Newton-Cotes quadratures

Extended midpoint (rectangle) method (interpolation with constant functions

$$\int_{x_0}^{x_{N-1}} f(x)dx = h[f_{1/2} + f_{3/2} + f_{5/2} + \cdots + f_{N-5/2} + f_{N-3/2}] \quad + O\left(\frac{1}{N^2}\right) \tag{4.1.19}$$

Order 2

Trapezoidal method (interpolation with linear functions)

$$\int_{x_0}^{x_{N-1}} f(x)dx = h\Big[\frac{1}{2}f_0 + f_1 + f_2 + \cdots + f_{N-2} + \frac{1}{2}f_{N-1}\Big] \quad + O\left(\frac{1}{N^2}\right) \tag{4.1.11}$$

Order 2

Simpsons method (interpolation with parabolas)

$$\int_{x_0}^{x_{N-1}} f(x)dx = h\Big[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{2}{3}f_2 + \frac{4}{3}f_3 + \cdots + \frac{2}{3}f_{N-3} + \frac{4}{3}f_{N-2} + \frac{1}{3}f_{N-1}\Big] \quad + O\left(\frac{1}{N^4}\right) \tag{4.1.13}$$

Order 4

Richardson extrapolation

(derivation of the results below is published in the weekly plan)

A(h) is a numerical approximation to an exact value A where h is the stepsize. For example for numerical integration.

Estimation of the order k:

$$\frac{A(h_1) - A(h_2)}{A(h_2) - A(h_3)} \approx \alpha^k \quad \text{for} \quad h_1/h_2 = h_2/h_3 = \alpha. \qquad h_1 > h_2 > h_3$$

Typically alpha=2.

Error estimation and extrapolation:

Extrapolation

$$\begin{aligned} A_R(h_2, h_1) &\equiv \frac{\alpha^k A(h_2) - A(h_1)}{\alpha^k - 1} \\ &= A(h_2) + \frac{A(h_2) - A(h_1)}{\alpha^k - 1}, \quad \alpha = \frac{h_1}{h_2} \qquad h_1 > h_2 \end{aligned}$$

Error estimate on $A(h_2)$

Exercises

$$\int_0^1 \cos(x^2)\exp(-x)dx$$

$$\int_0^1 \sqrt{x}\cos(x^2)\exp(-x)dx$$

$$\int_0^1 \frac{1}{\sqrt{x}}\cos(x^2)\exp(-x)dx$$

$$\int_0^1 1000\exp(-1/x)\exp(-1/(1-x))dx$$

Results from Trapezoidal method:

i	A(hi)	A(hi-1)-A(hi)	Rich-alp^k	A(hi)-A	Rich-fejl	Antal f-ber.
1.	0.593529	*	*	0.00347808	*	2.
2.	0.590981	0.00254788	*	0.000930202	*	3.
3.	0.590287	0.000694194	3.67027	0.000236008	0.000231398	5.
4.	0.59011	0.000176796	3.92653	0.0000592124	0.0000589319	9.
5.	0.590066	0.0000443962	3.98222	0.0000148161	0.0000147987	17.
6.	0.590055	0.0000111113	3.99559	3.70485×10^{-6}	3.70376×10^{-6}	33.
7.	0.590052	2.77859×10^{-6}	3.9989	9.26263×10^{-7}	9.26196×10^{-7}	65.
8.	0.590051	6.94694×10^{-7}	3.99973	2.31569×10^{-7}	2.31565×10^{-7}	129.
9.	0.590051	1.73677×10^{-7}	3.99993	5.78925×10^{-8}	5.78922×10^{-8}	257.
10.	0.590051	4.34193×10^{-8}	3.99998	1.44731×10^{-8}	1.44731×10^{-8}	513.

$$\int_0^1 \cos(x^2)\exp(-x)dx$$

i	A(hi)	A(hi-1)-A(hi)	Rich-alp^k	A(hi)-A
3	7.0303	-0.0374197	-57.8555	0.000445976
4	7.02981	0.000495216	-75.5623	-0.00004924
5	7.02986	-0.0000491767	-10.0701	-6.32668×10^{-8}
6	7.02986	-6.32622×10^{-8}	777.347	-4.56879×10^{-12}
7	7.02986	-4.55991×10^{-12}	13873.6	-8.88178×10^{-15}

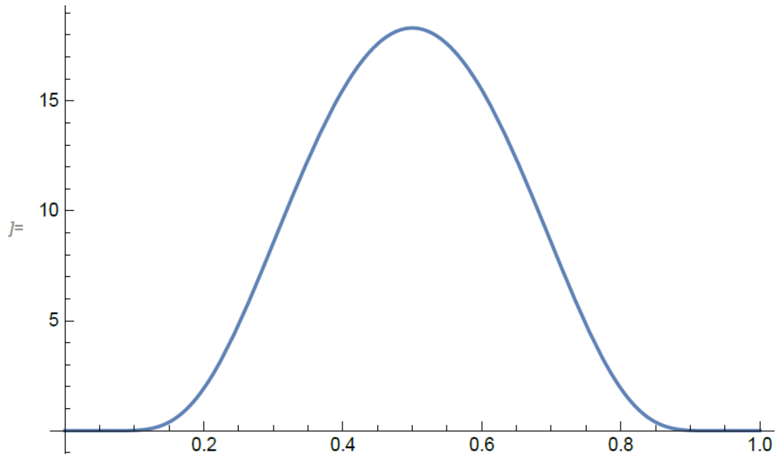
$$\int_0^1 1000\exp(-1/x)\exp(-1/(1-x))dx$$

$$\int_{x_0}^{x_{N-1}} f(x)dx = h\left[\frac{1}{2}f_0 + f_1 + f_2 + \cdots + f_{N-2} + \frac{1}{2}f_{N-1}\right] + O\left(\frac{(b-a)^3 f''}{N^2}\right) \tag{4.1.11}$$

