Euler-Maclaurin without analytic derivatives

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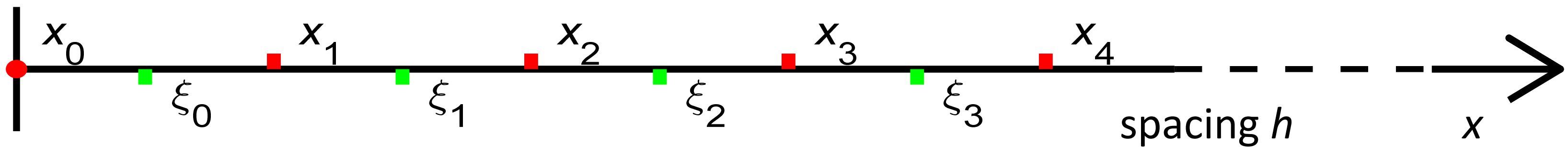
The Euler-Maclaurin formulas (for approximating infinite sums)



EM1 – Trapezoidal Rule

$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(x_k) \approx -\frac{h}{2} f(x_0) + \frac{h^2}{12} f^{(1)}(x_0) - \frac{h^4}{720} f^{(3)}(x_0) + \frac{h^6}{30240} f^{(5)}(x_0) - \frac{h^8}{1209600} f^{(7)}(x_0) + - \ldots$$

EM2 – Midpoint Rule

$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(\xi_k) \approx -\frac{h^2}{24} f^{(1)}(x_0) + \frac{7h^4}{5760} f^{(3)}(x_0) - \frac{31h^6}{967680} f^{(5)}(x_0) + \frac{127h^8}{154828800} f^{(7)}(x_0) + - \ldots$$

James Stirling

1692-1770

Colin Maclaurin

1698-1746

Leonhard Euler

1707-1783

Derivation of the EM1 formula (Part 1)

$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(x_k) \approx -\frac{h}{2} f(x_0) + \frac{h^2}{12} f^{(1)}(x_0) - \frac{h^4}{720} f^{(3)}(x_0) + \frac{h^6}{30240} f^{(5)}(x_0) - \frac{h^8}{1209600} f^{(7)}(x_0) + - \ldots$$

$$= \sum_{k=1}^{\infty} \frac{B_k}{k!} h^k f^{(k-1)}(x_0)$$

where the Bernoulli numbers B_k are defined by $\frac{z}{e^z - 1} = \sum_{k=0}^{\infty} \frac{B_k}{k!} z^k$

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_3 = 0, \quad B_4 = -\frac{1}{30}, \quad B_5 = 0, \quad B_6 = \frac{1}{42}, \quad B_7 = 0, \quad B_8 = -\frac{1}{30}, \quad B_9 = 0, \quad B_{10} = \frac{5}{66}, \quad \ldots$$

Neat identity:

Multiplying up the denominator: $z = \left(\frac{1}{1!} z + \frac{1}{2!} z^2 + \frac{1}{3!} z^3 + \ldots\right)\left(\frac{B_0}{0!} + \frac{B_1}{1!} z + \frac{B_2}{2!} z^2 + \ldots\right)$

Equate coefficients: Each coefficient corresponds to a whole diagonal in the identity matrix

$$\begin{bmatrix} \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots & \frac{B_{n-1}}{(n-1)!} \\ & \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots \\ & & \ddots & \ddots \\ & & & \frac{B_0}{0!} \end{bmatrix}_{n\times n} \times \begin{bmatrix} \frac{1}{1!} & \frac{1}{2!} & \ddots & \frac{1}{n!} \\ & \frac{1}{1!} & \frac{1}{2!} & \ddots \\ & & \ddots & \ddots \\ & & & \frac{1}{1!} \end{bmatrix}_{n\times n} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}_{n\times n}$$

Derivation of the EM1 formula (case of $h = 1$) (Part 2)

