Improving the accuracy of the Trapezoidal Rule

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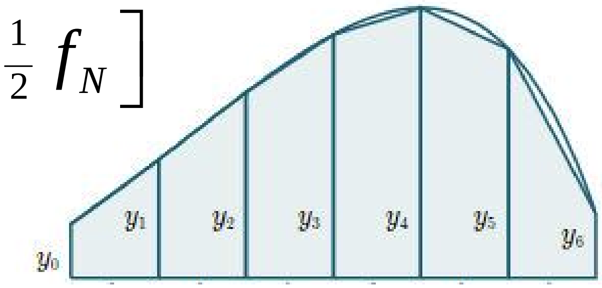
The trapezoidal rule

$$\int_{x_0}^{x_N} f(x)dx \approx h\left[\tfrac{1}{2} f_0 + f_1 + f_2 + \ldots + f_{N-1} + \tfrac{1}{2} f_N\right]$$



Babylonian astronomers, 50 BC

Error typically $O(h^2)$, but becomes spectrally accurate if the integrand is periodic. This follows from Euler-Maclaurin's formula (1740):

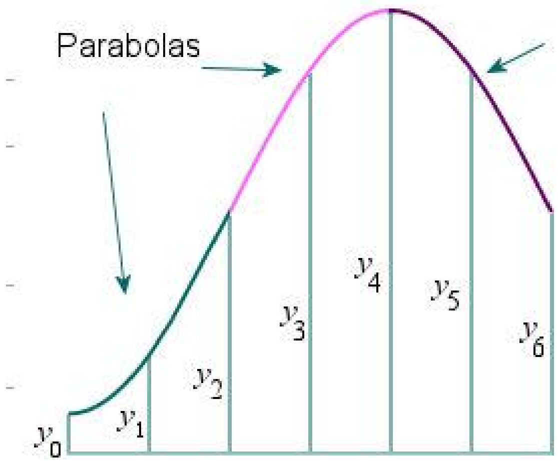
$$\int_{x_0}^{x_N} f(x)dx = h\left[\tfrac{1}{2} f_0 + f_1 + f_2 + \ldots + f_{N-1} + \tfrac{1}{2} f_N\right] +$$

$$+\frac{h^2}{12}\left[f_0^{I} - f_N^{I}\right] - \frac{h^4}{720}\left[f_0^{III} - f_N^{III}\right] + \frac{h^6}{30240}\left[f_0^{V} - f_N^{V}\right] - + \ldots$$

The coefficients can be obtained by the *generating function*

$$\frac{1}{1-e^{-z}} - \frac{1}{z} \quad = \quad \frac{1}{2} + \frac{1}{12}z - \frac{1}{720}z^3 + \frac{1}{30240}z^5 - \frac{1}{1209600}z^7 + - \ldots$$

Simpson and Newton-Cotes formulas



Trapezoidal rule: Fit by piecewise linear functions

Gives weights $h\left[\frac{1}{2}\ 1\ 1\ 1\ 1\ 1\ \ldots\ 1\ \frac{1}{2}\right]$

Simpson's rule: Fit by succession of quadratics

Simpson (1710-1761); however used by Kepler (1571-1630)

Gives weights $\frac{h}{3}[1\ 4\ 2\ 4\ 2\ 4\ 2\ldots\ 4\ 1]$

Newton-Cotes idea: Continue by using piecewise cubics, quartics, etc.

Newton (1642-1726), Cotes (1682-1716)

Orders of accuracy increases (from Trap. Rule) 2, 4, 4, 6, 6, 8, 8, ...

Concept flawed for several reasons:

- Essentially ALL errors in Trap. Rule comes from the ends; should do corrections there and NOT 'contaminate' throughout the whole interior.
- For periodic problem, Trap error ≈ (Simpson error)^2.
- Becomes very unstable for increasing orders.

Gregory's method

With notation

$$\Delta^0 f(x) = f(x) \qquad \nabla^0 f(x) = f(x)$$
$$\Delta^1 f(x) = f(x+h) - f(x) \qquad \nabla^1 f(x) = f(x) - f(x-h)$$
$$\Delta^2 f(x) = f(x+2h) - 2f(x+h) + f(x) \qquad \nabla^2 f(x) = f(x) - 2f(x-h) + f(x-2h)$$
$$\ldots \qquad \ldots$$

$$\int_{x_0}^{x_N} f(x)dx = h\left[f_0 + f_1 + f_2 + \ldots + f_{N-1} + f_N\right] +$$
$$-\tfrac{1}{2}\left[\Delta^0 f_0 + \nabla^0 f_N\right] + \tfrac{1}{12}\left[\Delta^1 f_0 - \nabla^1 f_N\right] - \tfrac{1}{24}\left[\Delta^2 f_0 - \nabla^2 f_N\right] + \tfrac{19}{720}\left[\Delta^3 f_0 - \nabla^3 f_N\right] - \tfrac{3}{160}\left[\Delta^4 f_0 - \nabla^4 f_N\right] + - \ldots$$

Non-trivial weights at left end; each term increases accuracy order by one.

