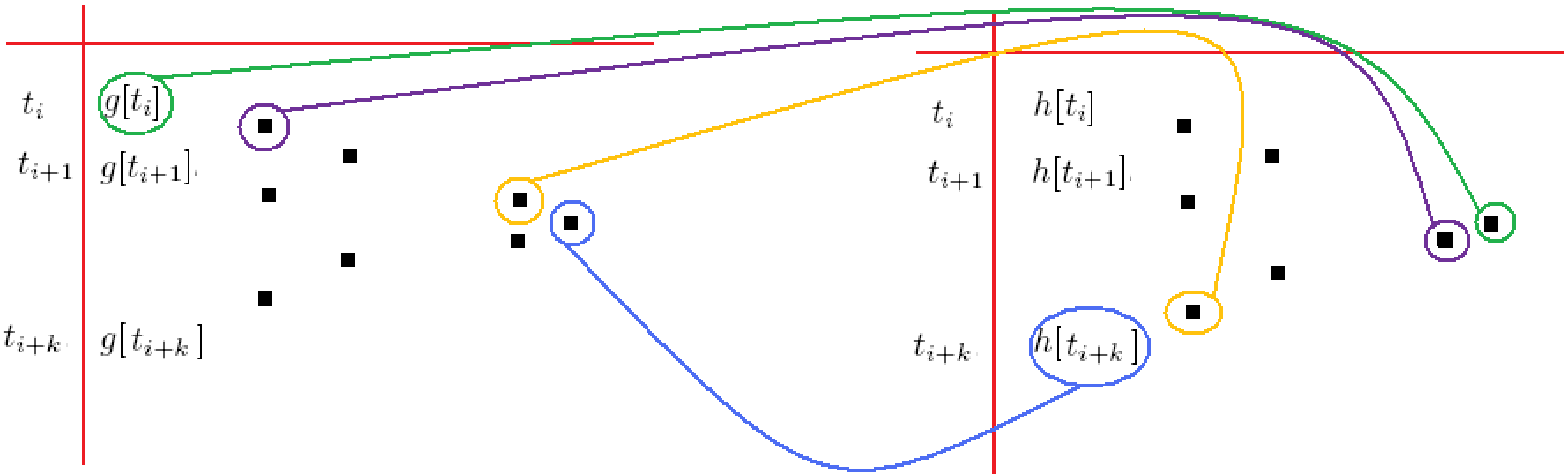
The Computation of B-Splines

Product Rule for Divided Differences.

Suppose $t_i \le t_{i+1} \le \cdots \le t_{i+k}$. *Assume further that the function* $f(t) = g(t)h(t)$ *is a product of two functions that are sufficiently often differentiable at* $t = t_j$, $j = i, \ldots, i+k$, *Then*

$$f[t_i, t_{i+1}, \ldots, t_{i+k}] = \sum_{r=i}^{i+k} g[t_i, t_{i+1}, \ldots, t_r] h[t_r, t_{r+1}, \ldots, t_{i+k}].$$



renormalize the B-splines $B_{i,r}(x)$

$$N_{i,r}(x) := \frac{B_{i,r}(x)}{t_{i+r} - t_i} \equiv f_x^{r-1}[t_i, t_{i+1}, \dots, t_{i+r}],$$

For $r \geq 2$ and $t_i < t_{i+r}$:

$$N_{i,r}(x) = \frac{x - t_i}{t_{i+r} - t_i} N_{i,r-1}(x) + \frac{t_{i+r} - x}{t_{i+r} - t_i} N_{i+1,r-1}(x).$$

PROOF. Suppose first $x \neq t_j$ for all j.

$$f_x^{r-1}(t) = (t - x)_+^{r-1} = (t - x)(t - x)_+^{r-2} = g(t) f_x^{r-2}(t).$$

$$g[t_i] = t_i - x, \quad g[t_i, t_{i+1}] = 1, \quad g[t_i, \dots, t_j] = 0 \quad \text{for } j > i + 1,$$

$$\begin{aligned} f_x^{r-1}[t_i, \dots, t_{i+r}] &= (t_i - x) f_x^{r-2}[t_i, \dots, t_{i+r}] + 1 \cdot f_x^{r-2}[t_{i+1}, \dots, t_{i+r}] \\ &= \frac{(t_i - x)}{t_{i+r} - t_i}(f_x^{r-2}[t_{i+1}, \dots, t_{i+r}] - f_x^{r-2}[t_i, \dots, t_{i+r-1}]) \\ &\quad + 1 \cdot f_x^{r-2}[t_{i+1}, \dots, t_{i+r}] \\ &= \frac{x - t_i}{t_{i+r} - t_i} f_x^{r-2}[t_i, \dots, t_{i+r-1}] + \frac{t_{i+r} - x}{t_{i+r} - t_i} f_x^{r-2}[t_{i+1}, \dots, t_{i+r}] \quad \blacksquare \end{aligned}$$

$$B_{i,r}(x) = \frac{x - t_i}{t_{i+r-1} - t_i}\, B_{i,r-1}(x) + \frac{t_{i+r} - x}{t_{i+r} - t_{i+1}}\, B_{i+1,r-1}(x)$$

To show this, let x be given. Then there is a $t_j \in \mathbf{t}$ with $t_j \leq x < t_{j+1}$. we know $B_{i,r}(x) = 0$ for all i, r with $x \notin [t_i, t_{i+r}]$, i.e., for $i \leq j - r$ and for $i \geq j + 1$. Therefore, in the following tableau of $B_{i,r} := B_{i,r}(x)$, the $B_{i,r}$ vanish at the positions denoted by 0:

$$\begin{array}{ccccc}
0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & B_{j-3,4} & \cdots \\
0 & 0 & B_{j-2,3} & B_{j-2,4} & \cdots \\
0 & B_{j-1,2} & B_{j-1,3} & B_{j-1,4} & \cdots \\
B_{j,1} & B_{j,2} & B_{j,3} & B_{j,4} & \cdots \\
0 & 0 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots &
\end{array}
\qquad
\boxed{\begin{array}{lcl}
B_{i,r-1} & \rightarrow & B_{i,r} \\
 & \nearrow & \\
B_{i+1,r-1} & &
\end{array}}$$

This method is numerically very stable because only nonnegative multiples of nonnegative numbers are added together.