Assuming that f is infinitely many times continuous differentiable on the complete integration interval, we have for the Trapezoidal method

$$\int_{x_0}^{x_{N-1}} f(x)dx = h\left[\frac{1}{2}f_0 + f_1 + f_2 + \cdots + f_{N-2} + \frac{1}{2}f_{N-1}\right] - \frac{B_2 h^2}{2!}(f'_{N-1} - f'_0) - \cdots - \frac{B_{2k} h^{2k}}{(2k)!}(f^{(2k-1)}_{N-1} - f^{(2k-1)}_0) - \cdots \quad (4.2.1)$$

where the B_{2k}'s are universal constants (hence independent of f, h and the integration interval !!)



$1000\exp(-1/x)\exp(1/(1-x)dx$

For the midpoint (rectangle) method, there is a similar formula

$$\int_{x_0}^{x_{N-1}} f(x)dx = h[f_{1/2} + f_{3/2} + f_{5/2} + \cdots + f_{N-5/2} + f_{N-3/2}] + \frac{B_2 h^2}{4}(f'_{N-1} - f'_0) + \cdots + \frac{B_{2k} h^{2k}}{(2k)!}(1 - 2^{-2k+1})(f^{(2k-1)}_{N-1} - f^{(2k-1)}_0) + \cdots \quad (4.4.1)$$

NOTICE: The errors in Eqs. 4.2.1 and 4.4.1 are asymptotic expansions and NOT Taylor series. If they would be Taylor series, the error for the Trapezoidal method for the above integrand would be ZERO for ANY stepsize as all derivatives vanishes at the endpoints.

Quadratures by variable transformation

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

Variable transformation:

$x = x(t)$, such that $x \in [a,b] \to t \in [c,d]$:

