4.2 Second order derivative

Back to Taylor expansion, we aim to find an approximation of $f"(x_i)$, we add (4.5) and (4.6):

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + h^2 f"(x_i) + \frac{2}{4!}h^4 f^{(4)}(x_i) + \dots$$
$$h^2 f"(x_i) = f(x_{i+1}) + f(x_{i-1}) - 2f(x_i) - \frac{2}{4!}h^4 f^{(4)}(x_i) + \dots$$
$$f"(x_i) = \frac{1}{h^2}(f(x_{i+1}) - 2f(x_i) + f(x_{i-1})) + O(h^2)$$

We define now $\delta_h^2(\cdot)$ as follows:

$$\delta_h^2 f(x_i) = f(x_{i+1}) - 2f(x_i) + f(x_{i-1})$$

Then, we define the second order derivative Richardson extrapolation:

$$\begin{cases} \Psi_h(\cdot) = \frac{1}{h^2}\delta_h^2(\cdot) \\ \Psi_h^k(\cdot) = \frac{2^{2k}\Psi_h^{k-1}(\cdot) - \Psi_{2h}^{k-1}(\cdot)}{2^{2k}-1} & , k \geq 1 \end{cases}$$

The error is of order h^{2k+2}.

Example 4.2.1 *In the same example, find the best approximation of $f"(0.4)$.*

Solution:

h	$\Psi_h f(x_2)$	$\Psi_h^1 f(x_2)$
0.1	20	25
0.2	5	–

$$\Psi_{0.1} f(x_2) = \frac{1}{0.01}(f(x_3) - 2f(x_2) + f(x_1)) = 20$$
$$\Psi_{0.2} f(x_2) = \frac{1}{0.04}(f(x_4) - 2f(x_2) + f(x_0)) = 5$$
$$\Psi_{0.1}^1 f(x_2) = \frac{2^2\Psi_{0.1} f(x_2) - \Psi_{0.2} f(x_2)}{2^2 - 1} = 25$$

The best approximation of $f"(0.4)$ is $f"(x_2) \approx \Psi_{0.1}^1 f(x_2) = 25$ with error of order h^4.

4.3 Numerical integration

This section aims to approximate the integral of f. Before we introduce methods, let's recall the following equality:

$$\int_a^b f(x)dx = \int_a^c f(x)dx + \int_c^b f(x)dx$$

Then, in our context, we can write the following:

$$I = \int_{x_0}^{x_n} f(x)dx = \sum_{k=0}^{n-1} \int_{x_x}^{x_{k+1}} f(x)dx$$

4.3.1 The midpoint rectangular approximation

This approximation can be used only when n is even i.e. $n = 2m$ for some integer m. By Figure 4.1, we can derive the following approximation:

$$I = \sum_{k=0}^{m-1} \int_{2k}^{2k+2} f(x)dx = \sum_{k=0}^{m-1} 2hf(x_{2k+1}) = 2h \sum_{k=0}^{m-1} f(x_{2k+1})$$

The error is of order h^2.

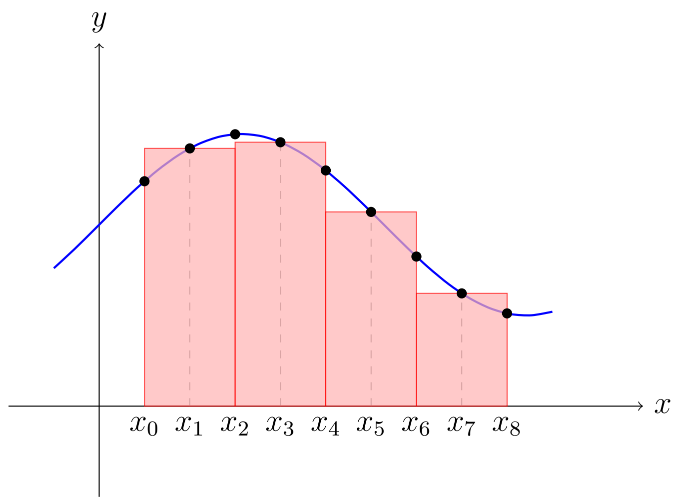

Figure 4.1: Midpoint Rule Approximation: Rectangles are constructed using midpoints of each subinterval.