EXAMPLE. For $t_i = i$, $i = 0, 1, \ldots$ and $x = 3.5 \in [t_3, t_4]$ the following tableau of values $B_{i,r} = B_{i,r}(x)$ is obtained.

$r =$	1	2	3	4
$i = 0$	0	0	0	1/48
$i = 1$	0	0	1/8	23/48
$i = 2$	0	1/2	6/8	23/48
$i = 3$	1	1/2	1/8	1/48
$i = 4$	0	0	0	0

For instance, $B_{2,4}$ is obtained from

$$B_{2,4} = B_{2,4}(3.5) = \frac{3.5-2}{5-2} \cdot \frac{6}{8} + \frac{6-3.5}{6-3} \cdot \frac{1}{8} = \frac{23}{48}.$$

interpolation problem for spline functions,

$$\mathbf{t} = (t_i)_{1 \leq i \leq N+r} \qquad t_1 \leq t_2 \leq \cdots \leq t_{N+r} \qquad t_i < t_{i+r} \text{ for } i = 1, 2, \ldots, N.$$

$B_i(x) \equiv B_{i,r,\mathbf{t}}(x)$, $i = 1, \ldots, N$, the associated B-splines,

$$\mathcal{S}_{r,\mathbf{t}} = \Big\{ \sum_{i=1}^{N} \alpha_i B_i(x) \mid \alpha_i \in \mathbb{R} \Big\},$$

given N pairs (ξ_j, f_j), $j = 1, \ldots, N$, of interpolation points

$$\xi_1 < \xi_2 < \cdots < \xi_N.$$

These are the data for the interpolation problem of finding a function $S \in \mathcal{S}_{r,\mathbf{t}}$ satisfying

$$S(\xi_j) = f_j, \quad j = 1, \ldots, N.$$

Since any $S \in \mathcal{S}_{r,\mathbf{t}}$ can be written as a linear combination of the B_i, $i = 1, \ldots, N$, this is equivalent to the problem of solving the linear equations

$$\sum_{i=1}^{N} \alpha_i B_i(\xi_j) = f_j, \quad j = 1, \ldots, N.$$

$$A = \begin{bmatrix} B_1(\xi_1) & \dots & B_N(\xi_1) \\ \vdots & & \vdots \\ B_1(\xi_N) & \dots & B_N(\xi_N) \end{bmatrix}$$

within the jth row of A all elements $B_i(\xi_j)$ with $t_{i+r} < \xi_j$ or $t_i > \xi_j$ are zero.
each row of A contains at most r elements different from 0,

Theorem. *The matrix* $A = (B_i(\xi_j))$ *of* (2.4.5.6) *is nonsingular if and only if all its diagonal elements* $B_i(\xi_i) \neq 0$ *are nonzero.*

It is possible to show [see Karlin (1968)] that the matrix A is *totally positive* in the following sense: all $r \times r$ submatrices B of A of the form

$$B = (a_{i_p, j_q})_{p,q=1}^{r} \quad \text{with} \quad r \geq 1, \ \ i_1 < i_2 < \cdots < i_r, \ \ j_1 < j_2 < \cdots < j_r,$$

have a nonnegative determinant, $\det(B) \geq 0$.

Gaussian elimination *without pivoting* is numerically stable [see de Boor and Pinkus (1977)].

Topics in Integration

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

The Integration Formulas of Newton and Cotes

$[a, b]$ $\quad x_i = a + i\,h, \quad i = 0,\ 1,\ \ldots,\ n, \quad h := (b-a)/n,\ n > 0$ integer,

P_n interpolating polynomial of degree n or less

$$P_n(x_i) = f_i := f(x_i) \quad \text{for} \quad i = 0,\ 1,\ \ldots,\ n.$$

Lagrange's interpolation formula

$$P_n(x) \equiv \sum_{i=0}^{n} f_i L_i(x), \quad L_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{x - x_k}{x_i - x_k},$$

introducing the new variable t such that $x = a + ht$:

$$L_i(x) = \varphi_i(t) := \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{t - k}{i - k}.$$

Integration gives

$$\int_a^b P_n(x)dx = \sum_{i=0}^{n} f_i \int_a^b L_i(x)dx$$
$$= h \sum_{i=0}^{n} f_i \int_0^n \varphi_i(t)dt$$
$$= h \sum_{i=0}^{n} f_i \alpha_i.$$

$$\alpha_i := \int_0^n \varphi_i(t)dt$$

depend solely on n

If $n = 2$ for instance, then

$$\alpha_0 = \int_0^2 \frac{t-1}{0-1}\frac{t-2}{0-2}dt = \frac{1}{2}\int_0^2 (t^2 - 3t + 2)dt = \frac{1}{2}\left(\frac{8}{3} - \frac{12}{2} + 4\right) = \frac{1}{3},$$
$$\alpha_1 = \int_0^2 \frac{t-0}{1-0}\frac{t-2}{1-2}dt = -\int_0^2 (t^2 - 2t)dt = -\left(\frac{8}{3} - 4\right) = \frac{4}{3},$$
$$\alpha_2 = \int_0^2 \frac{t-0}{2-0}\frac{t-1}{2-1}dt = \frac{1}{2}\int_0^2 (t^2 - t)dt = \frac{1}{2}\left(\frac{8}{3} - \frac{4}{2}\right) = \frac{1}{3},$$

$$\int_a^b P_2(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

Simpson's rule.

