CS412: Lecture #22

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Simpson's rule

This is a slightly more complicated algorithm, but the accuracy gains are so attractive that it has become somewhat of a golden standard for numerical integration. It is based on (piecewise) *quadratic* interpolation. Specifically, consider three equally spaced x-values:

$$x_1, x_2 = x_1 + h, x_3 = x_1 + 2h$$

with associated y-values, $y_i = f(x_i)$, $i = 1, 2, 3$. We will approximate $f(x)$ in $[x_1, x_3]$ with a *quadratic* $p(x) = c_2x^2 + c_1x + c_0$ that interpolates the three data points (x_1, y_1), (x_2, y_2), (x_3, y_3). Using Lagrange interpolation:

$$\begin{aligned}
l_1(x) &= \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} = \frac{(x-x_2)(x-x_3)}{(-h)(-2h)} = \frac{1}{2h^2}(x-x_2)(x-x_3) \\
l_2(x) &= \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} = -\frac{1}{h^2}(x-x_1)(x-x_3) \\
l_3(x) &= \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} = \frac{1}{2h^2}(x-x_1)(x-x_2)
\end{aligned}$$

and $p(x) = y_1l_1(x) + y_2l_2(x) + y_3l_3(x)$. We then proceed to approximate

$$\underbrace{\int_{x_1}^{x_3} f(x)dx}_{I} \approx \underbrace{\int_{x_1}^{x_3} p(x)dx}_{I_{\mathsf{simp}}} = \sum_{i=1}^{3} y_l \int_{x_1}^{x_3} l_i(x)dx$$

After some easy (yet tedious) analytic integration using the previous formulas, we get:

$$\int_{x_1}^{x_3} l_1(x)dx = \frac{h}{3}, \int_{x_1}^{x_3} l_2(x)dx = \frac{4h}{3}, \int_{x_1}^{x_3} l_3(x)dx = \frac{h}{3}$$

Thus,

$$\int_{x_1}^{x_3} p(x)dx = \frac{h}{3}(f(x_1) + 4f(x_2) + f(x_3))$$

This is Simpson's rule and is commonly written as:

$$\int_a^b f(x)dx \approx \frac{\overbrace{b-a}^{=2h}}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

In order to define the respective composite rule, we use a partitioning:

$$a = x_0 < x_1 < x_2 < \ldots < x_{2n-1} < x_{2n} = b$$

This time we define each interval $D_k = [x_{2k}, x_{2k+2}]$, and

$$I_k = \int_{x_{2k}}^{x_{2k+2}} f(x)dx \Rightarrow I = \sum_{k=0}^{n-1} I_k$$

Then,

$$I_{k,\mathsf{simp}} = \frac{h}{3}[f(x_{2k}) + 4f(x_{2k+1}) + f(x_{2k+2})]$$

and the composite rule $I_{\mathsf{simp}} = \sum_{k=0}^{n-1} I_{k,\mathsf{simp}}$ becomes:

$$I_{\mathsf{simp}} = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \ldots + 2f(x_{2n-2}) + 4f(x_{2n-1}) + f(x_{2n})]$$

In order to estimate the local error, we again try to use the formula for the interpolation error of passing a quadratic $p^{(k)}(x)$ through $(x_{2k}, f(x_{2k}))$, $(x_{2k+1}, f(x_{2k+1}))$, $(x_{2k+2}, f(x_{2k+2}))$.

$$f(x) - p^{(k)}(x) = \frac{f^{(3)}(c_k)}{3!}(x - x_{2k})(x - x_{2k+1})(x - x_{2k+2})$$

Thus,

$$\begin{aligned} e_k &= \left|\int_{x_{2k}}^{x_{2k+2}} [f(x) - p(x)]dx\right| \\ &\le \int_{x_{2k}}^{x_{2k+2}} \frac{|f^{(3)}(c_k)|}{3!}|(x - x_{2k})(x - x_{2k+1})(x - x_{2k+2})|dx \\ &\le \frac{1}{6}||f^{(3)}||_\infty \int_{x_{2k}}^{x_{2k+2}} |\underbrace{(x - x_{2k})(x - x_{2k+1})(x - x_{2k+2})}_{(\star)}|dx \end{aligned}$$

And with this we are at a dead end! We cannot simply remove the absolute value in the expression ($\star$) since it changes sign in $[x_{2k}, x_{2k+2}]$. Even if we break up this integral in sub-intervals, we will *at best* show that Simpson's rule is 3rd order accurate, where in fact it is even *more*, i.e., 4th order accurate!