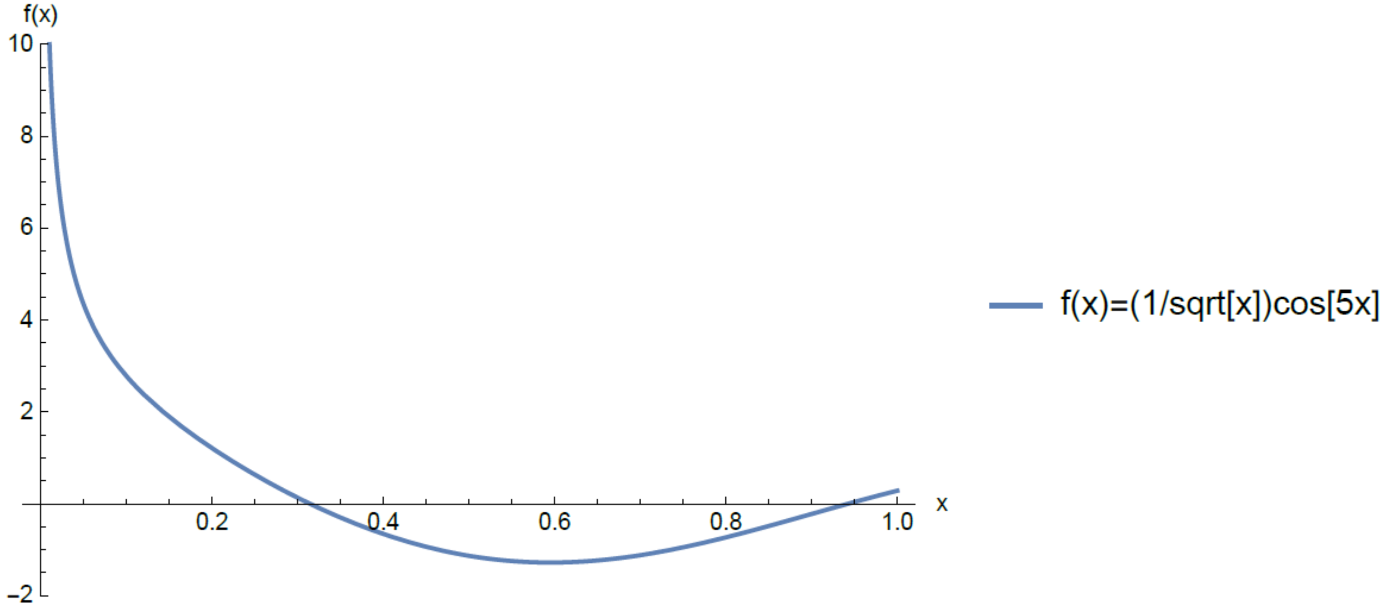
$$I = \int_c^d f[x(t)]\frac{dx}{dt}dt$$

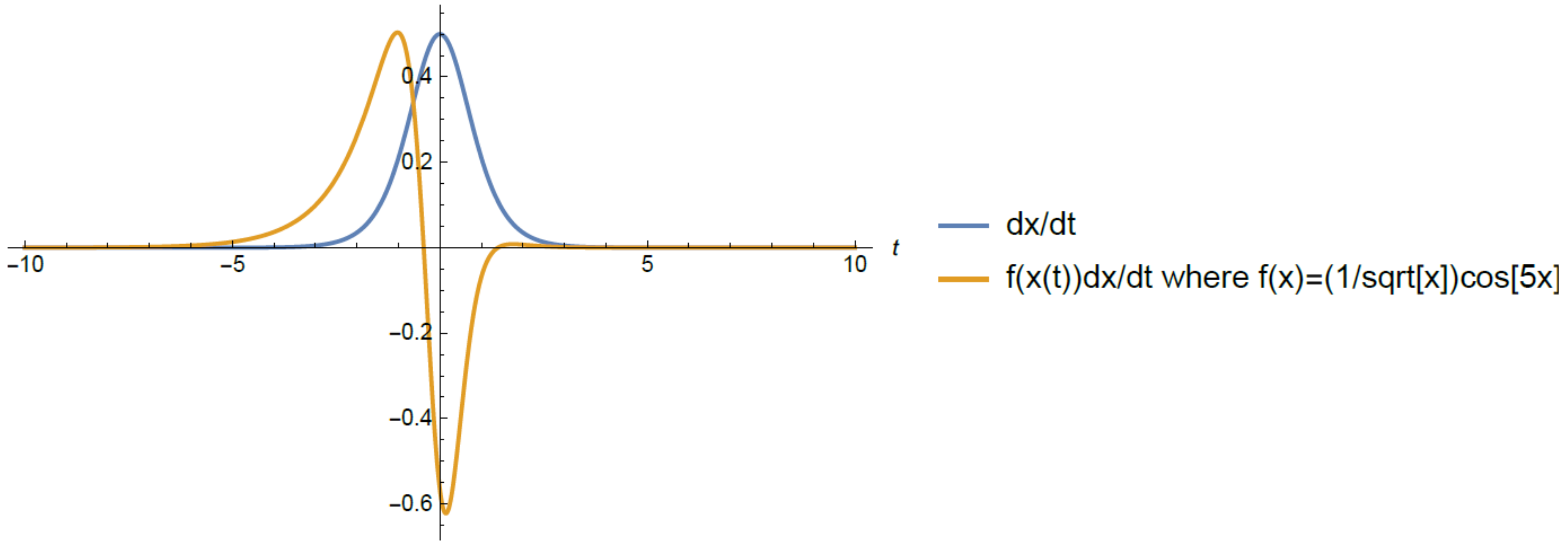
The first transformation of this kind was introduced by Schwartz [1] and has become known as the TANH rule:

$$\begin{aligned} x &= \frac{1}{2}(b+a) + \frac{1}{2}(b-a)\tanh t, \qquad x \in [a,b] \to t \in [-\infty,\infty] \\ \frac{dx}{dt} &= \frac{1}{2}(b-a)\,\mathrm{sech}^2\, t = \frac{2}{b-a}(b-x)(x-a) \end{aligned} \tag{4.5.3}$$

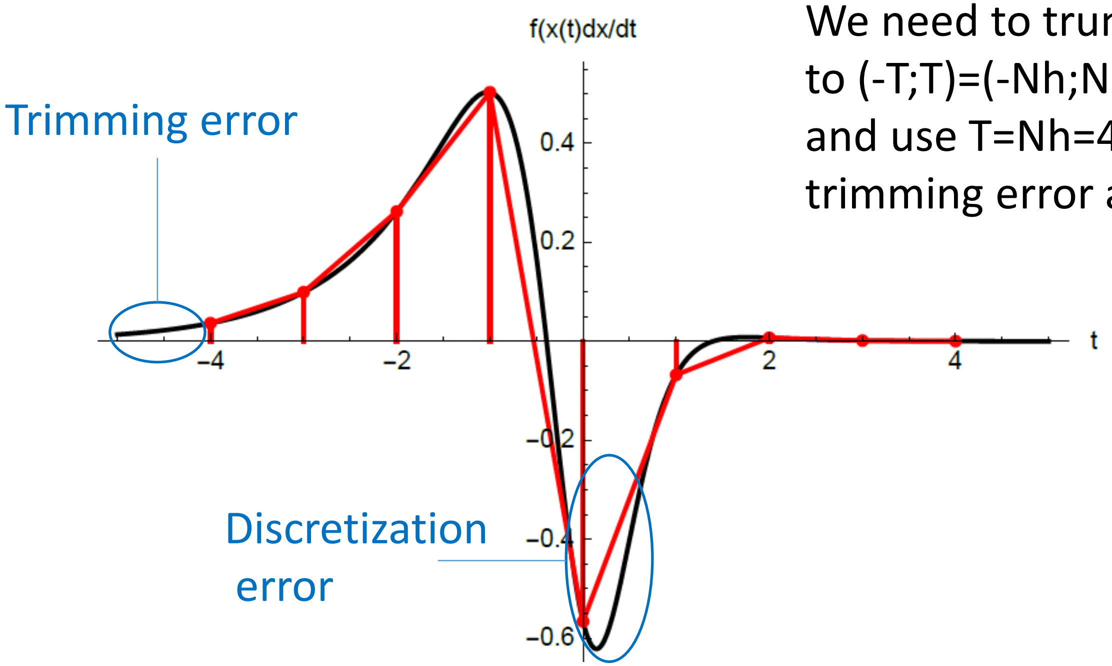
$$\mathrm{sech}(t) = \frac{2}{e^t + e^{-t}}$$