$$\int_a^b P_n(x)dx = h\sum_{i=0}^{n} f_i\alpha_i, \quad f_i := f(a+ih), \quad h := \frac{b-a}{n},$$

$$\sum_{i=0}^{n} \alpha_i = n.$$

$$\int_a^b P_n(x)dx = h\sum_{i=0}^{n} f_i\alpha_i, \quad f_i := f(a+ih), \quad h := \frac{b-a}{n},$$

$$\sum_{i=0}^{n} \alpha_i = n.$$

If s is a common denominator for the fractional weights α_i so that the numbers

$$\sigma_i := s\,\alpha_i, \quad i = 0,\ 1,\ \ldots,\ n,$$

are integers, then

$$\int_a^b P_n(x)dx = h\sum_{i=0}^{n} f_i\alpha_i = \frac{b-a}{ns}\sum_{i=0}^{n} \sigma_i f_i.$$

For sufficiently smooth functions $f(x)$ on the closed interval $[a,b]$ it can be shown [see Steffensen (1950)] that the approximation error may be expressed as follows:

$$\int_a^b P_n(x)dx - \int_a^b f(x)dx = h^{p+1}\cdot K\cdot f^{(p)}(\xi), \quad \xi\in(a,b).$$

n	σ_i							ns	Error	Name
1	1	1						2	$h^3 \frac{1}{12} f^{(2)}(\xi)$	Trapezoidal rule
2	1	4	1					6	$h^5 \frac{1}{90} f^{(4)}(\xi)$	Simpson's rule
3	1	3	3	1				8	$h^5 \frac{3}{80} f^{(4)}(\xi)$	3/8-rule
4	7	32	12	32	7			90	$h^7 \frac{8}{945} f^{(6)}(\xi)$	Milne's rule
5	19	75	50	50	75	19		288	$h^7 \frac{275}{12096} f^{(6)}(\xi)$	—
6	41	216	27	272	27	216	41	840	$h^9 \frac{9}{1400} f^{(8)}(\xi)$	Weddle's rule

integration rules may be found by Hermite interpolation $P \in \Pi_n$

$$P \in \Pi_3 \qquad \begin{array}{ll} P(a) = f(a), & P'(a) = f'(a), \\ P(b) = f(b), & P'(b) = f'(b) \end{array} \qquad a = 0,\ b = 1,$$

$$P(t) = f(0)[(t-1)^2 + 2t(t-1)^2] + f(1)[t^2 - 2t^2(t-1)]$$
$$+ f'(0)t(t-1)^2 + f'(1)t^2(t-1),$$

integration of which gives

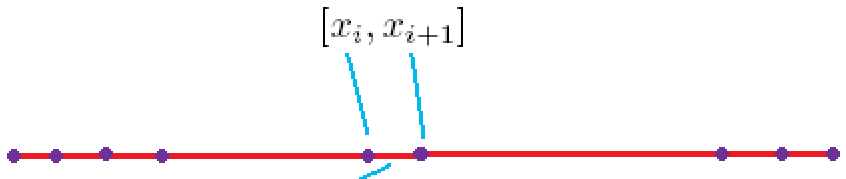
$$\int_0^1 P(t)dt = \tfrac{1}{2}(f(0) + f(1)) + \tfrac{1}{12}(f'(0) - f'(1)).$$

$$\int_a^b f(x)dx \approx M(h) := \frac{h}{2}(f(a) + f(b)) + \frac{h^2}{12}(f'(a) - f'(b)). \qquad h := b - a$$

If $f \in C^4[a, b]$ then

$$M(h) - \int_a^b f(x)dx = \frac{-h^5}{720} f^{(4)}(\xi), \quad \xi \in (a, b), \quad h := (b - a).$$

Composite Rule



The trapezoidal rule ($n = 1$)

$$I_i := \frac{h}{2}[f(x_i) + f(x_{i+1})]$$

$$x_i = a + ih,\ i = 0,\ 1,\ \ldots,\ N,$$

$$h := (b-a)/N$$

For the entire interval $[a, b]$, we obtain the approximation

trapezoidal sum

$$T(h) := \sum_{i=0}^{N-1} I_i \ = h\left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \cdots + f(b-h) + \frac{f(b)}{2}\right],$$

In each subinterval $[x_i, x_{i+1}]$, assuming $f \in C^2[a, b]$:

$$I_i - \int_{x_i}^{x_{i+1}} f(x)dx = \frac{h^3}{12} f^{(2)}(\xi_i), \quad \xi_i \in (x_i, x_{i+1}),$$

Summing these individual error terms gives

$$T(h) - \int_a^b f(x)dx = \frac{h^3}{12}\sum_{i=0}^{N-1} f^{(2)}(\xi_i) = \frac{h^2}{12}(b-a)\frac{1}{N}\sum_{i=0}^{N-1} f^{(2)}(\xi_i).$$

Since

$$\min_i f^{(2)}(\xi_i) \le \frac{1}{N}\sum_{i=0}^{N-1} f^{(2)}(\xi_i) \le \max_i f^{(2)}(\xi_i)$$

and $f^{(2)}(x)$ is continuous, there exists $\xi \in [\min_i \xi_i, \max_i \xi_i] \subset (a,b)$ with

$$f^{(2)}(\xi) = \frac{1}{N}\sum_{i=0}^{N-1} f^{(2)}(\xi_i).$$

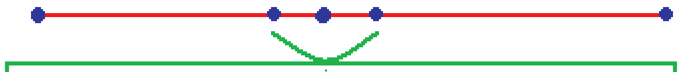
Thus

$$T(h) - \int_a^b f(x)dx = \frac{b-a}{12}h^2 f^{(2)}(\xi), \quad \xi \in (a,b).$$

h^2, order 2.

