DEN: Numerical derivation and integration (and $O(h^a)$)

Definition.
Consider some $a \in I\!R$ or $a = \pm\infty$, let f, g be functions defined on some (reduced) neighborhood of a. We say that $f = O(g)$ as $x \to a$ if there exist some constant C and a reduced neighborhood P of a such that $|f| \le C|g|$ on P.

Fact.
If $b \ge a \ge 0$ and $\alpha, \beta \in I\!R$, then
(i) $\beta h^b = O(h^a)$,
(ii) $\alpha h^2 + O(h^b) \sim \alpha h^a$
as $h \to 0$, resp. $h \to 0^+$.

Fact.
(i) For $b \ge a \ge 0$ and $\alpha, \beta \in I\!R$: $\alpha O(h^a) \pm \beta O(h^b) = O(h^a)$ as $h \to 0$.
(ii) For $a, b \ge 0$: $O(h^a) \cdot O(h^b) = O(h^{a+b})$ as $h \to 0$
(iii) For $b \ge a \ge 0$: $\dfrac{1}{h^a} O(h^b) = O(h^{b-a})$ as $h \to 0$.

Definition.
Consider a function f that is differentiable at a.
We consider the following approximating formulas for $f'(a)$:

$$f'(a) = \frac{f(a+h) - f(a)}{h} \qquad \text{(forward difference)},$$
$$f'(a) = \frac{f(a) - f(a-h)}{h} \qquad \text{(back difference)},$$
$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} \qquad \text{(central difference)}.$$

Fact.
Consider a function f that is three times continuously differentiable on some neighborhood of a point a. Then the following approximating formulas are true as $h \to 0$:

$$f'(a) = \frac{f(a+h) - f(a)}{h} + O(h),$$
$$f'(a) = \frac{f(a) - f(a-h)}{h} + O(h),$$
$$f'(a) = \frac{f(a+h) - f(a-h)}{2h} + O(h^2).$$

If f is four times continuously differentiable on some neighborhood of a, then

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

For $k \in I\!N$ and functions with derivatives of sufficient order we have

$$f^{(k)}(a) = \frac{1}{h^k} \sum_{i=1}^{k} (-1)^i \binom{k}{i} f(a + (k-i)h) + O(h)$$

(forward difference)

$$f^{(k)}(a) = \frac{1}{h^k} \sum_{i=1}^{k} (-1)^i \binom{k}{i} f(a - ih) + O(h)$$

(back difference)

$$f^{(k)}(a) = \frac{1}{(2h)^k} \sum_{i=1}^{k} (-1)^i \binom{k}{i} f(a + (k-2i)h) + O(h^2)$$

(central difference)

Definition.
Let f be a function integrable on an interval $[a,b]$. For $n \in I\!N$ denote $h = \frac{b-a}{n}$ and consider points $x_i = a + ih$.
By the **method of left rectangles** or **rectangle rule** with left endpoints for estimating the integral $\displaystyle\int_a^b f(x)\,dx$ we mean the formula

$$R_l(n) = h\sum_{i=0}^{n-1} f(x_i) = h\big[f(x_0) + \cdots + f(x_{n-1})\big].$$

By the **method of right rectangles** or **rectangle rule** with right endpoints for estimating the integral $\displaystyle\int_a^b f(x)\,dx$ we mean the formula

$$R_r(n) = h\sum_{i=1}^{n} f(x_i) = h\big[f(x_1) + \cdots + f(x_n)\big].$$

Theorem.
Consider a function f on an interval $[a,b]$, denote $M_1 = \max\limits_{x\in[a,b]} |f'(x)|$. If we approximate the integral $I = \displaystyle\int_a^b f(x)\,dx$ using a rectangle rule, then we have the following error estimates:

$$\begin{aligned} |I - R_l(n)| &\leq \frac{1}{2}(b-a)^2 M_1 \frac{1}{n} = \frac{1}{2}(b-a)M_1 h,\\ |I - R_r(n)| &\leq \frac{1}{2}(b-a)^2 M_1 \frac{1}{n} = \frac{1}{2}(b-a)M_1 h \end{aligned}$$

for $h = \frac{b-a}{n}$.