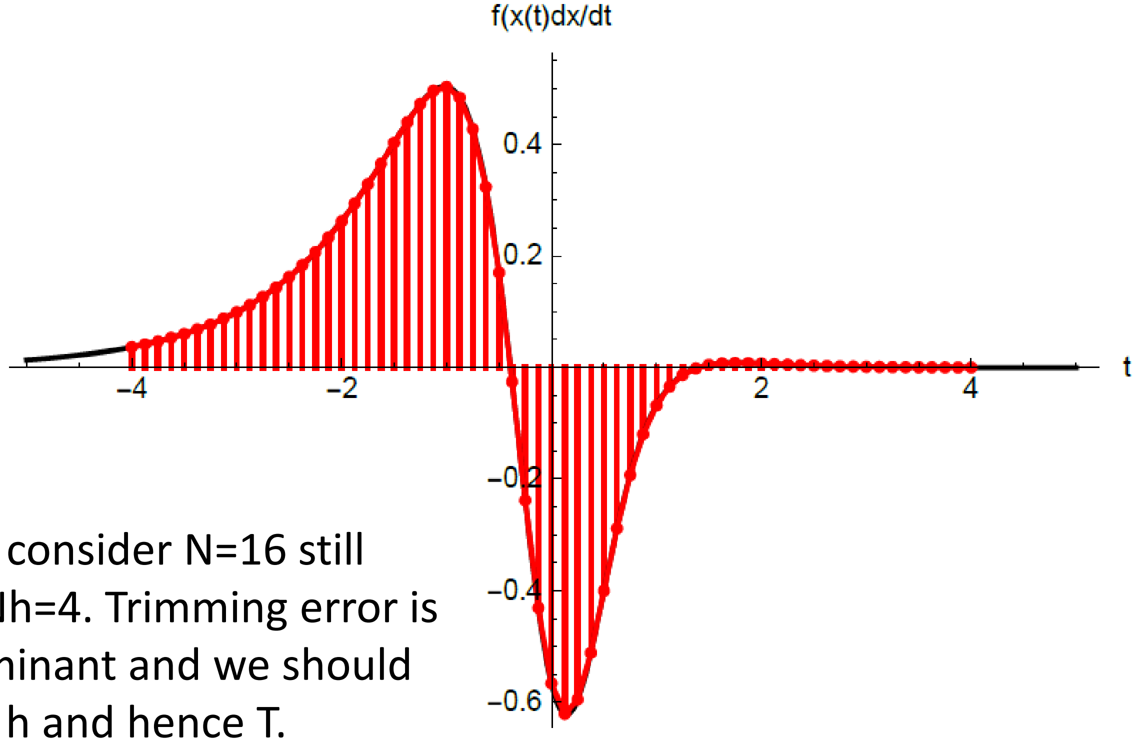
$$I = \int_a^b f(x)dx \longrightarrow \frac{1}{2}(b-a)\int_{-\infty}^{\infty} f(x(t))\mathrm{sech}^2(t)dt$$


f(x)
10
8
6
4
2
-2
0.2
0.4
0.6
0.8
1.0
x
f(x)=(1/sqrt[x])cos[5x]


0.4
0.2
-0.2
-0.4
-0.6
-10
-5
5
10
t
dx/dt
f(x(t))dx/dt where f(x)=(1/sqrt[x])cos[5x]

We need to truncate the infinite t-integral to (-T;T)=(-Nh;Nh). Here we consider N=4 and use T=Nh=4. We obtain a fairly similar trimming error and discretization error





Here we consider N=16 still with T=Nh=4. Trimming error is now dominant and we should increase h and hence T.

The first transformation of this kind was introduced by Schwartz [1] and has become known as the TANH rule:

$$\begin{aligned} x &= \frac{1}{2}(b+a) + \frac{1}{2}(b-a)\tanh t, \qquad x \in [a,b] \to t \in [-\infty, \infty] \\ \frac{dx}{dt} &= \frac{1}{2}(b-a)\operatorname{sech}^2 t = \frac{2}{b-a}(b-x)(x-a) \end{aligned} \tag{4.5.3}$$

$$\operatorname{sech}(t) = \frac{2}{e^t + e^{-t}}$$

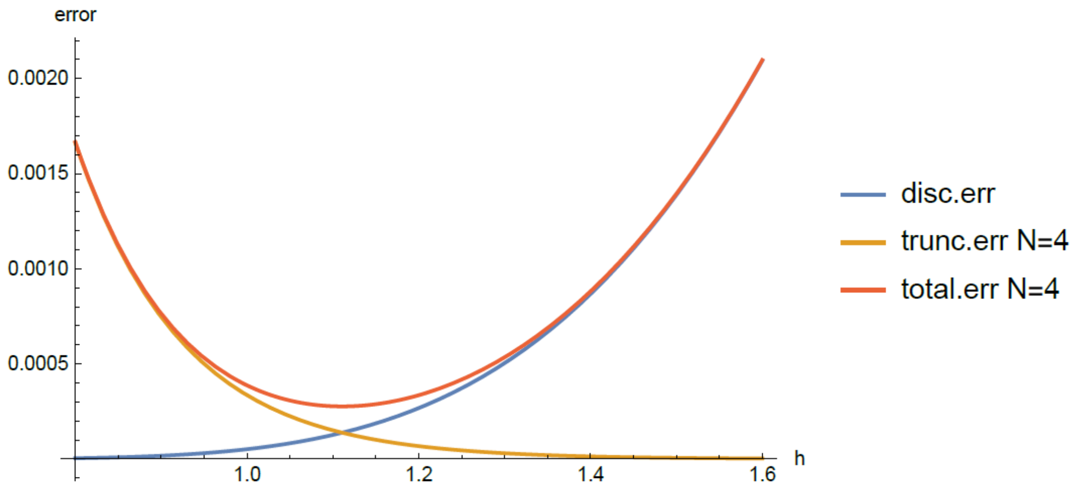
Discretization error (proved by Schwarz): $\epsilon_d \sim e^{-2\pi w/h}$

w is the distance from the real axis to the nearest singularity of the integrand.