If N is even, then Simpson's rule may be applied to each subinterval $[x_{2i}, x_{2i+2}]$, $i = 0, 1, \ldots, (N/2)-1$,

$[x_{2i}, x_{2i+2}]$



$$(h/3)(f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2})).$$

Summing these $N/2$ approximations results in the composite version of Simpson's rule

$$S(h) := \frac{h}{3}[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \cdots + 2f(b-2h) + 4f(b-h) + f(b)],$$

The error of $S(h)$ is the sum of all $N/2$ individual errors

$$S(h) - \int_a^b f(x)dx = \frac{h^5}{90} \sum_{i=0}^{(N/2)-1} f^{(4)}(\xi_i) = \frac{h^4}{90} \frac{b-a}{2} \frac{2}{N} \sum_{i=0}^{(N/2)-1} f^{(4)}(\xi_i),$$

we conclude that

$f \in C^4[a, b]$.

$$S(h) - \int_a^b f(x)dx = \frac{b-a}{180} h^4 f^{(4)}(\xi), \quad \xi \in (a, b),$$

order 4.

Extending the rule of integration $M(h)$

"interior" derivatives $f'(x_i)$, $0 < i < N$, cancel.

$$\int_{x_i}^{x_{i+1}} f(x)dx \quad \text{for} \quad i = 0, 1, \ldots, N-1$$

$$\begin{aligned} U(h) :&= h\left[\frac{f(a)}{2} + f(a+h) + \cdots + f(b-h) + \frac{f(b)}{2}\right] + \frac{h^2}{12}[f'(a) - f'(b)] \\ &= T(h) + \frac{h^2}{12}[f'(a) - f'(b)] \end{aligned}$$

correction to the trapezoidal sum $T(h)$.

$$U(h) - \int_a^b f(x)dx = -\frac{b-a}{720}h^4 f^{(4)}(\xi), \quad \xi \in (a,b), \qquad f \in C^4[a,b].$$

$$\hat{T}(h) := h\left[\tfrac{5}{12}f(a) + \tfrac{13}{12}f(a+h) + f(a+2h) + \cdots + f(b-2h) + \tfrac{13}{12}f(b-h) + \tfrac{5}{12}f(b)\right].$$

order 3

Peano's Error Representation

All integration rules considered so far are of the form

$$\tilde{I}(f) := \sum_{k=0}^{m_0} a_{k0} f(x_{k0}) + \sum_{k=0}^{m_1} a_{k1} f'(x_{k1}) + \cdots + \sum_{k=0}^{m_n} a_{kn} f^{(n)}(x_{kn}).$$

The integration error

$$R(f) := \tilde{I}(f) - \int_a^b f(x)dx$$

is a linear operator

$$R(\alpha f + \beta g) = \alpha R(f) + \beta R(g) \quad \text{for} \quad f, g \in V, \quad \alpha, \beta \in \mathbb{R}$$

$$V = \Pi_n,$$
$$V = C^n[a, b],$$

Theorem. *Suppose* $R(P) = 0$ *holds for all polynomials* $P \in \Pi_n$, *that is, every polynomial whose degree does not exceed* n *is integrated exactly. Then for all functions* $f \in C^{n+1}[a, b]$,

$$R(f) = \int_a^b f^{(n+1)}(t) K(t) dt,$$

where

$$K(t) := \frac{1}{n!} R_x[(x-t)_+^n], \quad (x-t)_+^n := \begin{cases} (x-t)^n & \text{for } x \geq t, \\ 0 & \text{for } x < t, \end{cases}$$

and

$$R_x[(x-t)_+^n]$$

denotes the error of $(x-t)_+^n$ *when the latter is considered as a function in* x.

The function $K(t)$ is called the *Peano kernel* of the operator R.

Simpson's rule $\qquad R(f) = \frac{1}{3}f(-1) + \frac{4}{3}f(0) + \frac{1}{3}f(1) - \int_{-1}^{1} f(x)dx.$

$P \in \Pi_3$ is integrated exactly.

proof. let $Q \in \Pi_2$ be the polynomial with

$$P(-1) = Q(-1),\ P(0) = Q(0),\ P(+1) = Q(+1).$$

Putting $S(x) := P(x) - Q(x)$, we have $R(P) = R(S)$.

degree of $S(x)$ is no greater then 3,

$S(x)$ has the three roots $-1, 0, +1$,

$$S(x) = a(x^2 - 1)x,$$

$$R(P) = R(S) = -a \int_{-1}^{1} x(x^2 - 1)dx = 0. \blacksquare$$

Thus Theorem can be applied with $n = 3$. The Peano kernel becomes

$$K(t) = \frac{1}{6}R_x[(x-t)_+^3] = \frac{1}{6}\left[\frac{1}{3}(-1-t)_+^3 + \frac{4}{3}(0-t)_+^3 + \frac{1}{3}(1-t)_+^3 - \int_{-1}^{1}(x-t)_+^3 dx\right].$$