$p =$	Non-trivial weights									
2	$\frac{1}{2}$									
3	$\frac{5}{12}$	$\frac{13}{12}$								
4	$\frac{3}{8}$	$\frac{7}{6}$	$\frac{23}{24}$							
5	$\frac{251}{720}$	$\frac{299}{240}$	$\frac{211}{240}$	$\frac{739}{720}$						
6	$\frac{95}{288}$	$\frac{317}{240}$	$\frac{23}{30}$	$\frac{739}{720}$	$\frac{157}{160}$					
7	$\frac{19087}{60480}$	$\frac{84199}{60480}$	$\frac{18869}{30240}$	$\frac{37621}{30240}$	$\frac{55031}{60480}$	$\frac{61343}{60480}$				
8	$\frac{5257}{17280}$	$\frac{22081}{15120}$	$\frac{54851}{120960}$	$\frac{103}{70}$	$\frac{89437}{120960}$	$\frac{16367}{15120}$	$\frac{23917}{24192}$			
9	$\frac{1070017}{3628800}$	$\frac{5537111}{3628800}$	$\frac{103613}{403200}$	$\frac{261115}{145152}$	$\frac{298951}{725760}$	$\frac{515677}{403200}$	$\frac{3349879}{3628800}$	$\frac{3662753}{3628800}$		
10	$\frac{25713}{89600}$	$\frac{1153247}{725760}$	$\frac{130583}{3628800}$	$\frac{903527}{403200}$	$-\frac{797}{5670}$	$\frac{6244961}{3628800}$	$\frac{56621}{80640}$	$\frac{3891877}{3628800}$	$\frac{1028617}{1036800}$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

James Gregory (1638-1675)

Extract from a letter by Gregory to John Collins, dated November 23, 1670:

Transcribed to print by Oxford Univ. Press, 1840
(with them introducing a typo, 164 in place of 160)

ponendo $AP = PO = c$

$PB = d$

$$\text{primam ex differentiis} \begin{cases} \text{primis} & = f \\ \text{secundis} & = h \\ \text{tertiis} & = i \\ \text{quartis} & = k \\ \text{quintis} & = l \end{cases}$$

et omnes differentias affici signo $+$, erit $ABP =$

$$\frac{dc}{2} - \frac{fc}{12} + \frac{hc}{24} - \frac{19ic}{720} + \frac{3kc}{164} - \frac{863\,lc}{60480} + \text{\&c. in infinitum.}$$

Gregory's exact derivation of this particular expansion is unknown, but he did extensive work on calculus, Taylor expansions, derivatives and integrals in the 1660's. He most likely obtained the coefficients from their *generating function*

$$\frac{1}{\log(1+z)} - \frac{1}{z} = \frac{1}{2} - \frac{1}{12}z + \frac{1}{24}z^2 - \frac{19}{720}z^3 + \frac{3}{160}z^4 - \frac{863}{60480}z^5 + - \ldots$$

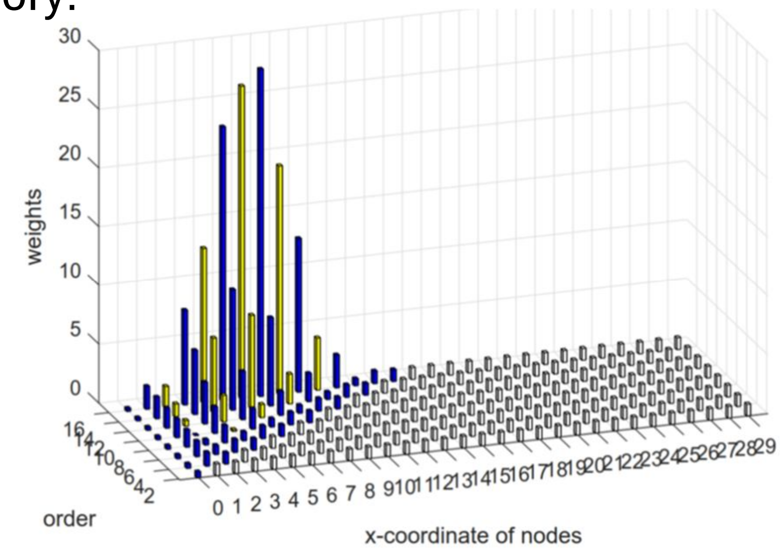
Note:

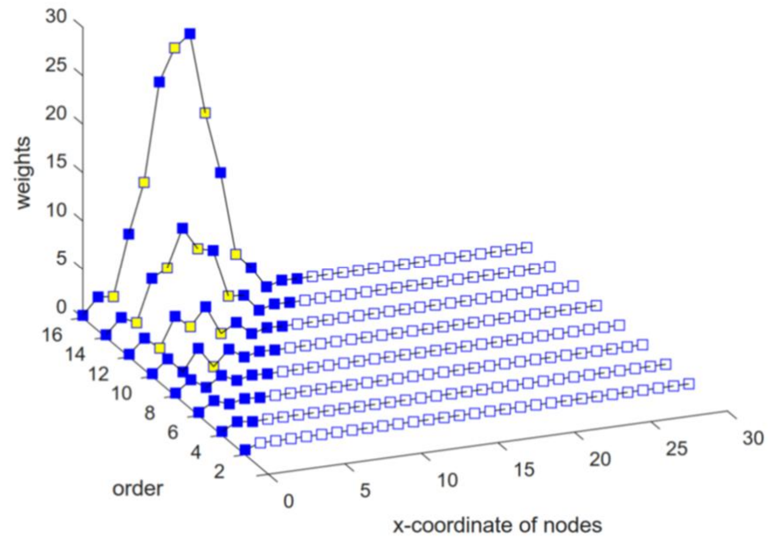
The first publications on calculus: Gottfried Leibnitz, 1684, Isaac Newton, 1687

Taylor expansions: Brook Taylor, 1715.