To achieve our goal, we will use a different (and more general) type of analysis. It is possible to show that:

Theorem 1. *If an integration rule integrates* exactly *any polynomial up to degree $(d-1)$, then the global error is $O(h^d)$ or better, i.e., the rule is at least d-order accurate.*

Methodology: We will test Simpson's rule on monomials $f(x) = x^d$, $d = 0, 1, 2, \ldots$

- $f(x) = 1$:

$$I_{\mathsf{simp}} = \frac{b-a}{6}[1+4+1] = (b-a) \equiv \int_a^b 1 \cdot dx \Rightarrow \text{correct!}$$

- $f(x) = x$:

$$I_{\mathsf{simp}} = \frac{b-a}{6}\left[a + 4f\left(\frac{a+b}{2}\right) + b\right] = \frac{b^2}{2} - \frac{a^2}{2} \equiv \int_a^b x dx \Rightarrow \text{correct!}$$

- $f(x) = x^2$:

$$I_{\mathsf{simp}} = \frac{b-a}{6}\left[a^2 + f\left(\frac{a+b}{2}\right)^2 + b^2\right] = \frac{b^3}{3} - \frac{a^3}{3} \equiv \int_a^b x^2 dx \Rightarrow \text{correct!}$$

- $f(x) = x^3$:

$$I_{\mathsf{simp}} = \frac{b-a}{6}\left[a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right] = \frac{b^4}{4} - \frac{a^4}{4} \equiv \int_a^b x^3 dx \Rightarrow \text{correct!}$$

- $f(x) = x^4$:

$$I_{\mathsf{simp}} = \frac{b-a}{6}\left[a^4 + 4\left(\frac{a+b}{2}\right)^4 + b^4\right]$$

  which is not equal to $\frac{b^5}{5} - \frac{a^5}{5} = \int_a^b x^4 dx$

Thus, Simpson's rule is $4th$ *order accurate*, i.e.,

$$e_{k,\mathsf{local}} \le O(h^5)$$
$$e_{k,\mathsf{global}} \le O(h^4)$$

Assessing order of accuracy in integration rules

Theorem 2. *If an integration rule integrates* exactly *any polynomial up to degree* $(d-1)$*, then the global error is* $O(h^d)$ *or better, i.e., the rule is at least d-order accurate.*

Methodology:

- Test the integration rule on *monomials* of degree $0, 1, 2, \ldots$, i.e., on $f(x) = 1$, $f(x) = x$, $f(x) = x^2, \ldots$
- If $f(x) = x^d$ is the 1st test function that is *not* integrated exactly, the order of accuracy is *equal* to d.

Example: Trapezoidal rule $I = \int_a^b f(x)dx \approx \frac{f(a)+f(b)}{2}(b-a)$.

- $f(x) = 1$:

$$I_{\mathsf{trap}} = \frac{1+1}{2}(b-a) = (b-a) \Rightarrow \text{exact!}$$

- $f(x) = x$:

$$I_{\mathsf{trap}} = \frac{a+b}{2}(b-a) = \frac{b^2}{2} - \frac{a^2}{2} \Rightarrow \text{exact!}$$

- $f(x) = x^2$:

$$I_{\mathsf{trap}} = \frac{a^2+b^2}{2}(b-a) \xrightarrow{\text{not exact}} \left(\int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} \right)$$

Thus, trapezoidal rule is 2nd order accurate!