By definition of $(x-t)_+^n$, we find that for $t \in [-1,1]$

$$\int_{-1}^{1}(x-t)_+^3 dx = \int_t^1 (x-t)^3 dx = \frac{(1-t)^4}{4},$$

$$(-1-t)_+^3 = 0, \quad (1-t)_+^3 = (1-t)^3,$$

$$(-t)_+^3 = \begin{cases} 0 & \text{if } t \geq 0, \\ -t^3 & \text{if } t < 0. \end{cases}$$

The Peano kernel for Simpson's rule in the interval $[-1,1]$ is then

$$K(t) = \begin{cases} \frac{1}{72}(1-t)^3(1+3t) & \text{if } 0 \leq t \leq 1, \\ K(-t) & \text{if } -1 \leq t \leq 0. \end{cases}$$

Proof of Theorem. Consider the Taylor expansion of $f(x)$ at $x = a$:

$$f(x) = f(a) + f'(a)(x-a) + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + r_n(x).$$

$$r_n(x) = \frac{1}{n!}\int_a^x f^{(n+1)}(t)(x-t)^n dt = \frac{1}{n!}\int_a^b f^{(n+1)}(t)(x-t)_+^n dt.$$

$$R(f(x) = R(f(a)) + R(f'(a)(x-a)) + \cdots + R(\frac{f^{(n)}(a)}{n!}(x-a))^n + R(r_n(x))$$

since $R(P) = 0$ for $P \in \Pi_n$.

0

$$R(f) = R(r_n) = \frac{1}{n!}R_x\left(\int_a^b f^{(n+1)}(t)(x-t)_+^n dt\right),$$

Change order

we show first that

$$\frac{d^k}{dx^k}\left[\int_a^b f^{(n+1)}(t)(x-t)_+^n dt\right] = \int_a^b f^{(n+1)}(t)\left[\frac{d^k}{dx^k}[(x-t)_+^n]\right] dt \qquad 1 \le k \le n.$$

- $(x-t)_+^n$ is $n-1$ times continuously differentiable. $\Longrightarrow$ For $k < n$ it is true.
- Proof for the case $k = n$:

For $k = n-1$ we have

$$\frac{d^{n-1}}{dx^{n-1}}\left[\int_a^b f^{(n+1)}(t)(x-t)_+^n dt\right] = \int_a^b f^{(n+1)}(t)\frac{d^{n-1}}{dx^{n-1}}[(x-t)_+^n]dt$$

and therefore

$$\begin{aligned}\frac{d^{n-1}}{dx^{n-1}}\left[\int_a^b f^{(n+1)}(t)(x-t)_+^n dt\right] &= n!\int_a^b f^{(n+1)}(t)(x-t)_+ dt \\ &= n!\underbrace{\int_a^x f^{(n+1)}(t)(x-t)dt.}_{\text{differentiable as a function of } x,}\end{aligned}$$

$$
\begin{aligned}
\frac{d^n}{dx^n}\left[\int_a^b f^{(n+1)}(t)(x-t)_+^n dt\right] &= \frac{d}{dx}\left[\frac{d^{n-1}}{dx^{n-1}}\int_a^b f^{(n+1)}(t)(x-t)_+^n dt\right] \\
&= \frac{d}{dx}n!\int_a^x f^{(n+1)}(t)(x-t)dt \\
&= n!f^{(n+1)}(x)(x-x) + n!\int_a^x f^{(n+1)}(t)dt \\
&= \int_a^b f^{(n+1)}(t)\left[\frac{d^n}{dx^n}(x-t)_+^n\right]dt. \quad \blacksquare
\end{aligned}
$$

Thus the differential operators

$$
\frac{d^k}{dx^k}, \quad k = 1, \ \ldots, \ n,
$$

commute with integration. Because $I(f) = I_x(f)$ is a linear combination of differential operators, it also commutes with integration.

Finally the continuity properties of the integrand $f^{(n+1)}(t)(x-t)_+^n$ are such that the following two integrations can be interchanged:

$$\int_a^b \left[\int_a^b f^{(n+1)}(t)(x-t)_+^n \, dt\right] dx = \int_a^b f^{(n+1)}(t) \left[\int_a^b (x-t)_+^n \, dx\right] dt.$$

This then shows the entire operator R_x commutes with integration, and we obtain the desired result

$$R(f) = \frac{1}{n!} \int_a^b f^{(n+1)}(t) R_x((x-t)_+^n) dt. \quad \blacksquare$$

For a surprisingly large class of integration rules, the Peano kernel $K(t)$ has constant sign on $[a, b]$. In this case, the mean-value theorem of integral calculus gives

$$R(f) = f^{(n+1)}(\xi) \int_a^b K(t)dt \quad \text{for some} \quad \xi \in (a, b).$$

The above integral of $K(t)$ does not depend on f, and can therefore be determined by applying R, for instance, to the polynomial $f(x) := x^{n+1}$. This gives

$$R(f) = \frac{R(x^{n+1})}{(n+1)!} f^{(n+1)}(\xi) \quad \text{for some} \quad \xi \in (a, b).$$

In the case of Simpson's rule, $K(t) \geq 0$ for $-1 \leq t \leq 1$.

$$\frac{R(x^4)}{4!} = \frac{1}{24}\left(\tfrac{1}{3}\cdot 1 + \tfrac{4}{3}\cdot 0 + \tfrac{1}{3}\cdot 1 - \int_{-1}^{1} x^4 dx\right) = \frac{1}{90},$$

error of Simpson's formula

$$\tfrac{1}{3}f(-1) + \tfrac{4}{3}f(0) + \tfrac{1}{3}f(1) - \int_{-1}^{1} f(t)dt = \tfrac{1}{90}f^{(4)}(\xi), \quad \xi \in (a,b).$$

Newton-Cotes formulas of degree n is exact for
- $P \in \Pi_n$ if n is odd,
- $P \in \Pi_{n+1}$ if n is even

The Peano kernels for the Newton-Cotes formulas are of constant sign.

