CENG 216 – Numerical Computation

Numerical Differentiation and Integration

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Slide Credits

Slides are based on material from the main textbook:

"Numerical Analysis", The new international edition, 2ed, by Timothy Sauer

Numerical Differentiation

The Need to Compute Numerical Derivatives

- When solving problems with methods that require derivatives such as Newton's Method, an explicit analytical formula for $f'(x)$ may not be always available.

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- For some complex functions, analytical derivatives are not available or difficult to compute.
- Numerical derivatives are easy to compute, so we can check analytical derivatives by comparing their results to numerical ones.

Def: Forward Difference Formula

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$$\begin{aligned} f'(x) &= \frac{f(x+0.1) - f(x)}{0.1} \\ f'(2) &= \frac{\frac{1}{2.1} - \frac{1}{2}}{0.1} \\ &\approx -0.2381 \quad \text{(Forward difference result)} \end{aligned}$$

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\begin{aligned}
f'(x) = -x^{-2} \rightarrow f'(2) = -0.25 \quad \text{(Analytical formula)} \\
\|-0.2381 - (-0.25)\| = 0.0119 \quad \text{(Forward error)}
\end{aligned}
$$

Backward and Centered Differences

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(c) \text{ (Forward difference)}$$

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$$\approx \frac{f(x+h) - f(x-h)}{2h}, \quad \text{(Centered difference formula)}$$

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$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x-h)}{2h} \\ f'(2) &= \frac{\frac{1}{2.1} - \frac{1}{1.9}}{0.2} \\ &\approx -0.2506 \end{aligned}$$

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$$\approx -0.2506$$
$$\|-0.2506 - (-0.25)\| = 0.0006 \quad \text{(Centered difference error)}$$

Second Derivative Formulas

$$\begin{aligned} f''(x) &= \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} \underbrace{- \frac{h^2}{12} f^{(\text{iv})}(c)}_{\mathcal{O}(h^2)} \\ &\approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} \end{aligned}$$

Rounding Errors in Finite Differences

Ex: Approximate the derivative of $f(x) = e^x$ at $x = 0$.

$$f'(x) \approx \frac{e^{x+h} - e^x}{h}, \quad (\star)$$

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h	$\star$	Error in $\star$	$\star\star$	Error in $\star\star$
10^{-5}	1.00000500000696	−0.00000500000696	1.00000000001210	−0.00000000001210
10^{-6}	1.00000049996218	−0.00000049996218	0.99999999997324	0.00000000002676
10^{-7}	1.00000004943368	−0.00000004943368	0.99999999947364	0.00000000052636
10^{-8}	0.99999999392253	0.00000000607747	0.99999999392253	0.00000000607747
10^{-9}	1.00000008274037	−0.00000008274037	1.00000002722922	−0.00000002722922
10^{-10}	1.00000008274037	−0.00000008274037	1.00000008274037	−0.00000008274037
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Error drops as h gets smaller but then it starts to increase. Why?

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$$\left.\begin{aligned}\hat{f}(x+h) &= f(x+h) + \epsilon_1 \\ \hat{f}(x-h) &= f(x-h) + \epsilon_2\end{aligned}\right\} |\epsilon_1|, |\epsilon_2| \approx \epsilon_{\text{mach}}, \text{ rounding errors}$$

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$$f'_{\text{correct}}(x) - f'_{\text{machine}}(x) = f'(x) - \frac{\hat{f}(x+h) - \hat{f}(x-h)}{2h}$$

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As h gets smaller, error in the finite difference formulas becomes smaller, but the rounding error grows. There is an optimal h where the sum of the two error is at a minimum.

Numerical Integration

- Given a complex function $f(x)$, sample the function at n points: $(x_1, y_1), \ldots, (x_n, y_n)$.

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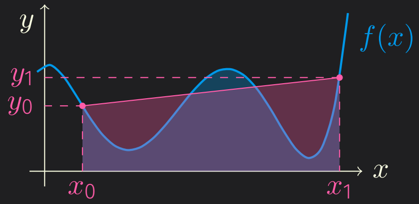
- Approximate the true integral $\int_a^b f(x)\,dx$ by $\int_a^b P(x)\,dx$.
- Compute $\int_a^b P(x)\,dx$ by the true analytical expression since it is easy to integrate polynomials.