Often, due to $\operatorname{sech}^2 t$, we have $w = \pi/2$

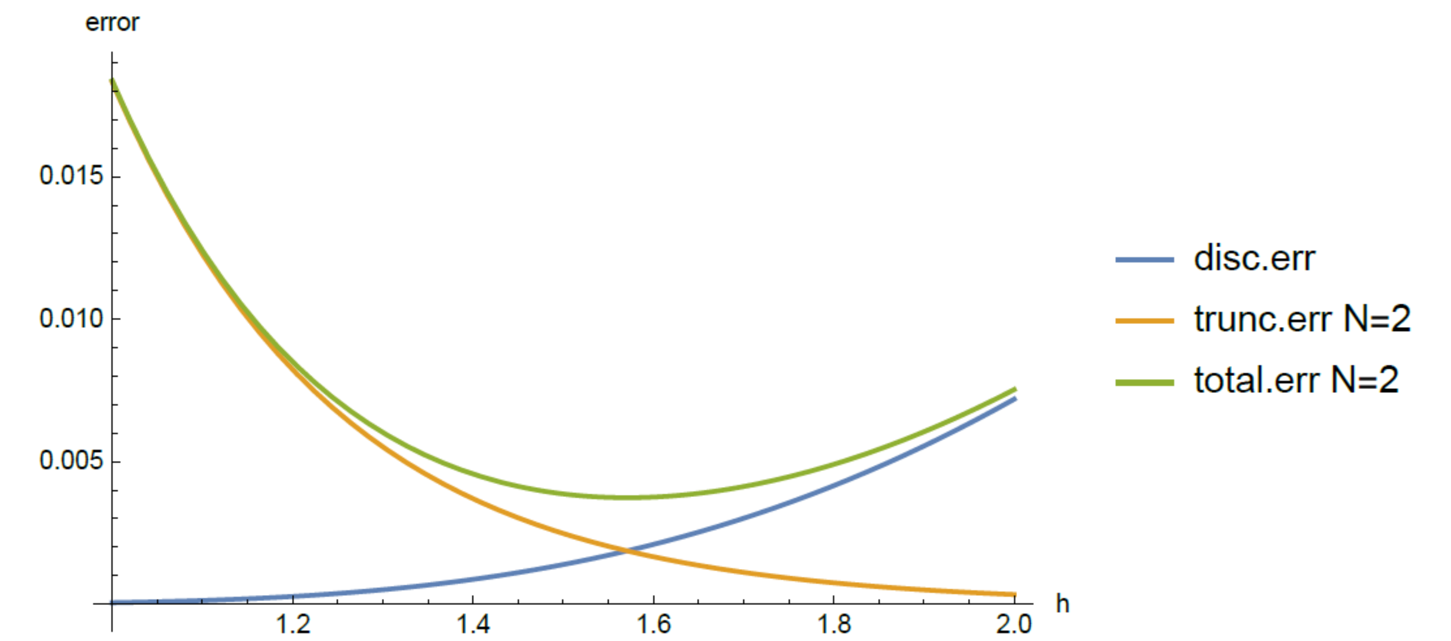
Trimming error (truncation of infinite interval): $\epsilon_t \sim \operatorname{sech}^2 t_N \sim e^{-2Nh}$

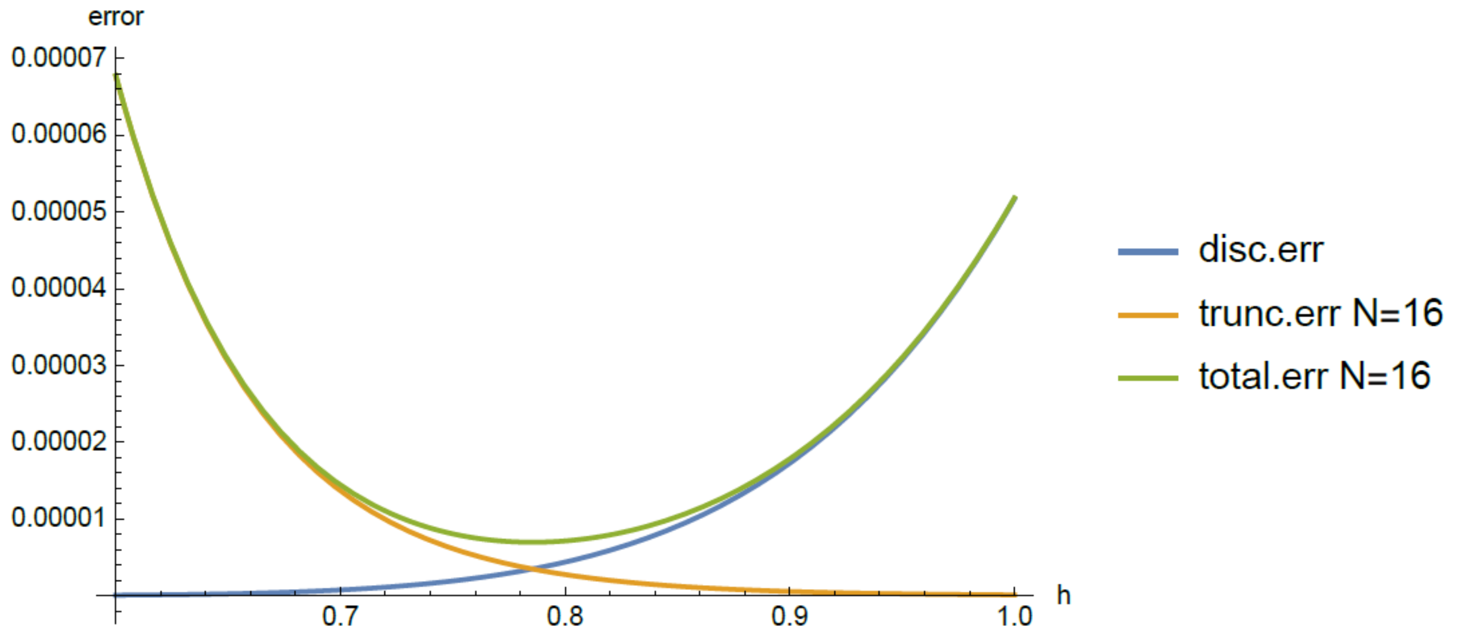
For a given number of steps N. What is the optimal stepsize h ?