Steffensen (1950)

$$R_n(f) = \begin{cases} \dfrac{R_n(x^{n+1})}{(n+1)!} f^{(n+1)}(\xi), & \text{if } n \text{ is odd}, \\ \dfrac{R_n(x^{n+2})}{(n+2)!} f^{(n+2)}(\xi), & \text{if } n \text{ is even}. \end{cases} \quad \xi \in (a,b),$$

$$R(f) = \frac{h}{2}(f(a) + f(b)) + \frac{h^2}{12}(f'(a) - f'(b)) - \int_b^b f(x)dx, \quad h := b - a,$$

vanishes for all polynomials $P \in \Pi_3$.

For $n = 3$, Peano kernel:

$$\begin{aligned} K(t) &= \frac{1}{6} R_x((x-t)_+^3) \\ &= \frac{1}{6}\left[\frac{h}{2}((a-t)_+^3 + (b-t)_+^3) + \frac{h^2}{4}((a-t)_+^2 - (b-t)_+^2) - \int_a^b (x-t)_+^3 dx\right] \\ &= \frac{1}{6}\left[\frac{h}{2}(b-t)^3 - \frac{h^2}{4}(b-t)^2 - \frac{1}{4}(b-t)^4\right] \\ &= -\tfrac{1}{24}(b-t)^2(a-t)^2 \le 0 \end{aligned}$$

We find for $a = 0$, $b = 1$ that

$$\frac{R(x^4)}{4!} = \tfrac{1}{24}(\tfrac{1}{2} \cdot 1 + \tfrac{1}{12} \cdot (-4) - \tfrac{1}{5}) = -\tfrac{1}{720}.$$

$$R(f) = -\frac{1}{24}\int_a^b f^{(4)}(t)(b-t)^2(a-t)^2 dt = -\frac{(b-a)^5}{720} f^{(4)}(\xi), \quad \xi \in (a, b),$$

The Euler–Maclaurin Summation Formula

for $g \in C^{2m+2}[0,1])$

$$\int_0^1 g(t)dt = \frac{g(0)}{2} + \frac{g(1)}{2} + \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!}(g^{(2l-1)}(0) - g^{(2l-1)}(1))$$
$$- \frac{B_{2m+2}}{(2m+2)!} g^{(2m+2)}(\xi), \quad 0 < \xi < 1.$$

Here B_k are the classical *Bernoulli numbers*

$$B_2 = \tfrac{1}{6}, \quad B_4 = -\tfrac{1}{30}, \quad B_6 = \tfrac{1}{42}, \quad B_8 = -\tfrac{1}{30}, \ \ldots,$$

for $g \in C^{2m+2}[0,N]$

$$\int_0^N g(t)dt = \frac{g(0)}{2} + g(1) + \cdots + g(N-1) + \frac{g(N)}{2}$$
$$+ \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!}(g^{(2l-1)}(0) - g^{(2l-1)}(N))$$
$$- \frac{B_{2m+2}}{(2m+2)!} N g^{(2m+2)}(\xi), \quad 0 < \xi < N.$$

$$
\begin{aligned}
&\frac{g(0)}{2} + g(1) + \cdots + g(N-1) + \frac{g(N)}{2} \\
&= \int_0^N g(t)dt + \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!}(g^{(2l-1)}(N) - g^{(2l-1)}(0)) \\
&\quad + \frac{B_{2m+2}}{(2m+2)!} N g^{(2m+2)}(\xi), \quad 0 < \xi < N.
\end{aligned}
$$

For a general uniform partition $x_i = a + ih$, $i = 0, \ldots, N$, $x_N = b$, of the interval $[a, b]$,

$$
\begin{aligned}
T(h) = \int_a^b f(t)dt &+ \sum_{l=1}^{m} h^{2l} \frac{B_{2l}}{(2l)!}(f^{(2l-1)}(b) - f^{(2l-1)}(a)) \\
&+ h^{2m+2} \frac{B_{2m+2}}{(2m+2)!}(b-a) f^{(2m+2)}(\xi), \quad a < \xi < b, \quad h = (b-a)/N,
\end{aligned}
$$

where $T(h)$ denotes the trapezoidal sum

$$
T(h) = h\left[\frac{f(a)}{2} + f(a+h) + \cdots + f(b-h) + \frac{f(b)}{2}\right].
$$

Properties of the Bernoulli polynomials

23.1.1 $$\frac{te^{xt}}{e^t-1}=\sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!} \qquad |t|<2\pi$$

23.1.2 $$B_n=B_n(0) \qquad n=0, 1, \ldots$$

23.1.3 $$B_0=1,\ B_1=-\frac{1}{2},\ B_2=\frac{1}{6},\ B_4=-\frac{1}{30}$$

23.1.4 $$\sum_{k=1}^{m} k^n=\frac{B_{n+1}(m+1)-B_{n+1}}{n+1} \qquad m, n=1, 2,$$

23.1.5 $$B_n'(x)=nB_{n-1}(x) \qquad n=1, 2, \ldots$$

23.1.6 $$B_n(x+1)-B_n(x)=nx^{n-1} \qquad n=0, 1, \ldots$$

23.1.7 $$B_n(x+h)=\sum_{k=0}^{n}\binom{n}{k} B_k(x)h^{n-k} \qquad n=0, 1, \ldots$$