Taylor expand $f(x)$ around $x = k$:

$$f(x) = f(k) + \frac{1}{1!}(x-k)f'(k) + \frac{1}{2!}(x-k)^2 f''(k) + \dots$$

This implies:

$$\begin{bmatrix} \int_k^{k+1} f(x)dx \\ f(k+1) - f(k) \\ f'(k+1) - f'(k) \\ \vdots \end{bmatrix} = \begin{bmatrix} \frac{1}{1!} & \frac{1}{2!} & \frac{1}{3!} & \ddots \\ & \frac{1}{1!} & \frac{1}{2!} & \ddots \\ & & \frac{1}{1!} & \ddots \\ & & & \ddots \end{bmatrix} \begin{bmatrix} f(k) \\ f'(k) \\ f''(k) \\ \vdots \end{bmatrix}$$

Add these relations for $k = 0,1,2,\dots$

$$\begin{bmatrix} \int_0^{\infty} f(x)dx \\ -f(0) \\ -f'(0) \\ \vdots \end{bmatrix} = \begin{bmatrix} \frac{1}{1!} & \frac{1}{2!} & \frac{1}{3!} & \ddots \\ & \frac{1}{1!} & \frac{1}{2!} & \ddots \\ & & \frac{1}{1!} & \ddots \\ & & & \ddots \end{bmatrix} \begin{bmatrix} \sum_{k=0}^{\infty} f(k) \\ \sum_{k=0}^{\infty} f'(k) \\ \sum_{k=0}^{\infty} f''(k) \\ \vdots \end{bmatrix}$$

Use the 'Neat Identity':

$$\begin{bmatrix} \frac{B_0}{0!} & \frac{B_1}{1!} & \frac{B_2}{2!} & \ddots \\ & \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots \\ & & \frac{B_0}{0!} & \ddots \\ & & & \ddots \end{bmatrix} \times \begin{bmatrix} \frac{1}{1!} & \frac{1}{2!} & \frac{1}{3!} & \ddots \\ & \frac{1}{1!} & \frac{1}{2!} & \ddots \\ & & \frac{1}{1!} & \ddots \\ & & & \ddots \end{bmatrix} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots \end{bmatrix}$$

Multiply by Bernoulli matrix from left:

$$\begin{bmatrix} \frac{B_0}{0!} & \frac{B_1}{1!} & \frac{B_2}{2!} & \ddots \\ & \frac{B_0}{0!} & \frac{B_1}{1!} & \ddots \\ & & \frac{B_0}{0!} & \ddots \\ & & & \ddots \end{bmatrix} \begin{bmatrix} \int_0^{\infty} f(x)dx \\ -f(0) \\ -f'(0) \\ \vdots \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{\infty} f(k) \\ \sum_{k=0}^{\infty} f'(k) \\ \sum_{k=0}^{\infty} f''(k) \\ \vdots \end{bmatrix}$$

Now read off EM1 from the top row in this equation.

Other early Euler-Maclaurin pioneers

Amedeo Plana
1781-1864

Niels Henrik Abel
1802-1829

Abel-Plana formula (1820):

$$\sum_{k=0}^{\infty} f(k) = \int_0^{\infty} f(x)dx + \frac{1}{2} f(0) + i \int_0^{\infty} \frac{f(it) - f(-it)}{e^{2\pi t} - 1} dt$$

$$\sum_{k=0}^{\infty} (-1)^k f(k) = \frac{1}{2} f(0) + i \int_0^{\infty} \frac{f(it) - f(-it)}{2\sinh(\pi t)} dt$$

Siméon Poisson
1781-1840

Provided in 1820 the first precise error term
For truncated Euler-Maclaurin expansions