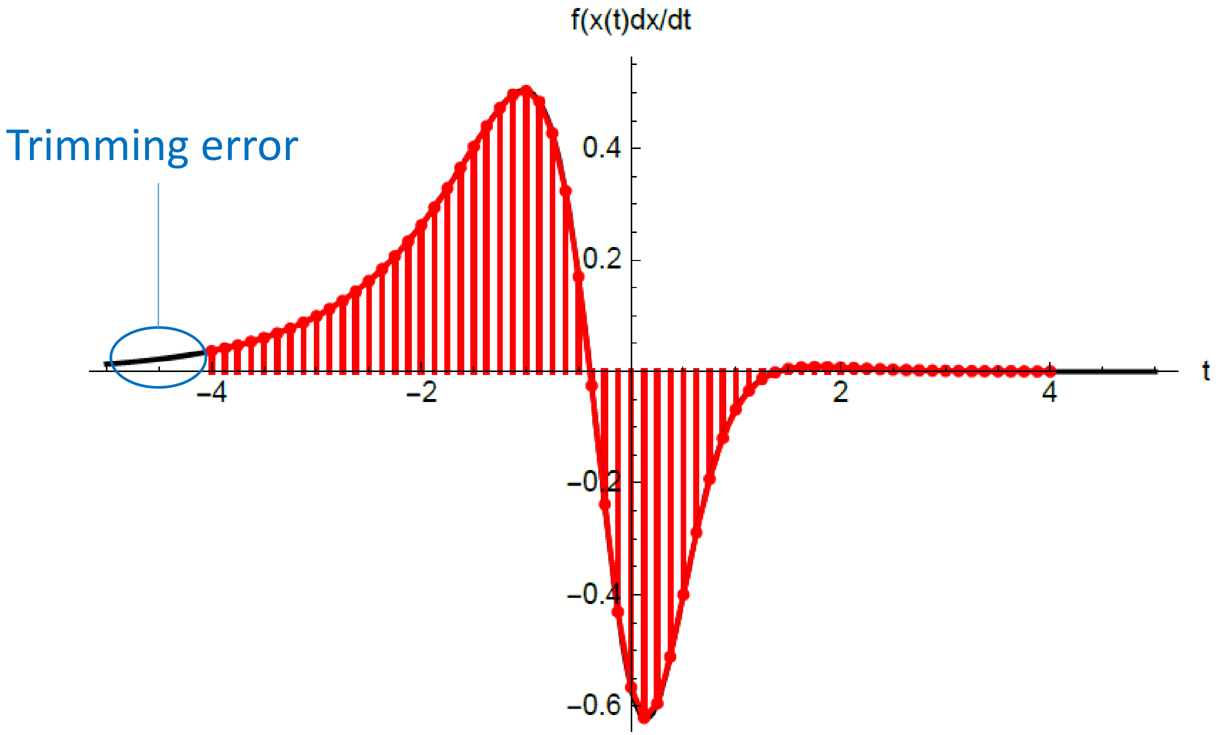


Setting $\epsilon_d \sim \epsilon_t$, we find

$$h \sim \frac{\pi}{(2N)^{1/2}}, \qquad \epsilon \sim e^{-\pi(2N)^{1/2}}$$


error
0.015
0.010
0.005
1.2
1.4
1.6
1.8
2.0
h
disc.err
trunc.err N=2
total.err N=2


error
0.00007
0.00006
0.00005
0.00004
0.00003
0.00002
0.00001
0.7
0.8
0.9
1.0
h
disc.err
trunc.err N=16
total.err N=16



Trimming error due to singularity at x=0.

The question is:
Can we find an even better transformation of the integral ?

