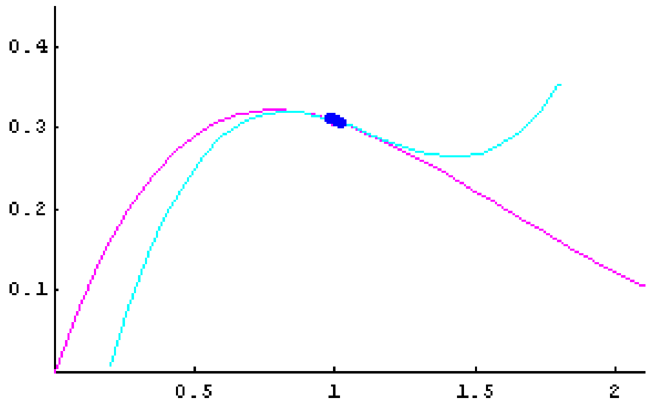
$$f''[x] = -2\,e^{-x}\,Cos[x]$$
$$f'''[x] = 2\,e^{-x}\,Cos[x] + 2\,e^{-x}\,Sin[x]$$
$$f'''[1.] = 1.01665197$$
$$h = 0.05$$
$$f'''[1.] \approx (-f[1.-0.1] + 2f[1.-0.05] - 2f[1.+0.05] + f[1.+0.1])/(0.00025) = 1.01692832$$



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f'''[x] = 2\,e^{-x}\,\mathrm{Cos}[x] + 2\,e^{-x}\,\mathrm{Sin}[x]$$
$$f'''[1.] = 1.01665197$$
$$h = 0.02$$
$$f'''[1.] \approx (-f[1.-0.04] + 2f[1.-0.02] - 2f[1.+0.02] + f[1.+0.04])/(0.000016) = 1.01669627$$



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\mathrm{Cos}[x]$$
$$f'''[x] = 2\,e^{-x}\,\mathrm{Cos}[x] + 2\,e^{-x}\,\mathrm{Sin}[x]$$
$$f'''[1.] = 1.01665197$$
$$h = 0.01$$
$$f'''[1.] \approx (-f[1.-0.02] + 2f[1.-0.01] - 2f[1.+0.01] + f[1.+0.02])/(2.\times 10^{-6}) = 1.01666305$$