Main complication when applying the EM formulas

$$\int_{x_0}^{\infty} f(x)dx - h\sum_{k=0}^{\infty} f(x_k) \approx -\frac{h}{2} f(x_0) + \frac{h^2}{12} f^{(1)}(x_0) - \frac{h^4}{720} f^{(3)}(x_0) + \frac{h^6}{30240} f^{(5)}(x_0) - \frac{h^8}{1209600} f^{(7)}(x_0) + - \dots$$

Formula contains a large number of derivatives (we often want, say, 50 or 100 terms):

> *In general the calculation of the higher derivatives involved in the Euler-Maclaurin expansion is not possible.*

(Süli and Mayers, *An Introduction to Numerical Analysis*, Cambridge University Press, 2003)

Do we actually need to?
Can one simply replace the derivatives in EM with regular finite difference approximations?

Rest of this presentation:

1. Summary of some standard finite difference (FD) schemes
2. Error analysis suggesting that FD actually ought to work just fine in this context
3. Two verification tests
4. Conclusions

Some finite difference (FD) and Hermite-FD (HFD) formulas

'Regular' centered FD weights

Order of derivative	Order of accuracy	Approximations at $x=0$; x coordinates at nodes: -4	-3	-2	-1	0	1	2	3	4
0	∞					1				
1	2				$-\frac{1}{2}$	0	$\frac{1}{2}$			
	4			$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$		
	6		$-\frac{1}{60}$	$\frac{3}{20}$	$-\frac{3}{4}$	0	$\frac{3}{4}$	$-\frac{3}{20}$	$\frac{1}{60}$	
	8	$\frac{1}{280}$	$-\frac{4}{105}$	$\frac{1}{5}$	$-\frac{4}{5}$	0	$\frac{4}{5}$	$-\frac{1}{5}$	$\frac{4}{105}$	$-\frac{1}{280}$
2	2				1	-2	1			
	4			$-\frac{1}{12}$	$\frac{4}{3}$	$-\frac{5}{2}$	$\frac{4}{3}$	$-\frac{1}{12}$		
	6		$\frac{1}{90}$	$-\frac{3}{20}$	$\frac{3}{2}$	$-\frac{49}{18}$	$\frac{3}{2}$	$-\frac{3}{20}$	$\frac{1}{90}$	
	8	$-\frac{1}{560}$	$\frac{8}{315}$	$-\frac{1}{5}$	$\frac{8}{5}$	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$
3	2			$-\frac{1}{2}$	1	0	-1	$\frac{1}{2}$		
	4		$\frac{1}{8}$	-1	$\frac{13}{8}$	0	$-\frac{13}{8}$	1	$-\frac{1}{8}$	
	6	$-\frac{7}{240}$	$\frac{3}{10}$	$-\frac{169}{120}$	$\frac{61}{30}$	0	$-\frac{61}{30}$	$\frac{169}{120}$	$-\frac{3}{10}$	$\frac{7}{240}$
4	2			1	-4	6	-4	1		
	4		$-\frac{1}{6}$	2	$-\frac{13}{2}$	$\frac{28}{3}$	$-\frac{13}{2}$	2	$-\frac{1}{6}$	
	6	$\frac{7}{240}$	$-\frac{2}{5}$	$\frac{169}{60}$	$-\frac{122}{15}$	$\frac{91}{8}$	$-\frac{122}{15}$	$\frac{169}{60}$	$-\frac{2}{5}$	$\frac{7}{240}$