DE (double exponential) rule:

$$x = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)\tanh(c\sinh t), \qquad x \in [a,b] \to t \in [-\infty, \infty]$$

$$\frac{dx}{dt} = \frac{1}{2}(b-a)\,\mathrm{sech}^2(c\sinh t)c\cosh t \sim \exp(-c\exp|t|) \quad \text{as} \quad |t| \to \infty$$

Use c=1

Trimming error and Discretization error (what NR writes is rubbish and inconsistent with their implementation):

NR uses a constant $Nh \equiv h_{max}$ and the Trapezoidal method with quadrature points

$$t_j = jh \quad j = -N, \ldots, N \tag{1}$$

where $h = h_{max}/N$. We then get a trimming error (putting $c = 1$):

$$\epsilon_t \simeq [f(x(-h_{max})) + f(x(h_{max}))]\exp(-\exp(h_{max})) \tag{2}$$

and a discretization error as for the Tanh method

$$\epsilon_d \simeq \exp(-2\pi\omega/h) = \exp(-\pi^2 N/h_{max}) \tag{3}$$

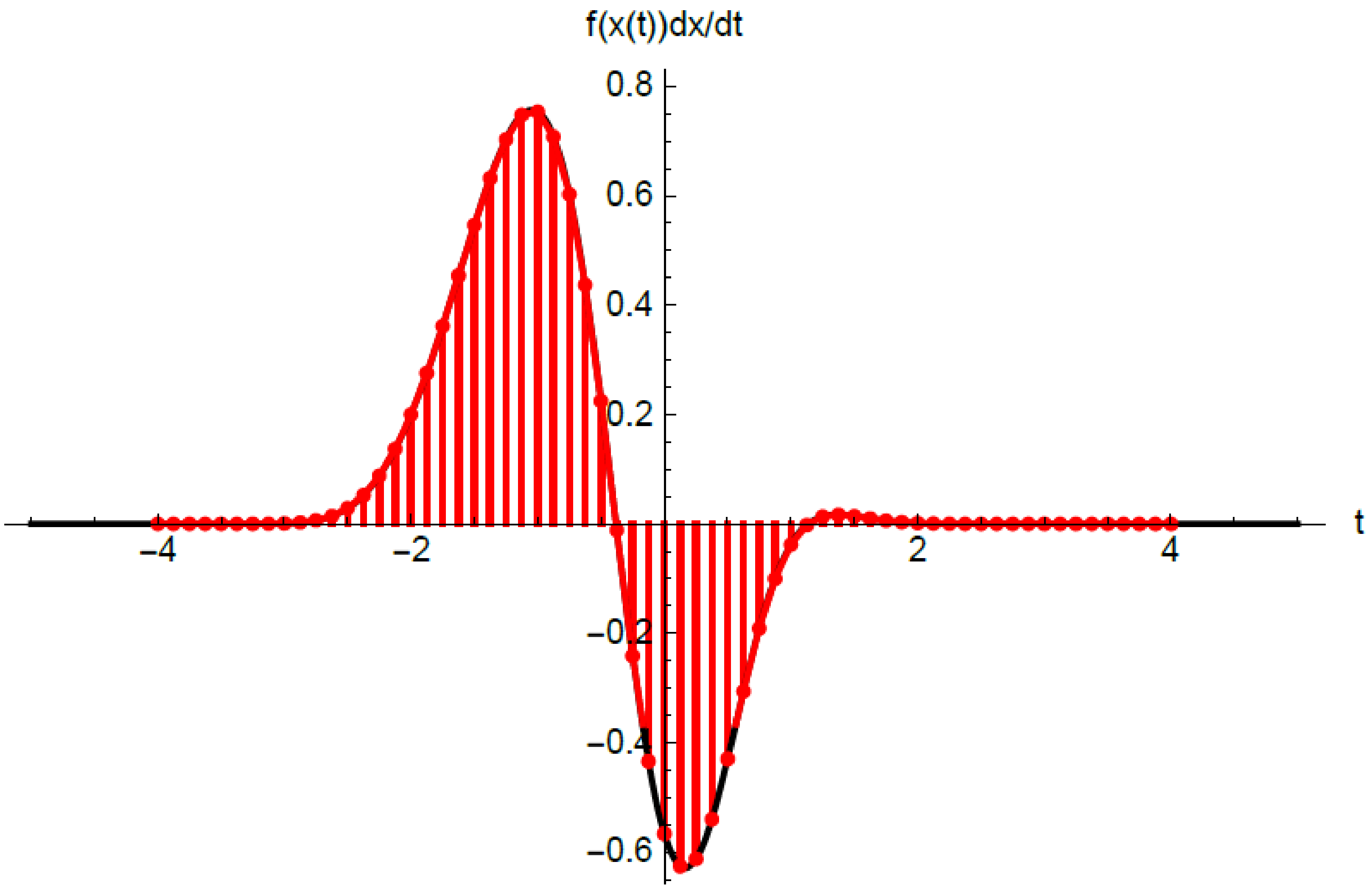
where we assume that $\omega = \pi/2$ (nearest singularity of dx/dt when $c = 1$). The trimming error is constant and negligible even for strong singularities when selecting $h_{max} = 4.3$. Hence, the error is given by the discretization error alone, which decays exponentially with N.