Example 4.3.1 *In the same example, approximate* $\int_{0.2}^{0.6} f(x)dx$ *using the midpoint rectangular approximation.*

Solution:

$$\begin{aligned} I &= \int_{0.2}^{0.6} f(x)dx \\ &\approx 2h \sum_{k=0}^{1} f(x_{2k+1}) \\ &= 2(0.1)(f(x_1) + f(x_3)) \\ &= 0.2(1.3 + 1.7) \\ &= 0.6 \end{aligned}$$

4.3.2 Trapezoid approximation

By Figure 4.2, we can derive the following approximation:

$$
\begin{aligned}
I = T(h) &= \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} f(x)dx \\
&= \sum_{k=0}^{n-1} \frac{h}{2}(f(x_k) + f(x_{k+1})) \\
&= \frac{h}{2}(f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n))
\end{aligned}
$$

The error is of order h^2.

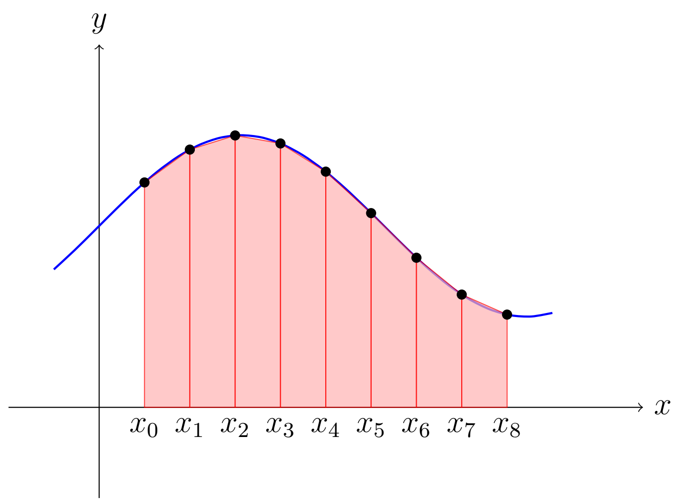

Figure 4.2: Trapezoid Rule Approximation

Example 4.3.2 *In the same example, approximate* $\int_{0.2}^{0.6} f(x)dx$ *using the trapezoid approximation.*

Solution:

$$
\begin{aligned}
I &= \int_{0.2}^{0.6} f(x)dx \\
&\approx \frac{h}{2}(f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + f(x_4)) \\
&= 0.59
\end{aligned}
$$

Example 4.3.3 *Approximate* $I = \int_0^1 e^{x^2} dx$ *using a set of points with distance* $h = 0.25$.

Solution:
We set the table of points:

i	0	1	2	3	4
x_i	0	0.25	0.5	0.75	1
y_i	1	1.0644	1.284	1.755	2.7182

Now, we use the trapezoid approximation:

$$\begin{aligned} I &= \int_0^1 f(x)dx \\ &\approx \frac{h}{2}(f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + f(x_4)) \\ &= 1.49 \end{aligned}$$

Finally, we introduce the integral Richardson extrapolation as follows:

$$\begin{cases} R^0(h) = T(h) \\ R^k(h) = \frac{2^{2k}R^{k-1}(h) - R^{k-1}(2h)}{2^{2k}-1} \end{cases}, \; k \geq 1$$

The error is of order h^{2k+2}.

Example 4.3.4 *In the same example, find the best possible approximation of* $\int_{0.2}^{0.6} f(x)dx$ *using Richardson extrapolation.*

h	$R^0(h)$	$R^1(h)$	$R^2(h)$
0.1	0.59	0.5933	0.5937
0.2	0.58	0.5866	–
0.4	0.6	–	–

$$\begin{aligned} R^0(0.1) &= T(0.1) = 0.59 \\ R^0(0.2) &= T(0.2) = \frac{0.2}{2}(f(x_0) + 2f(x_2) + f(x_4)) = 0.58 \\ R^0(0.4) &= T(0.4) = \frac{0.4}{2}(f(x_0) + f(x_4)) = 0.6 \\ R^1(0.1) &= \frac{2^2R^0(0.1) - R^0(0.2)}{2^2-1} = 0.5933 \\ R^1(0.2) &= \frac{2^2R^0(0.2) - R^0(0.4)}{2^2-1} = 0.5866 \\ R^2(0.1) &= \frac{2^4R^1(0.1) - R^1(0.2)}{2^4-1} = 0.5937 \end{aligned}$$

The best possible approximation of I is $I \approx R^2(0.1) = 0.5937$ with error of order h^6.