Centered Hermite weights

Weights for	Order of derivative	Order of accuracy	Approximations at $x=0$; x coordinates at nodes: -4	-3	-2	-1	0	1	2	3	4
$f(x_i)$	0	∞					1				
	1	∞					0				
	2	4				2	-4	2			
		8			$\frac{7}{54}$	$\frac{64}{27}$	-5	$\frac{64}{27}$	$\frac{7}{54}$		
		12		$\frac{157}{18000}$	$\frac{69}{250}$	$\frac{39}{16}$	$-\frac{49}{9}$	$\frac{39}{16}$	$\frac{69}{250}$	$\frac{157}{18000}$	
		16	$\frac{199}{343000}$	$\frac{11824}{385875}$	$\frac{48}{125}$	$\frac{304}{125}$	$-\frac{205}{36}$	$\frac{304}{125}$	$\frac{48}{125}$	$\frac{11824}{385875}$	$\frac{199}{343000}$
	3	4				$-\frac{15}{2}$	0	$\frac{15}{2}$			
		8			$-\frac{31}{144}$	$-\frac{88}{9}$	0	$\frac{88}{9}$	$\frac{31}{144}$		
		12		$-\frac{167}{18000}$	$-\frac{963}{2000}$	$-\frac{171}{16}$	0	$\frac{171}{16}$	$\frac{963}{2000}$	$\frac{167}{18000}$	
		16	$-\frac{2493}{5488000}$	$-\frac{12944}{385875}$	$-\frac{87}{125}$	$-\frac{1392}{125}$	0	$\frac{1392}{125}$	$\frac{87}{125}$	$\frac{12944}{385875}$	$\frac{2493}{5488000}$
$f'(x_i)$	0	∞					0				
	1	∞					1				
	2	4				$\frac{1}{2}$	0	$-\frac{1}{2}$			
		8			$\frac{1}{36}$	$\frac{8}{9}$	0	$-\frac{8}{9}$	$-\frac{1}{36}$		
		12		$\frac{1}{600}$	$\frac{9}{100}$	$\frac{9}{8}$	0	$-\frac{9}{8}$	$-\frac{9}{100}$	$-\frac{1}{600}$	
		16	$\frac{1}{9800}$	$\frac{32}{3675}$	$\frac{4}{25}$	$\frac{32}{25}$	0	$-\frac{32}{25}$	$-\frac{4}{25}$	$-\frac{32}{3675}$	$-\frac{1}{9800}$
	3	4				$-\frac{3}{2}$	-12	$-\frac{3}{2}$			
		8			$-\frac{1}{24}$	$-\frac{8}{3}$	-15	$-\frac{8}{3}$	$-\frac{1}{24}$		
		12		$-\frac{1}{600}$	$-\frac{27}{200}$	$-\frac{27}{8}$	$-\frac{49}{3}$	$-\frac{27}{8}$	$-\frac{27}{200}$	$-\frac{1}{600}$	
		16	$-\frac{3}{39200}$	$-\frac{32}{3675}$	$-\frac{6}{25}$	$-\frac{96}{25}$	$-\frac{205}{12}$	$-\frac{96}{25}$	$-\frac{6}{25}$	$-\frac{32}{3675}$	$-\frac{3}{39200}$

Very fast and stable algorithms available to calculate weights also in the case of irregularly spaced nodes.

Apparent difficulty when applying FD formulas

Applying FD formulas for high order derivatives is notoriously ill-conditioned numerically

Say we want to approximate $f^{(50)}(0)$ by FD:

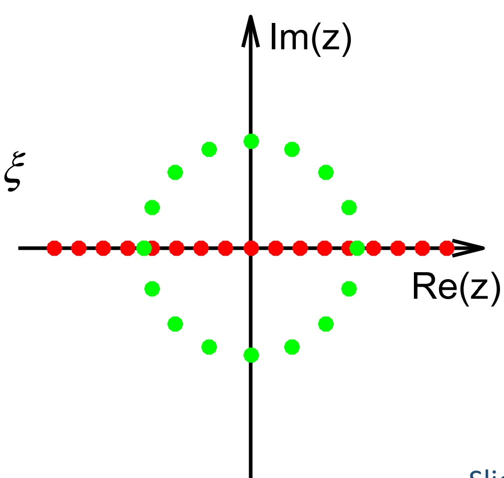
$$f^{(50)}(0) \approx \frac{w_{-n} f(-nh) + \ldots + w_{-1} f(-h) + w_0 f(0) + w_1(h) + \ldots + w_n f(nh)}{h^{50}}$$

A derivative is a local property of a function, so the stencil needs to be narrow, which implies

- h must be extremely small
- h^{50} is vastly much smaller still
- Extreme loss of significant digits in numerator (to produce an $O(1)$-sized result).