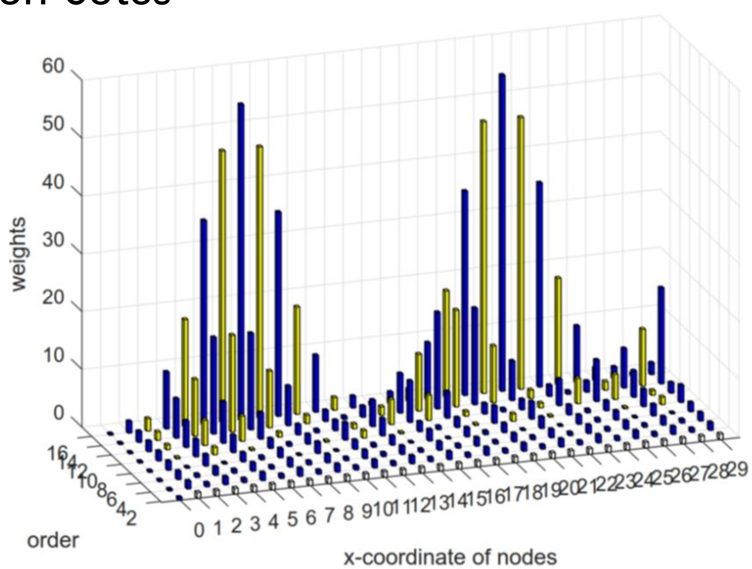
Comparison of weights, Gregory vs. Newton-Cotes methods

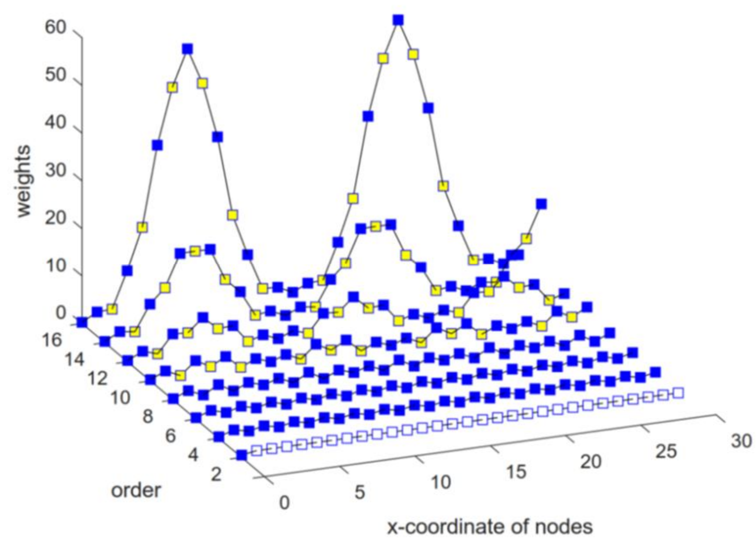
Gregory:



