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 $|f| \leq C|g|$ on P.

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

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

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

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 $\int_a^b f(x)\,dx$ 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 $\int_a^b f(x)\,dx$ 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 $I = \int_a^b f(x)\,dx$ using a rectangle rule, then we have the following error estimates:

$$|I - R_l(n)| \le \frac{1}{2}(b-a)^2 M_1 \frac{1}{n} = \frac{1}{2}(b-a)M_1 h,$$
$$|I - R_r(n)| \le \frac{1}{2}(b-a)^2 M_1 \frac{1}{n} = \frac{1}{2}(b-a)M_1 h$$

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

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

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

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

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

Rectangle rule $\qquad E = O(h)$

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

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

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

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

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

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 $n \in \mathbb{N}$ 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 $\dfrac{2^p I_{2n} - I_n}{2^p - 1}$ is an approximation of I of order q.

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