We will NOT assume here that *f*(*z*) is available as an analytic function in the complex plane
If it is available; two options:

1. Use the Abel-Plana formulas
2. Use Cauchy's integral formula: $f^{(k)}(z) = \frac{k!}{2\pi i} \oint_\Gamma \frac{f(\xi)}{(\xi - z)^{k+1}} d\xi$



  - No need for path to be close to the center
  - Trigonometric basis functions are orthogonal
  - If the path is circular, FFT is available

EM2 example using 'regular' centered FD approximations

Define $F(x) = -\int_x^{\infty} f(t)dt$ The EM2 formula then becomes

$$\sum_{k=0}^{\infty} f(k+\tfrac{1}{2}) = -F(0) + \frac{1}{24}F^{(2)}(0) - \frac{7}{5760}F^{(4)}(0) + \frac{31}{96780}F^{(6)}(0) - \frac{127}{154828800}F^{(8)}(0) + \ldots$$

Suppose we want to approximate the RHS using $F(x)$ at 5 nodes $x = \left\{-1, -\frac{1}{2},\ 0, +\frac{1}{2}, +1\right\}$

$$F^{(0)}(0) \approx (\quad 1\,F(0) \quad)$$

$$F^{(2)}(0) \approx 2^2\left(-\tfrac{1}{12}F(-1) \ +\tfrac{4}{3}F(-\tfrac{1}{2}) \ -\tfrac{5}{2}F(0) \ +\tfrac{4}{3}F(\tfrac{1}{2}) \ -\tfrac{1}{12}F(1) \right)$$

$$F^{(4)}(0) \approx 2^4\left(1\,F(-1) \ -4F(-\tfrac{1}{2}) \ 6\,F(0) \ -4F(\tfrac{1}{2}) \ +1\,F(1) \right)$$

We can use only μ = 3 terms of EM2.
Combine together according to coefficients in the EM2 formula; get weights

$$\left\{-\frac{1}{30}, \ \frac{3}{10}, \ -\frac{23}{15}, \ \frac{3}{10}, \ -\frac{1}{30}\right\}$$

Generalize to using different number of EM2 terms

μ	$-\frac{5}{2}$	-2	$-\frac{3}{2}$	-1	$-\frac{1}{2}$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
	Weights for $F(x)$ at x-locations										
1						-1					
2					$\frac{1}{6}$	$-\frac{4}{3}$	$\frac{1}{6}$				
3				$-\frac{1}{30}$	$\frac{3}{10}$	$-\frac{23}{15}$	$\frac{3}{10}$	$-\frac{1}{30}$			
4			$\frac{1}{140}$	$-\frac{8}{105}$	$\frac{57}{140}$	$-\frac{176}{105}$	$\frac{57}{140}$	$-\frac{8}{105}$	$\frac{1}{140}$		
5		$-\frac{1}{630}$	$\frac{5}{252}$	$-\frac{38}{315}$	$\frac{125}{252}$	$-\frac{563}{315}$	$\frac{125}{252}$	$-\frac{38}{315}$	$\frac{5}{252}$	$-\frac{1}{630}$	
6	$\frac{1}{2772}$	$-\frac{2}{385}$	$\frac{25}{693}$	$-\frac{568}{3465}$	$\frac{1585}{2772}$	$-\frac{6508}{3465}$	$\frac{1585}{2772}$	$-\frac{568}{3465}$	$\frac{25}{693}$	$-\frac{2}{385}$	$\frac{1}{2772}$

Coefficients stay much simpler than the EM2 ones; μ = 6, cf. $\frac{73}{3503554560}$.