Definition.
Let f be a function integrable on an interval $[a,b]$. For $n \in I\!N$ denote $h = \frac{b-a}{n}$ and consider points $x_i = a + ih$.
By the **trapezoid rule** for estimating the integral $\displaystyle\int_a^b f(x)\,dx$ we mean the formula

$$T(n) = \frac{1}{2}h\Big[\sum_{i=0}^{n-1} f(x_i) + \sum_{i=1}^{n} f(x_i)\Big] = \frac{1}{2}h\Big[f(x_0) + \sum_{i=1}^{n-1} 2f(x_i) + f(x_n)\Big].$$

Theorem.
Consider a function f on an interval $[a,b]$, denote $M_2 = \max\limits_{x\in[a,b]} |f''(x)|$. If we approximate the integral $I = \displaystyle\int_a^b f(x)\,dx$ using the trapezoid rule, then we have the following error estimate:

$$|I - T(n)| \leq \frac{1}{12}(b-a)^3 M_2 \frac{1}{n^2} = \frac{1}{12}(b-a)M_2 h^2$$

for $h = \frac{b-a}{n}$.

Definition.
Let f be a function integrable on an interval $[a,b]$. For $n\in I\!N$, n even, denote $h=\frac{b-a}{n}$ and consider points $x_i=a+ih$.

By the **Simpson rule** for estimating the integral $\int_a^b f(x)\,dx$ we mean the formula

$$\begin{aligned}S(n)&=\frac{1}{3}h\Big[f(x_0)+4\sum_{i=1}^{n/2}f(x_{2i-1})+2\sum_{i=1}^{n/2-1}f(x_{2i})+f(x_n)\Big]\\&=\frac{1}{3}h\Big[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\dots+4f(x_{n-1})+f(x_n)\Big].\end{aligned}$$

Theorem.
Consider a function f on an interval $[a,b]$, denote $M_4=\max\limits_{x\in[a,b]}|f''''(x)|$. If we approximate the integral $I=\int_a^b f(x)\,dx$ using the Simpson rule, then we have the following error estimate

$$|I-S(n)|\le\frac{1}{180}(b-a)^5M_4\frac{1}{n^4}=\frac{1}{180}(b-a)M_4h^4\text{ for }h=\frac{b-a}{n}.$$

Numerical integration overview:
$I=\int\limits_a^b f(x)\,dx,\quad a=x_0<x_1<\dots<x_n=b,\quad x_{i+1}-x_i=h=\frac{b-a}{n}$

Rectangle rule $E=O(h)$

$$R_l(n)=\sum_{i=0}^{n-1}hf(x_i)$$
$$R_r(n)=\sum_{i=1}^{n}hf(x_i)$$

Trapezoid rule $E=O(h^2)$

$$T(n)=\tfrac{1}{2}h\Big[f(x_0)+\sum_{i=1}^{n-1}2f(x_i)+f(x_n)\Big]$$

Simpson rule $E=O(h^4)$

$$S(n)=\tfrac{1}{3}h\Big[f(x_0)+\sum_{i=1}^{n/2}4f(x_{2i-1})+\sum_{i=1}^{n/2-1}4f(x_{2i})+f(x_n)\Big]$$

Definition.
We say that a method I_n for approximating an integral is of **order** p for $p\in I\!N$, provided that for every function f on an interval $[a,b]$ there is $C>0$ such that

$$\Big|\int\limits_a^b f(x)\,dx-I_n\Big|\le C\frac{1}{n^p}.$$

That is, $|I-I_n|$ is $O(h^p)$ as $h\to 0^+$.

Fact.
Let f be a function integrable on some interval $[a,b]$. Let I_n for $n\in I\!N$ be an approximation of the integral $I=\int_a^b f(x)\,dx$ by some method of order p, assume that the error estimate is of the form

$$|I-I_n|\sim Ch^p+O(h^q).$$

Then the formula $\dfrac{2^pI_{2n}-I_n}{2^p-1}$ is an approximation of I of order q.

Moreover, $\dfrac{I_{2n}-I_n}{2^p-1}$ is a good estimate of the error $I-I_{2n}$.