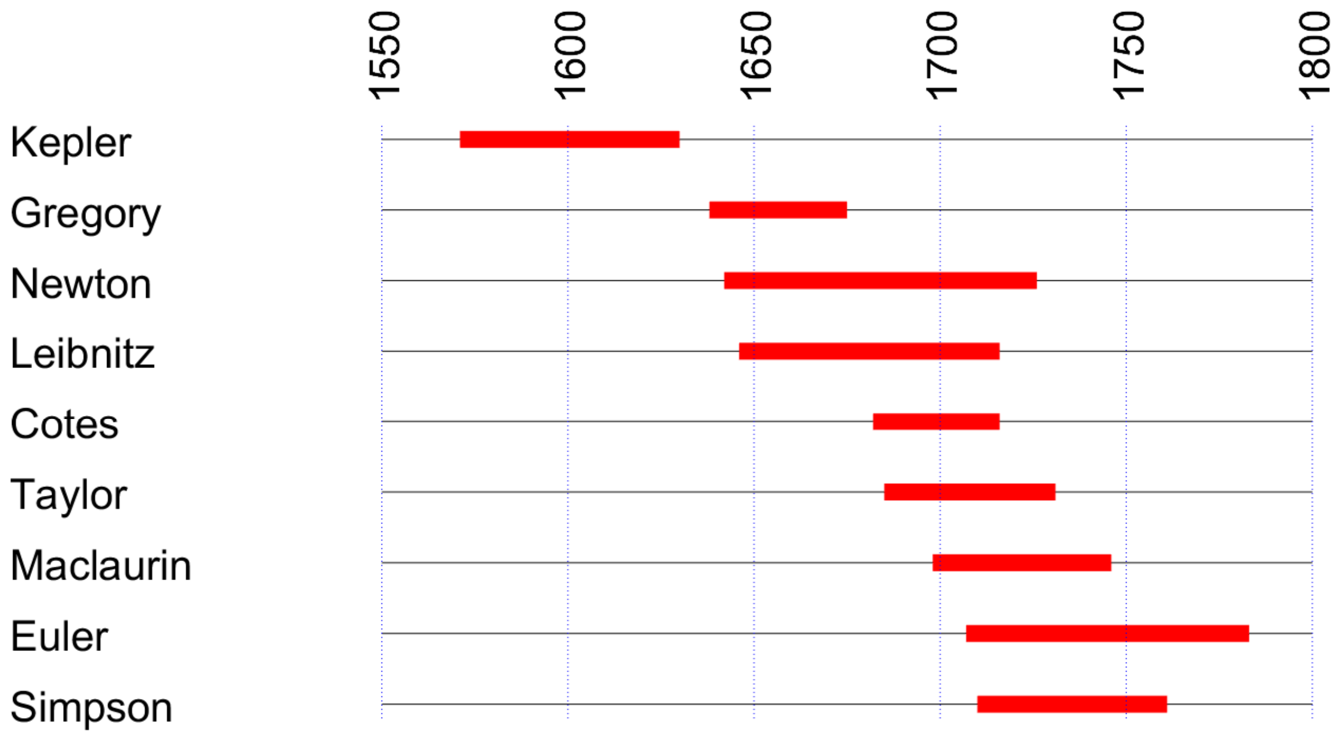


Newton-Cotes



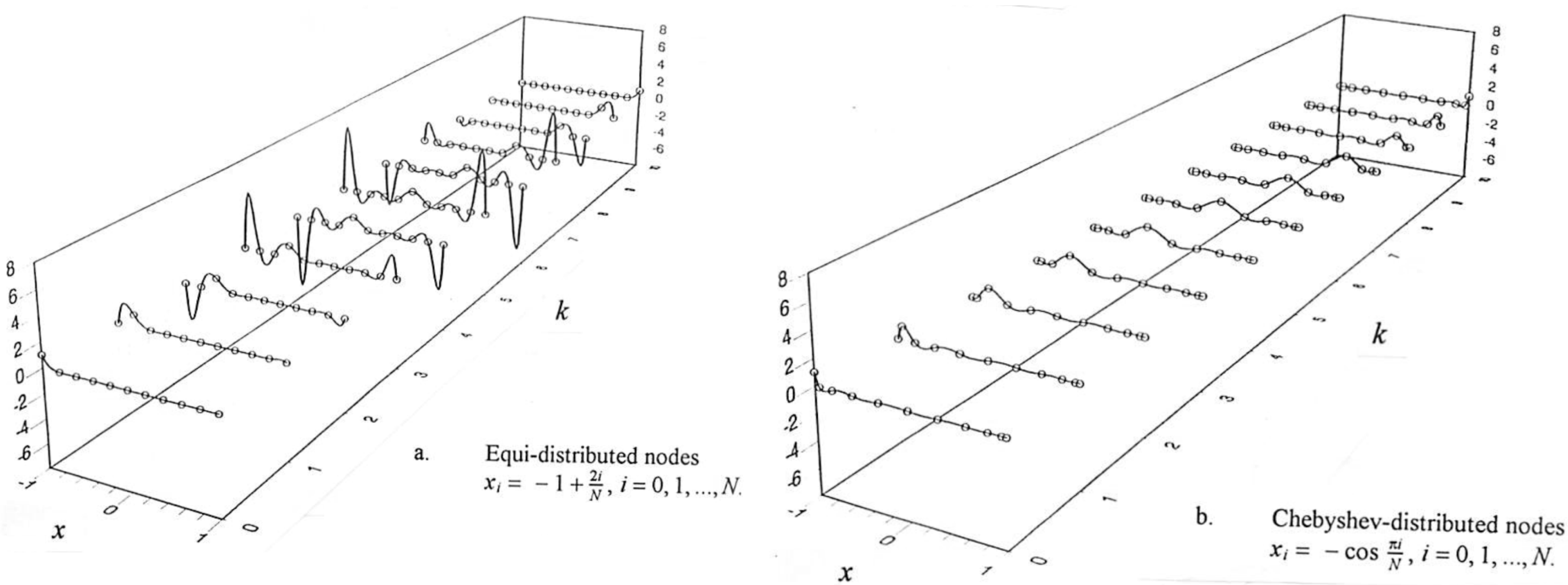


Timeline of the pioneers of numerical quadrature



The Runge phenomenon (Runge 1901)

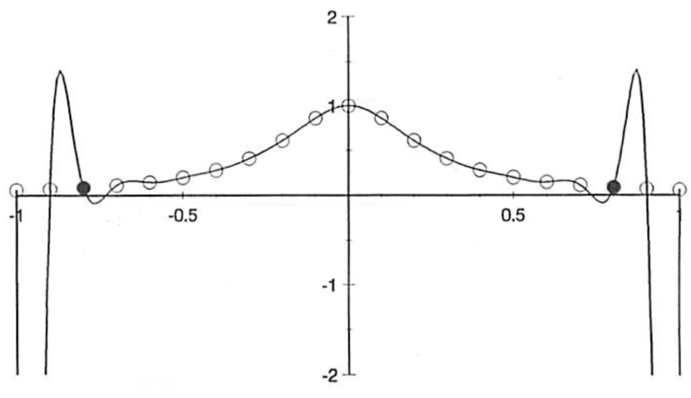
Polynomial *cardinal functions*; 11 nodes over [-1,1]



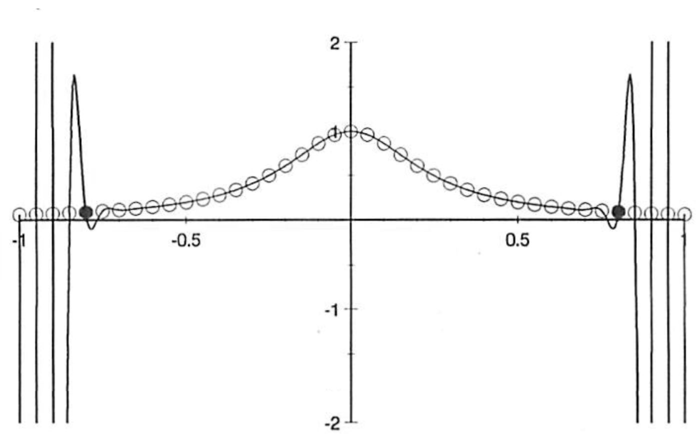
Node clustering remedy not available – committed here to equispaced node layout.