Closed form for coefficients contains no Bernoulli numbers:

$$w_{\mu,k} = (-1)^{k+1} \sum_{n=|k|}^{\mu-1} \frac{(n!)^2}{(2n+1)(n+k)!(n-k)!}$$

Weights stay small however far the table is extended, implying no danger ever of numerical cancellations.

Are these approximations accurate? (We have NOT let h -> 0)

Error when using μ terms of the EM2 formula, μ = 1,2,3,...

EM2 with exact analytic derivatives: $$\text{EM2}_{\text{Error}} \approx \frac{B_{2\mu}}{(2\mu)!} F^{(2\mu)}(0) \approx \frac{2}{(2\pi)^{2\mu}} F^{(2\mu)}(0)$$

FD approximation (using *h* = 1/2): $$\text{FD}_{\text{Error}} \approx \frac{(\mu!)^2 \, 2^{-2\mu}}{(2\mu+1)!} F^{(2\mu)}(0) \approx \frac{1}{4^{2\mu}} \sqrt{\frac{\pi}{2\mu}} F^{(2\mu)}(0)$$

Only essential difference: Factor $(2\pi)^{2\mu}$ vs. $4^{2\mu}$

In words: Given μ (number of EM terms), changing analytical derivatives to regular FD approximations (with *h* =1/2), loses only about $2\mu \log_{10}\left(\frac{\pi}{2}\right) \approx 0.39\mu$ decimal digits.

All numerical cancellations in high derivative calculations have been eliminated, since all the weights we apply to function values stayed small.

Even this accuracy loss becomes virtually eliminated when changing from regular FD to Hermite-FD approximations.

Regular FD vs. Hermite FD (HFD) approximations

Using regular FD, μ = 3 EM2 terms:

$$\left\{-F(0)+\frac{1}{24}F^{(2)}(0)-\frac{7}{5760}F^{(4)}(0)\right\}\approx\left\{-\frac{1}{30}F(-1)+\frac{3}{10}F\left(-\tfrac{1}{2}\right)-\frac{23}{15}F(0)+\frac{3}{10}F\left(\tfrac{1}{2}\right)-\frac{1}{30}F(1)\right\}$$

Using Hermite FD, μ = 3 EM2 terms:

Recall $F(x)=-\int_x^\infty f(t)dt,$ i.e. $F'(x)=f(x).$

The $f(x)$ function is also available to us without differentiation (the function to be summed).

	Weights at									
	$x=$	$-\frac{1}{2}$	0	$\frac{1}{2}$		$x=$	$-\frac{1}{2}$	0	$\frac{1}{2}$	
$F(0)\approx$	[	0	1	0	] F	+[	0	0	0	] f
$F^{(2)}(0)\approx$	8 [	1	-2	1	] F	+[	1	0	-1	] f
$F^{(4)}(0)\approx$	192 [	-1	-2	-1	] F	+48 [	-1	0	1	] f

$$\left\{-F(0)+\frac{1}{24}F^{(2)}(0)-\frac{7}{5760}F^{(4)}(0)\right\}\approx\left\{\frac{17}{30}F\left(-\tfrac{1}{2}\right)-\frac{32}{15}F(0)+\frac{17}{30}F\left(\tfrac{1}{2}\right)\right\}+\left\{\frac{1}{10}f\left(-\tfrac{1}{2}\right)+0\,f(0)-\frac{1}{10}f\left(\tfrac{1}{2}\right)\right\}$$

Same formal order of accuracy, and same number of function evaluations, but higher accuracy due to more local information.

