Simpson Rule

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April 2019

Given a real-valued function $f(x)$. We would like to estimate the integral

$$I = \int_a^b f(x)dx, a < b$$

The Simpson Rule aims to fit $f(x)$ by using quadratic function.

1 Derivation of the simplest case

The simplest case is to use one single quadratic function to fit $f(x)$. We wish the quadratic function to pass through $f(x_0)$, $f(x_1)$ and $f(x_2)$, where $x_0 = a$, $x_1 = \frac{a+b}{2}$ and $x_2 = b$.

We first find the quadratic function by Lagrange interpolation.

Step 1 - Find the Lagrange Basis

$$\begin{aligned}
l_0(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-\frac{a+b}{2})(x-b)}{(a-\frac{a+b}{2})(a-b)} = \frac{x^2 - \frac{a+3b}{2}x + \frac{b(a+b)}{2}}{\frac{(a-b)^2}{2}} = \frac{2x^2-(a+3b)x+b(a+b)}{(b-a)^2} \\
l_1(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-a)(x-b)}{(\frac{a+b}{2}-a)(\frac{a+b}{2}-b)} = \frac{x^2-(a+b)x+ab}{-\frac{(a-b)^2}{4}} = \frac{-4x^2+4(a+b)x-4ab}{(b-a)^2} \\
l_2(x) &= \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-a)(x-\frac{a+b}{2})}{(b-a)(b-\frac{a+b}{2})} = \frac{x^2 - \frac{(3a+b)}{2}x + \frac{a(a+b)}{2}}{\frac{(b-a)^2}{2}} = \frac{2x^2-(3a+b)x+a(a+b)}{(b-a)^2}
\end{aligned}$$

Step 2 - Find the Fitting Polynomials

$$\begin{aligned}
p(x) &= f(x_0)l_0(x) + f(x_1)l_1(x) + f(x_2)l_2(x) \\
&= \frac{2x^2-(a+3b)x+b(a+b)}{(b-a)^2}f(x_0) + \frac{-4x^2+4(a+b)x-4ab}{(b-a)^2}f(x_1) + \frac{2x^2-(3a+b)x+a(a+b)}{(b-a)^2}f(x_2) \\
&= \frac{1}{(b-a)^2}(Ax^2+Bx+C)
\end{aligned}$$

where

$$\begin{aligned}
A &= 2f(x_0) - 4f(x_1) + 2f(x_2) \\
B &= -(a+3b)f(x_0) + 4(a+b)f(x_1) - (3a+b)f(x_2) \\
C &= b(a+b)f(x_0) - 4abf(x_1) + a(a+b)f(x_2)
\end{aligned}$$

Step 3 - Integration

$$\begin{aligned}
I = \int_a^b f(x)dx \approx \int_a^b p(x)dx &= \frac{1}{(b-a)^2}\left[\frac{A}{3}x^3 + \frac{B}{2}x^2 + Cx\right]_a^b \\
&= \frac{1}{(b-a)^2}\left(\frac{A}{3}(b^3-a^3) + \frac{B}{2}(b^2-a^2) + C(b-a)\right) \\
&= \frac{1}{b-a}\left(\frac{A}{3}(b^2+ab+a^2) + \frac{B}{2}(b+a) + C\right)
\end{aligned}$$

Here

$$\begin{aligned}\frac{A}{3}(b^2+ab+a^2) &= \frac{1}{3}((2a^2+2ab+2b^2)f(x_0)-4(a^2+ab+b^2)f(x_1)+(2a^2+2ab+2b^2)f(x_2))\\ \frac{B}{2}(b+a) &= \frac{1}{2}(-(a^2+4ab+3b^2)f(x_0)+4(a^2+2ab+b^2)f(x_1)-(3a^2+4ab+b^2)f(x_2))\\ C &= (ab+b^2)f(x_0)-4abf(x_1)+(a^2+ab)f(x_2)\end{aligned}$$

Therefore

$$\begin{aligned}I \approx \int_a^b p(x)dx &= \frac{1}{b-a}\left(\left(\frac{1}{6}a^2-\frac{1}{3}ab+\frac{1}{6}b^2\right)f(x_0)+4\left(\frac{1}{6}a^2-\frac{1}{3}ab+\frac{1}{6}b^2\right)+\left(\frac{1}{6}a^2-\frac{1}{3}ab+\frac{1}{6}b^2\right)\right)\\ &= \frac{1}{6(b-a)}((a-b)^2f(x_0)+(a-b)^2f(x_1)+(a-b)^2f(x_2))\\ &= \frac{b-a}{6}(f(x_0)+4f(x_1)+f(x_2))\\ &= \frac{b-a}{6}\left(f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right)\end{aligned}$$

This is the formula for simplest case of simpson rule.

2 Relation to Richardson Extrapolation

Recall that I could be estimated using trapezoidal rule. When $n=1$, we have $I \approx I_1 = (b-a)\frac{f(a)+f(b)}{2}$ with error $\sim h_1^2 = (b-a)^2$. When $n=2$, we have $I \approx I_2 = \frac{b-a}{2}\left(\frac{f(a)}{2}+f(\frac{a+b}{2})+\frac{f(b)}{2}\right)$ with error $\sim h_2^2 = \left(\frac{b-a}{2}\right)^2$. Therefore a better estimate is given by

$$\tilde{I} = \frac{\frac{h_2^2}{h_1^2}I_2 - I_1}{\frac{h_2^2}{h_1^2}-1} = \frac{4I_2-I_1}{3} = \frac{b-a}{6}\left(f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right)$$

3 Composite Simpson Rule

Given sampling points $a = x_0 < x_1 < x_2 < ... < x_{2n} = b$. (need odd number of sampling points!) which are equally spaced (i.e. $\forall i, x_i - x_{i-1} = h = \frac{b-a}{2n}$). We wish to perform *piecewise* quadratic interpolation on data $\{x_0, x_1, x_2\}$, $\{x_2, x_3, x_4\}$, ..., $\{x_{2n-2}, x_{2n-1}, x_{2n}\}$ separately, then estimate the integral pieces by pieces. In such case we have $\frac{x_{2i}+x_{2(i+1)}}{2} = x_{2i+1}$,

$$\begin{aligned}I &= \int_a^b f(x)dx\\ &= \sum_{i=0}^{n-1}\int_{x_{2i}}^{x_{2(i+1)}} f(x)dx\\ &\approx \sum_{i=0}^{n-1}\frac{2h}{6}\left(f(x_{2i})+4f\left(\frac{x_{2i}+x_{2(i+1)}}{2}\right)+f(x_{2(i+1)})\right)\\ &= \frac{h}{3}\sum_{i=0}^{n-1}\left(f(x_{2i})+4f(x_{2i+1})+f(x_{2(i+1)})\right)\\ &= \frac{b-a}{6n}(f(x_0)+4f(x_1)+f(x_2)+f(x_2)+4f(x_3)+f(x_4)+...+f(x_{2(i-1)})+4f(x_{2i-1})+f(x_{2i}))\\ &= \frac{b-a}{6n}(f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+...+2f(x_{2(i-1)})+4f(x_{2i-1})+f(x_{2i}))\end{aligned}$$