The Runge phenomenon

Commonly used demonstration function $f(x) = \dfrac{1}{1+16x^2}$



$N = 20$



$N = 40$

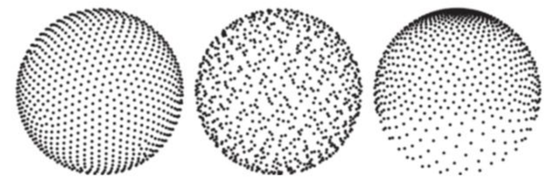
For equispaced interpolation on [-1,1]:

Error: $E(z,N) \approx e^{N(\psi(z_0)-\psi(z))}$ where $\psi(z) = -\dfrac{1}{2}\mathrm{Re}\left[(1-z)\log(1-z)-(-1-z)\log(-1-z)\right]$

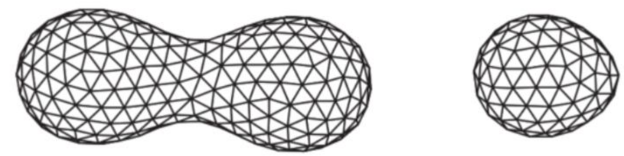
Here z need not be on the real axis; z_0 is the location of the nearest singularity (in the example, $z_0 = \pm\dfrac{i}{4}$).

RBF-FD papers for numerical quadrature over various surfaces

J.A. Reeger and BF: Numerical quadrature over the surface of a sphere, *Studies in Appl. Math.*, 2015



J.A. Reeger, BF and M.L. Watts: Numerical quadrature over smooth closed surfaces, *Proc. R. Soc. A*, 2017



J.A. Reeger and BF: Numerical quadrature over smooth surfaces with boundaries, *J. Comput. Phys*. 2018

In all cases: Accuracy $O(h^7)$ with h a `typical' node separation.
With N nodes, total cost for all weights $O(N \log N)$ operations

In last case, when increasing the accuracy order further, no Runge phenomenon arose (in spite of no node clustering towards the boundary).

When simplified first to flat surface patch and then to a 1-D interval with equispaced nodes, method produced a 'Gregory-like' scheme, of high order of accuracy but still free from the Runge phenomenon.

Motivated current project: Can one derive such Gregory-type schemes by some more direct (not RBF-based) approach?

Revisit Gregory-type quadrature schemes

Consider

$$\int_0^\infty f(x)\,dx \approx \sum_{k=0}^{\infty} w_k\, f(k) \tag{1}$$

where all weights w_k are 1 from $k = N+1$ and onwards.

If $f(x)$ is defined on $[-\infty, \infty]$, its Fourier modes are $e^{i\omega x}$, ω real.
The counterpart modes for $[0, \infty]$ are e^{-zx}, Re $z \geq 0$. Thus, substitute $f(x) = e^{-zx}$ into (1):

$$\frac{1}{z} = \sum_{k=0}^{\infty} w_k e^{-zk} \tag{2}$$

Subtract from (2) the identity

$$\frac{1}{1-e^{-z}} = \sum_{k=0}^{\infty} 1 \cdot e^{-zk} \tag{3}$$

Let $d_k = w_k - 1$. Task becomes choosing coefficients d_k , $k = 0, 1, 2, \ldots , N$ so that

$$\frac{1}{z} - \frac{1}{1-e^{-z}} = \sum_{k=0}^{N} d_k e^{-zk} \tag{4}$$

becomes as accurate as possible around $z = 0$.

For every power of z we can match the Taylor expansions of the LHS and RHS of (4), we gain one order of accuracy in the quadrature formula (1).

Derive matching conditions

$$\frac{1}{z}-\frac{1}{1-e^{-z}}=\sum_{k=0}^{N} d_k e^{-zk}$$

LHS:

$$\frac{1}{z}-\frac{1}{1-e^{-z}}=-\frac{1}{2}-\frac{z}{12}+\frac{z^3}{720}-\frac{z^5}{30240}+\frac{z^7}{1209600}-+\dots$$

(Same as the generating function for the Euler-Maclaurin formula)

RHS: Taylor expand each exponential. Matching powers $k = 0,1,2,\dots,n \le N$ gives

$$\begin{bmatrix} 0^0 & 1^0 & 2^0 & \cdots & N^0 \\ 0^1 & 1^1 & 2^1 & \cdots & N^1 \\ \vdots & \vdots & & & \vdots \\ 0^n & 1^n & 2^n & \cdots & N^n \end{bmatrix} \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ d_n \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} -1/2 \\ 1/12 \\ 0 \\ -1/120 \\ 0 \\ \vdots \end{bmatrix}$$

RHS column vector entries are $B_{k+1}/(k+1)$ where the B_k are the Bernoulli numbers.

This (generally underdetermined) Vandermonde linear system can be rearranged to upper triangular form

Matching conditions

Equivalent system:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & \cdots & \cdots & \cdots \\ & 1 & 2 & 3 & 4 & \cdots & \cdots & \cdots \\ & & 1 & 3 & 6 & \cdots & \cdots & \cdots \\ & & & 1 & 4 & \cdots & \cdots & \cdots \\ & & & & 1 & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ d_n \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} -1/2 \\ 1/12 \\ -1/24 \\ 19/720 \\ -3/160 \\ \vdots \end{bmatrix}$$

RHS column vector contains the exact Gregory coefficients:

$$\int_{x_0}^{x_N} f(x)dx = h\left[f_0 + f_1 + f_2 + \ldots + f_{N-1} + f_N \right] - \tfrac{1}{2}\left[\Delta^0 f_0 + \nabla^0 f_N\right] + \tfrac{1}{12}\left[\Delta^1 f_0 - \nabla^1 f_N\right] - \tfrac{1}{24}\left[\Delta^2 f_0 - \nabla^2 f_N\right] + \tfrac{19}{720}\left[\Delta^3 f_0 - \nabla^3 f_N\right] - + \ldots$$