23.1.8 $$B_n(1-x)=(-1)^nB_n(x) \qquad n=0, 1, \ldots$$

23.1.9 $$(-1)^nB_n(-x)=B_n(x)+nx^{n-1} \qquad n=0, 1, \ldots$$

23.1.10 $$B_n(mx)=m^{n-1}\sum_{k=0}^{m-1} B_n\left(x+\frac{k}{m}\right) \qquad n=0, 1, \ldots \quad m=1, 2, \ldots$$

23.1.11 $$\int_a^x B_n(t)dt=\frac{B_{n+1}(x)-B_{n+1}(a)}{n+1}$$

23.1.12 $$\int_0^1 B_n(t)B_m(t)dt=(-1)^{n-1}\frac{m!n!}{(m+n)!}B_{m+n}$$

$$m, n=1, 2, \ldots$$

23.1.13 $|B_{2n}|>|B_{2n}(x)| \qquad n=1, 2, \ldots, \qquad 1>x>0$

23.1.14

$$\frac{2(2n+1)!}{(2\pi)^{2n+1}}\left(\frac{1}{1-2^{-2n}}\right)>(-1)^{n+1}B_{2n+1}(x)>0$$

$$n=1, 2, \ldots, \qquad \tfrac{1}{2}>x>0$$

23.1.15

$$\frac{2(2n)!}{(2\pi)^{2n}}\left(\frac{1}{1-2^{1-2n}}\right)>(-1)^{n+1}B_{2n}>\frac{2(2n)!}{(2\pi)^{2n}}$$

23.1.16

$$B_n(x)=-2\frac{n!}{(2\pi)^n}\sum_{k=1}^{\infty}\frac{\cos(2\pi kx-\tfrac{1}{2}\pi n)}{k^n}$$

$$n>1, 1\geq x\geq 0$$

$$n=1, 1>x>0$$

23.1.17

$$B_{2n-1}(x)=\frac{(-1)^n 2(2n-1)!}{(2\pi)^{2n-1}}\sum_{k=1}^{\infty}\frac{\sin 2k\pi x}{k^{2n-1}}$$

$$n>1, 1\geq x\geq 0$$

$$n=1, 1>x>0$$

23.1.18

$$B_{2n}(x)=\frac{(-1)^{n-1}2(2n)!}{(2\pi)^{2n}}\sum_{k=1}^{\infty}\frac{\cos 2k\pi x}{k^{2n}}$$

$$n=1,2, \ldots, \qquad 1\geq x\geq 0$$

23.1.19 $B_{2n+1}=0 \qquad n=1,2,\ldots$

23.1.20 $B_n(0)=(-1)^n B_n(1)$

$=B_n \qquad n=0,1,\ldots$

23.1.21 $B_n(\tfrac{1}{2})=-(1-2^{1-n})B_n \qquad n=0,1,\ldots$

23.1.22 $B_n(\tfrac{1}{4})=(-1)^n B_n(\tfrac{3}{4})$

$=-2^{-n}(1-2^{1-n})B_n-n4^{-n}E_{n-1}$

$n=1,2,\ldots$

23.1.23 $B_{2n}(\tfrac{1}{3})=B_{2n}(\tfrac{2}{3})$

$=-2^{-1}(1-3^{1-2n})B_{2n} \qquad n=0,1,\ldots$

23.1.24 $B_{2n}(\tfrac{1}{6})=B_{2n}(\tfrac{5}{6})$

$=2^{-1}(1-2^{1-2n})(1-3^{1-2n})B_{2n}$

$n=0,1,\ldots$

from:
Abramowitz, Stegun
Handbook of Mathematical Functions with
Formulas, Graphs, and Mathematical Tables

Properties of the Bernoulli polynomials that we need in the proof of the Euler-Maclaurin Theorem

- $B'_{n+1}(x) \quad = \quad (n+1)B_n(x), \quad n = 0, 1, 2, \ldots.$

$$\begin{aligned}
\frac{te^{xt}}{e^t - 1} &= \sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!} \qquad \Rightarrow \qquad B_0(x) = 1. \\
\frac{d}{dx}\frac{te^{xt}}{e^t - 1} &= \frac{d}{dx}\sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!} \\
\frac{t^2e^{xt}}{e^t - 1} &= \sum_{n=1}^{\infty} B'_n(x)\frac{t^n}{n!} = \sum_{n=0}^{\infty} B'_{n+1}(x)\frac{t^{n+1}}{(n+1)!} \\
\frac{te^{xt}}{e^t - 1} &= \sum_{n=0}^{\infty} B'_{n+1}(x)\frac{t^n}{(n+1)!} \\
B'_{n+1}(x) &= (n+1)B_n(x), \quad n = 0, 1, 2, \ldots.
\end{aligned}$$

- $(-1)^n B_n(1-x) = B_n(x).$

$$\begin{aligned}
\sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!} &= \frac{te^{xt}}{e^t-1} \\
\sum_{n=0}^{\infty}(-1)^n B_n(1-x)\frac{t^n}{n!} &= \sum_{n=0}^{\infty} B_n(1-x)\frac{(-t)^n}{n!} = \frac{-te^{(1-x)(-t)}}{e^{-t}-1} \\
\sum_{n=0}^{\infty}(-1)^n B_n(1-x)\frac{t^n}{n!} &= \frac{-te^{(1-x)(-t)}}{e^{-t}-1}.\frac{e^t}{e^t} = \frac{te^{xt}}{e^t-1} = \sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!} \\
(-1)^n B_n(1-x) &= B_n(x).
\end{aligned}$$