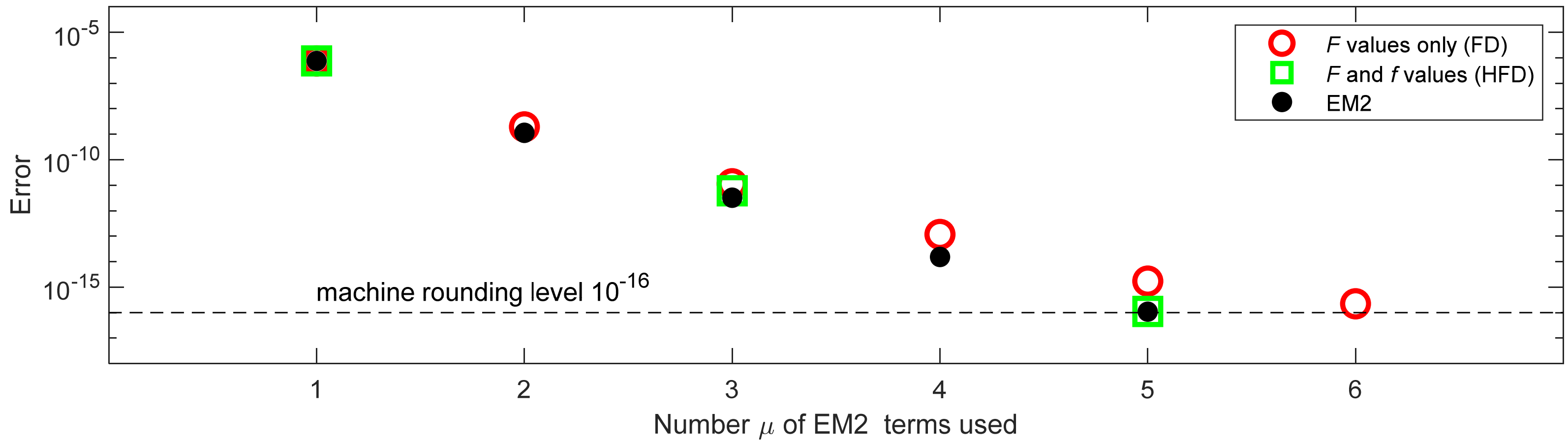
Example 1

Approximate: $\sum_{k=1}^{\infty} f(k) \approx 0.2590385692623903923 7$

where $f(x) = \dfrac{x \,\mathrm{erfinv}\left(\arctan \dfrac{1}{\sqrt{1+x^2}}\right)}{(x^2+2)\sqrt{1+x^2}}$, $\quad F(x) = \dfrac{e^{-\left(\mathrm{erfinv}\left(\arctan \frac{1}{\sqrt{1+x^2}}\right)\right)^2} - 1}{\sqrt{\pi}}$

To reach error around 10^{-16} by direct summation requires approximately 100,000,000 terms.

Instead, sum directly $\sum_{k=1}^{19} f(x)$ and apply EM2 to $\sum_{k=20}^{\infty} f(x)$.



μ = 5 terms of EM2 requires a total of 9 function evaluations (FD or HFD), or evaluation of up to 7th derivative of *f*(*x*) (EM2).

The error loss by replacing analytic derivatives with FD/HFD approximations is insignificant.