Multiply by Pascal triangle inverse from left:

$$\left[\begin{array}{ccccc|ccc} 1 & & & & & \cdots & \cdots & \cdots \\ & 1 & & & & \cdots & \cdots & \cdots \\ & & 1 & & & \cdots & B & \cdots \\ & & & 1 & & \cdots & \cdots & \cdots \\ & & & & 1 & \cdots & \cdots & \cdots \end{array}\right] \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ d_n \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 & -1 & 1 \\ & 1 & -2 & 3 & -4 \\ & & 1 & -3 & 6 \\ & & & 1 & -4 \\ & & & & 1 \end{bmatrix} \begin{bmatrix} -1/2 \\ 1/12 \\ -1/24 \\ 19/720 \\ -3/160 \\ \vdots \end{bmatrix} = \begin{bmatrix} g_0 \\ g_1 \\ g_2 \\ \vdots \\ \vdots \\ g_n \end{bmatrix}$$

Matching conditions

Relation to be satisfied for our quadrature weights to be accurate of order $p = n+2$:

$$\left[\begin{array}{ccccc|ccc} 1 &&&&& \cdots & \cdots & \cdots \\ & 1 &&&& \cdots & \cdots & \cdots \\ && 1 &&& \cdots & B & \cdots \\ &&& 1 && \cdots & \cdots & \cdots \\ &&&& 1 & \cdots & \cdots & \cdots \end{array}\right] \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ d_n \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 & -1 & 1 \\ & 1 & -2 & 3 & -4 \\ && 1 & -3 & 6 \\ &&& 1 & -4 \\ &&&& 1 \end{bmatrix} \begin{bmatrix} -1/2 \\ 1/12 \\ -1/24 \\ 19/720 \\ -3/160 \\ \vdots \end{bmatrix} = \begin{bmatrix} g_0 \\ g_1 \\ g_2 \\ \vdots \\ \vdots \\ g_n \end{bmatrix}$$

Explicit values are available for the B-matrix:
and also for the RHS vector:

$$B_{i,j} = \frac{(-1)^i j}{n+i-j} \binom{n+j}{j} \binom{n}{i}$$

Gregory weights w_k:

$p =$							
2	$\frac{1}{2}$						
3	$\frac{5}{12}$	$\frac{13}{12}$					
4	$\frac{3}{8}$	$\frac{7}{6}$	$\frac{23}{24}$				
5	$\frac{251}{720}$	$\frac{299}{240}$	$\frac{211}{240}$	$\frac{739}{720}$			
6	$\frac{95}{288}$	$\frac{317}{240}$	$\frac{23}{30}$	$\frac{739}{720}$	$\frac{157}{160}$		
7	$\frac{19087}{60480}$	$\frac{84199}{60480}$	$\frac{18869}{30240}$	$\frac{37621}{30240}$	$\frac{55031}{60480}$	$\frac{61343}{60480}$	
8	$\frac{5257}{17280}$	$\frac{22081}{15120}$	$\frac{54851}{120960}$	$\frac{103}{70}$	$\frac{89437}{120960}$	$\frac{16367}{15120}$	$\frac{23917}{24192}$

Gregory ‘corrections’ from weights all one; $d_k = w_k - 1$

$p =$							
2	$-\frac{1}{2}$						
3	$-\frac{7}{12}$	$\frac{1}{12}$					
4	$-\frac{5}{8}$	$\frac{1}{6}$	$-\frac{1}{24}$				
5	$-\frac{469}{720}$	$\frac{59}{240}$	$-\frac{29}{240}$	$\frac{19}{720}$			
6	$-\frac{193}{288}$	$\frac{77}{240}$	$-\frac{7}{30}$	$\frac{73}{720}$	$-\frac{3}{160}$		
7	$-\frac{41393}{60480}$	$\frac{23719}{60480}$	$-\frac{11371}{30240}$	$\frac{7381}{30240}$	$-\frac{5449}{60480}$	$\frac{863}{60480}$	
8	$-\frac{12023}{17280}$	$\frac{6961}{15120}$	$-\frac{66109}{120960}$	$\frac{33}{70}$	$-\frac{31523}{120960}$	$\frac{1247}{15120}$	$-\frac{275}{24192}$

The g-column is the corresponding row in the Gregory ‘correction table’.

Example: Create a quadrature scheme with weights $d_0, d_1, \dots, d_9$ of order $p = 8$:

Write

$$\left[\begin{array}{ccccc|ccc} 1 & & & & & \cdots & \cdots & \cdots \\ & 1 & & & & \cdots & \cdots & \cdots \\ & & 1 & & & \cdots & B & \cdots \\ & & & \ddots & & \cdots & \cdots & \cdots \\ & & & & 1 & \cdots & \cdots & \cdots \end{array}\right] \begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ \vdots \\ d_6 \\ \vdots \\ d_9 \end{bmatrix} = \begin{bmatrix} g_0 \\ g_1 \\ g_2 \\ \vdots \\ g_6 \end{bmatrix}$$

where $N = 9$ and $n = 6$ in the form

$$\begin{bmatrix} d_0 \\ d_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ d_6 \end{bmatrix} = \begin{bmatrix} -12023/17280 \\ 6961/15120 \\ -66109/120960 \\ 33/70 \\ -31523/120960 \\ 1247/15120 \\ -275/24192 \end{bmatrix} - \begin{bmatrix} 1 & 7 & 28 \\ -7 & -48 & -189 \\ 21 & 140 & 540 \\ -35 & -224 & -840 \\ 35 & 210 & 756 \\ -21 & -112 & -378 \\ 7 & 28 & 84 \end{bmatrix} \begin{bmatrix} d_7 \\ d_8 \\ d_9 \end{bmatrix}$$

By choosing *N* somewhat larger than *n*, we have an under-determined system, and we can then find a solution that minimizes the *d*-coefficients

and

we have a set-up for finding weight sets containing only relatively simple rational number weights.