Trapezoid Rule ($n = 2$)



$$f(x) \approx y_0 \frac{x - x_1}{x_0 - x_1} + y_1 \frac{x - x_0}{x_1 - x_0}$$

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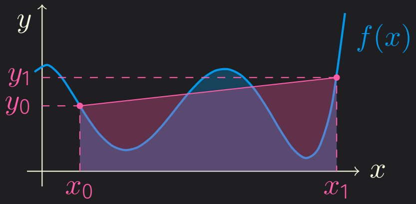

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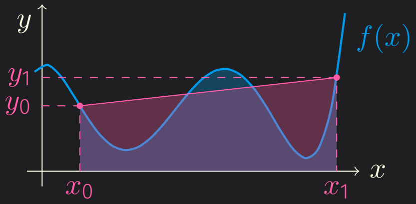

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&\approx y_0 \int_0^{x_1 - x_0} \frac{u + x_0 - x_1}{x_0 - x_1}\,du + y_1 \int_{x_0 - x_1}^{0} \frac{v + x_1 - x_0}{x_1 - x_0}\,dv \qquad \begin{pmatrix} u = x - x_0, \\ v = x - x_1 \end{pmatrix}
\end{aligned}$$

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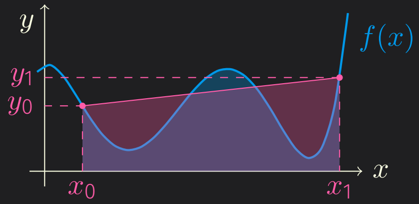

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&\approx y_0 \int_{0}^{h} \frac{u - h}{-h}\,du + y_1 \int_{-h}^{0} \frac{v + h}{h}\,dv \quad (h = x_1 - x_0)
\end{aligned}$$

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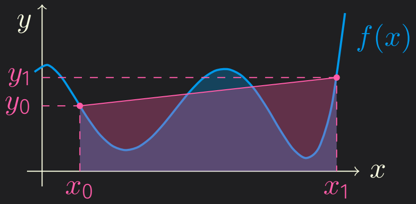

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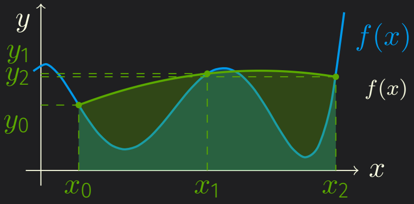
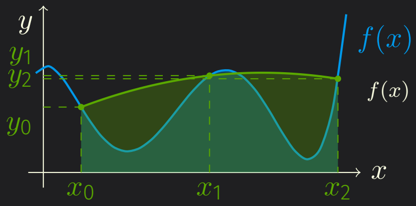
&\approx -y_0 \left. \frac{\frac{u^2}{2} - hu}{h} \right|_0^h + y_1 \left. \frac{\frac{v^2}{2} + hv}{h} \right|_{-h}^0 = y_0 \frac{h}{2} + y_1 \frac{h}{2} = h \frac{(y_0 + y_1)}{2}.
\end{aligned}$$



$$f(x) \approx y_0 \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} + y_1 \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} + y_2 \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$



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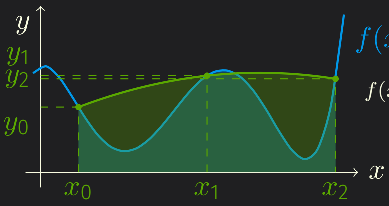
Simpson's Rule ($n = 3$)



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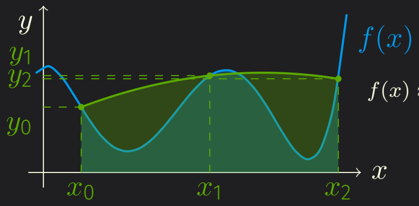

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&\quad + y_2 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}\,dx \\
&= y_0 \frac{h}{3} + y_1 \frac{4h}{3} + y_2 \frac{h}{3} \qquad (h = x_2 - x_1 = x_1 - x_0) \\
&= \frac{h}{3}(y_0 + 4y_1 + y_2).
\end{aligned}$$

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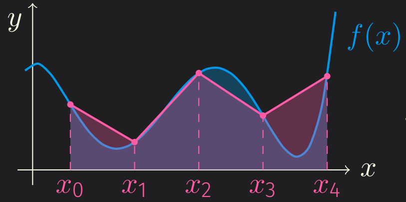
Composite Trapezoid Rule



$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{m-1} f(x_i)\right],$$

$$m = 4, a = x_0, b = x_4, h = \frac{b-a}{m}.$$

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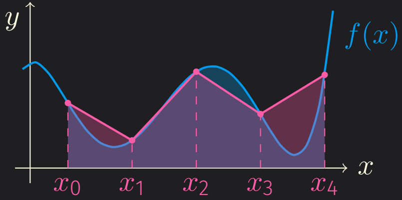

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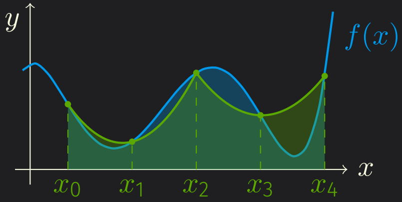
Composite Simpson's Rule



$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(a)+f(b)+4\sum_{i=1}^{m} f(x_{2i-1}) + 2\sum_{i=1}^{m-1} f(x_{2i})\right],$$

$$m=2, a=x_0, b=x_4, h=\frac{b-a}{2m}.$$