- $(-1)^n B_n(1) = B_n(0).$

by induction:

$$B_0(x) \equiv 1,$$

$$B_1(x) \equiv x - \tfrac{1}{2},$$

$$B_2(x) \equiv x^2 - x + \tfrac{1}{6},$$

$$B_3(x) \equiv x^3 - \tfrac{3}{2}x^2 + \tfrac{1}{2}x,$$

$$B_4(x) \equiv x^4 - 2x^3 + x^2 - \tfrac{1}{30}, \ \ldots$$

$$\vdots$$

Bernoulli polynomials.

$$B_{2l+1}(0) = B_{2l+1}(1) = 0 \quad \text{for } l > 0,$$

$$B_k(0) = B_k(1) = B_k \quad \text{for } k > 1, \qquad \text{for even } k.$$

$$B_k = B_k(0)$$

Bernoulli numbers

This gives

$$\int_0^1 B_k(t)dt = \frac{1}{k+1}(B_{k+1}(1) - B_{k+1}(0)) = 0 \quad \text{for } k \geq 1.$$

by induction:

a)	$(-1)^m B_{2m-1}(x) > 0$	for $0 < x < \frac{1}{2}$,
b)	$(-1)^m (B_{2m}(x) - B_{2m}) > 0$	for $0 < x < 1$,
c)	$(-1)^{m+1} B_{2m} > 0.$	

proof. (a) holds for $m = 1$. Suppose it holds for some $m \geq 1$. Then for $0 < x \leq \frac{1}{2}$,

$$\frac{(-1)^m}{2m}(B_{2m}(x) - B_{2m}) = (-1)^m \int_0^x B_{2m-1}(t)dt > 0. \quad + \quad \boxed{(-1)^k B_k(1-x) = B_k(x).} \longrightarrow \text{(b)}$$

$$(-1)^{m+1} B_{2m} = (-1)^m \int_0^1 (B_{2m}(t) - B_{2m})dt > 0, \quad \longrightarrow \quad \text{(c)}$$

We must now prove (a) for $m+1$.

$B_{2m+1}(0) = 0$

$B_{2m+1}(\frac{1}{2}) = 0$

$\exists\ \bar{x}$ between 0 and $\frac{1}{2}$ $\quad B_{2m-1}(\bar{x}) = 0$,

in violation of the induction hypothesis.

The sign of $B_{2m+1}(x)$ in $0 < x < \frac{1}{2}$ is equal to the sign of its first derivative at zero, whose value is $(2m+1)B_{2m}(0) = (2m+1)B_{2m}$. The sign of the latter is $(-1)^{m+1}$ by (c).

Proof We will use integration by parts and successively determine polynomials $B_k(x)$, starting with $B_1(x) \equiv x - \frac{1}{2}$, such that

$$\int_0^1 g(t)dt = B_1(t)g(t)\Big|_0^1 - \int_0^1 B_1(t)g'(t)dt,$$

$$\int_0^1 B_1(t)g'(t)dt = \frac{1}{2}B_2(t)g'(t)dt\Big|_0^1 - \frac{1}{2}\int_0^1 B_2(t)g''(t)dt,$$

$$\vdots$$

$$\int_0^1 B_{k-1}(t)g^{(k-1)}(t)dt = \frac{1}{k}B_k(t)g^{(k-1)}(t)\Big|_0^1 - \frac{1}{k}\int_0^1 B_k(t)g^{(k)}(t)dt,$$

where

$$B'_{k+1}(x) = (k+1)B_k(x), \quad k = 1,\ 2,\ \ldots\ .$$

Combining the first $2m+1$ relations we get

$$\int_0^1 g(t)dt = \frac{g(0)}{2} + \frac{g(1))}{2} + \sum_{l=1}^{m} \frac{B_{2l}}{(2l)!}(g^{(2l-1)}(0) - g^{(2l-1)}(1)) + r_{m+1},$$

where the error term r_{m+1} is given by the integral

$$r_{m+1} := \frac{-1}{(2m+1)!}\int_0^1 B_{2m+1}(t)g^{(2m+1)}(t)dt.$$

We use integration by parts once more to transform the error term:

$$\int_0^1 B_{2m+1}(t)g^{(2m+1)}(t)dt = \frac{1}{2m+2}(B_{2m+2}(t) - B_{2m+2})g^{(2m+1)}(t)\Big|_0^1$$
$$- \frac{1}{2m+2}\int_0^1 (B_{2m+2}(t) - B_{2m+2})g^{(2m+2)}(t)dt.$$

$$r_{m+1} = \frac{1}{(2m+2)!}\int_0^1 (B_{2m+2}(t) - B_{2m+2})g^{(2m+2)}(t)dt.$$

$(B_{2m+2}(t) - B_{2m+2})$ does not change its sign between 0 and 1.

Since the function $B_{2m+2}(x) - B_{2m+2}$ does not change its sign in the interval of integration, there exists ξ, $0 < \xi < 1$, such that

$$r_{m+1} = \frac{g^{(2m+2)}(\xi)}{(2m+2)!} \int_0^1 (B_{2m+2}(t) - B_{2m+2})dt.$$

$$r_{m+1} = -\frac{B_{2m+2}}{2m+2)!} g^{(2m+2)}(\xi),$$