Minimization solutions to the under-determined system

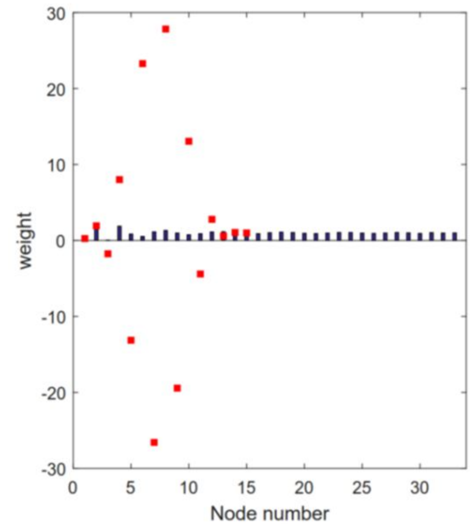
Choose desired accuracy order p , then take $n = p - 2$, and let $N > n$. For example, minimize:

L2: Matlab *lsqmin*
or use pseudoinverse

$$\sum_{k=0}^{N} s^{2k} d_k^2$$

L1: Mathematica *NMinimize*

$$\sum_{k=0}^{N} s^2 \, | \, d_k \, |$$



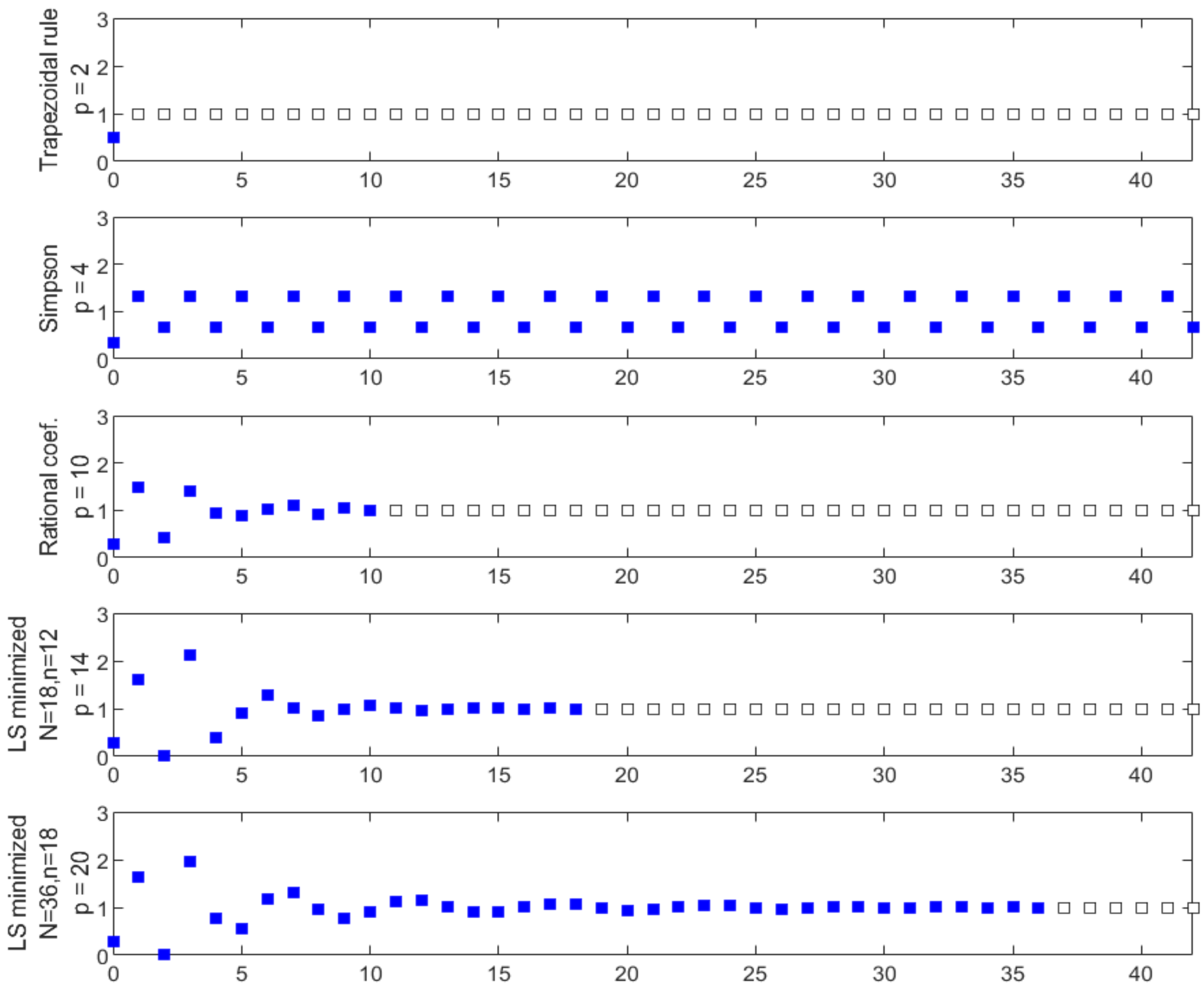
Order $p = 16$ schemes,
Gregory vs. L_2-generated

Example of a rational number solution

The following set of d_k 'correction' coefficients (weights $w_k = 1 + d_k$) gives an order $p = 10$ scheme:

$$\frac{1}{96}\left\{-\frac{26911}{400},\frac{628}{1350},-\frac{10421}{189},\frac{33487}{840},-\frac{31441}{4725},-\frac{16873}{1512},\frac{10567}{4200},\frac{10451}{1080},-\frac{28613}{3024},\frac{5099}{1400},-\frac{107}{200}\right\}$$