Example 2

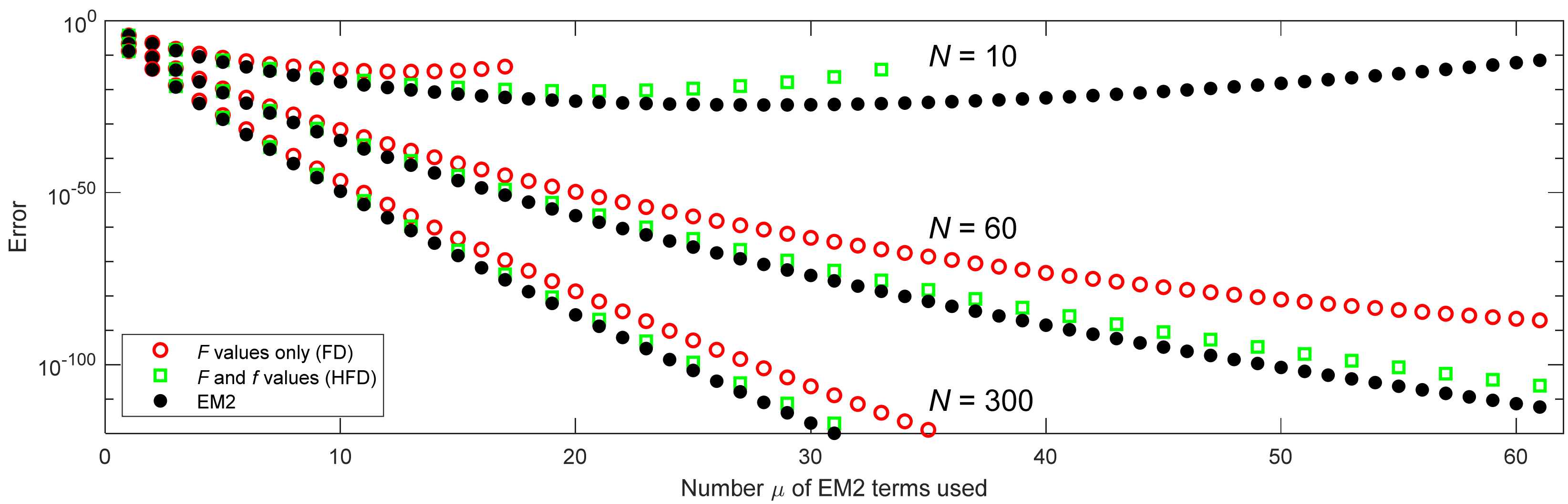
Evaluate to high precision Euler's constant

$$\gamma = \lim_{n\to\infty}\left(\sum_{k=1}^{n}\frac{1}{k} - \log n\right) = 1 + \sum_{k=2}^{\infty}\left(\frac{1}{k} + \log\left(1-\frac{1}{k}\right)\right) \approx 0.5772156649015328606\,1$$

Here: $f(x) = \frac{1}{x} + \log\left(1-\frac{1}{x}\right), \quad F(x) = 2(x-1)\operatorname{arccoth}(2x-1) - 1.$

Reaching error 10^{-100} by direct summation requires about 10^{100} terms.

Sum explicitly $\sum_{k=2}^{N-1} f(k)$, then apply EM2 to $\sum_{k=N}^{\infty} f(k)$.



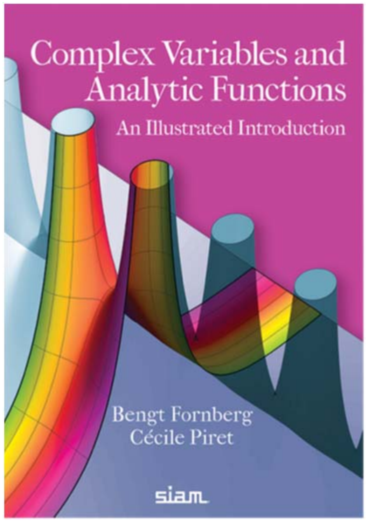
Some conclusions

Historical notes:

- The pioneering works by Euler, Maclaurin, Plana, Abel, Poisson, etc. were carried out between 200 and 300 years ago.
- Surprisingly little (if any) attention has been given to simplifying the numerical use of the Euler-Maclaurin expansions.

Some aspects of the present numerical approach:

- FD approximations of low order derivatives to high orders of accuracy is common for ODEs and PDEs. In contrast, FD approximations of very high order derivatives are rare.
- High accuracies for EM expansions can be reached with standard FD approximations, and *without* resorting to small step sizes when approximating the derivatives.
- Even when using real-valued arithmetic, it is unnecessary to do any analytic differentiations when using EM expansions to approximate infinite sums.



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(with residue calculus derivations of both the EM and the Abel-Plana formulas) → → → →
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