Illustration of weight sets that will be used in following test



Weight range in Gregory schemes of matching order *p*

[-0.14, 2.24]

[-7.8, 10.2]

[-276, 273]

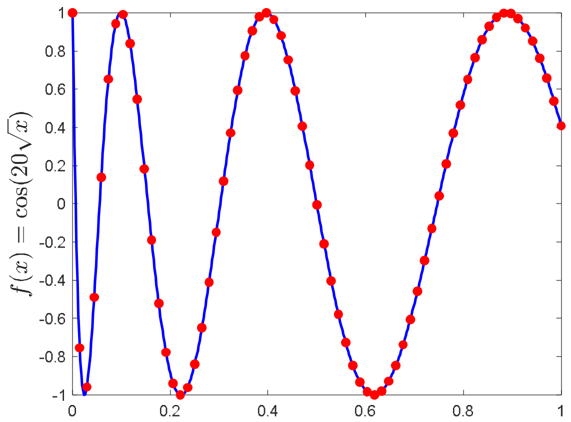
Corrections from the two sides can overlap.
For example rational coefficient scheme can be used on any equispaced node set of 11 or more nodes.

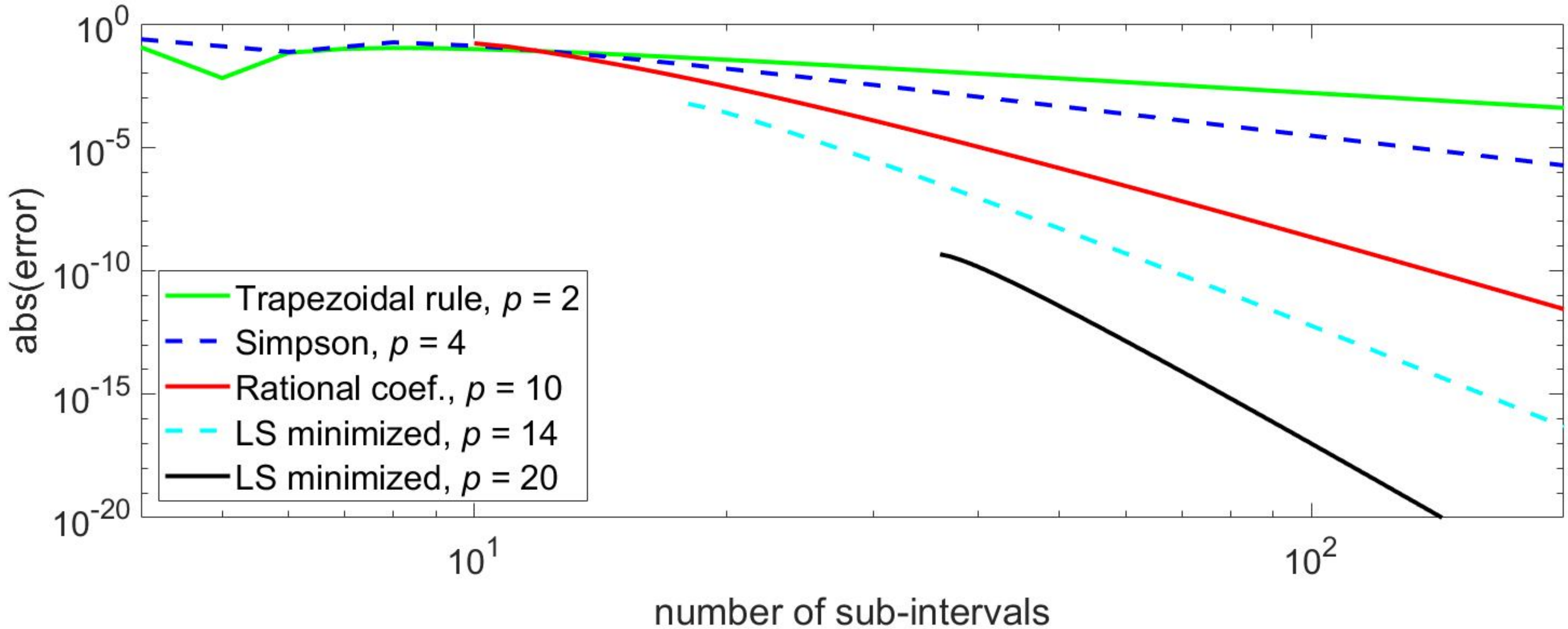
Numerical quadrature methods applied to a test function

Test function: $f(x) = \cos(20\sqrt{x})$

$$\int_0^1 f(x)dx = \frac{1}{200}(\cos(20) + 20\sin(20) - 1)$$

Test function with $N = 68$; gives error < 10^{-16}





Some conclusions

Historical notes:

- Several of Gregory's pioneering works around 1670 deserve much more recognition than is nowadays customary – including his pioneering works in calculus, use of Taylor expansions and, as focused on here, his quadrature method.

- Gregory's quadrature compares in most aspects favorably against the Newton and Cotes approach.

Specific to the present work:

- The Runge phenomenon is not quite as unavoidable as often portrayed.

- Allowing Gregory-type quadrature formulas to feature non-trivial weights in a somewhat wider interval than minimally needed avoids weights becoming negative, or wildly oscillatory.

Publications:

BF and J.A. Reeger, *An improved Gregory-like method for 1-D quadrature*, Numerische Mathematik (2019)
BF, *Improving the accuracy of the trapezoidal rule* (submitted, 2019)