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

$$\downarrow$$

$$\frac{1}{2}(b-a)\int_{-\infty}^{\infty} f(x(t))\mathrm{sech}^2(\sinh(t))\cosh(t)dt$$

Killing the singularity…



Implementation issues

Implement f(x(t)) as F(t) in the following way (derivation is left out):

```
q = Exp[-2 Sinh[t]];

d[t_] = (b - a) q / (1 + q)
```

$$\frac{e^{-2\,\mathrm{Sinh}[t]}}{1 + e^{-2\,\mathrm{Sinh}[t]}}$$

```
F[t_] = If[t < 0, f[a + d[-t]], f[b - d[t]]];
```

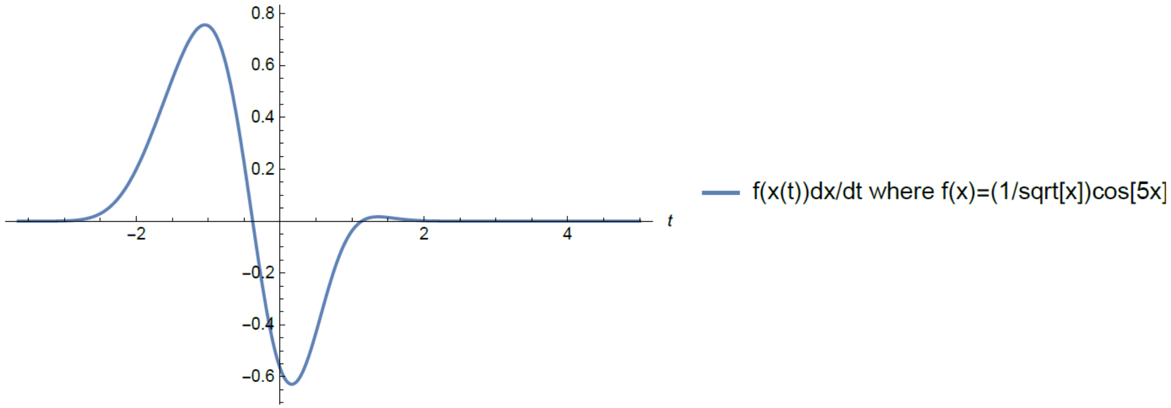
```
Plot[{Legended[f[x[t]] dxdt, "f(x(t))dx/dt where f(x)=(1/sqrt[x])cos[5x]"]},
 {t, -5, 5}, PlotRange → All, AxesLabel → {t, ""}]
```

Power: Infinite expression $\frac{1}{\sqrt{0.}}$ encountered.

Power: Infinite expression $\frac{1}{\sqrt{0.}}$ encountered.

Power: Infinite expression $\frac{1}{\sqrt{0.}}$ encountered.

General: Further output of Power::infy will be suppressed during this calculation.



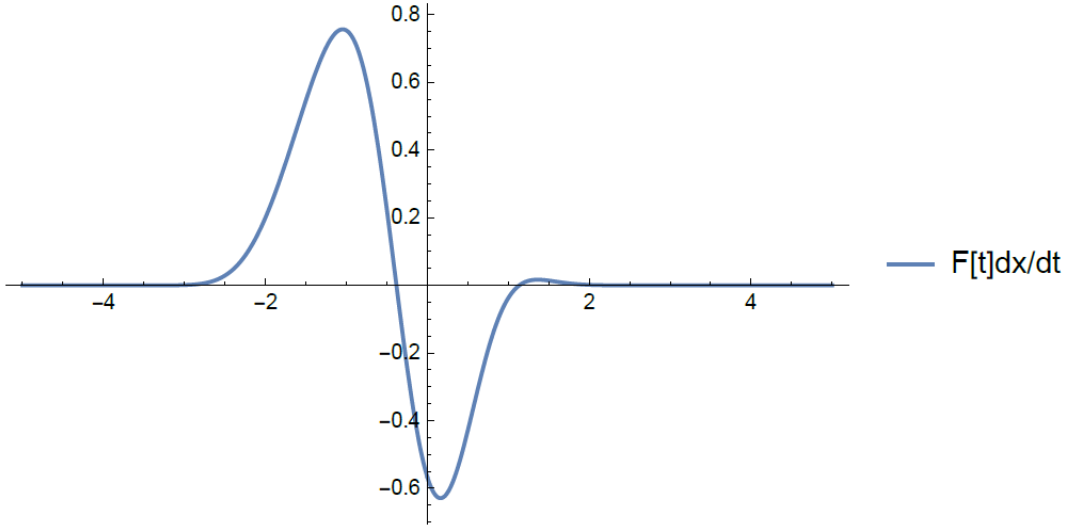
$$x = \frac{1}{2}(b + a) + \frac{1}{2}(b - a)\tanh(c \sinh t)$$

a=0; b=1:

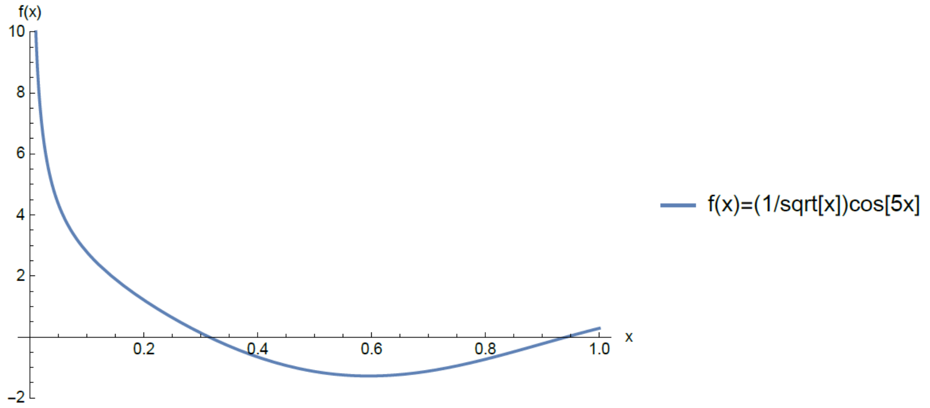
```
{x[-3.6], x[-3.7]} // N
```

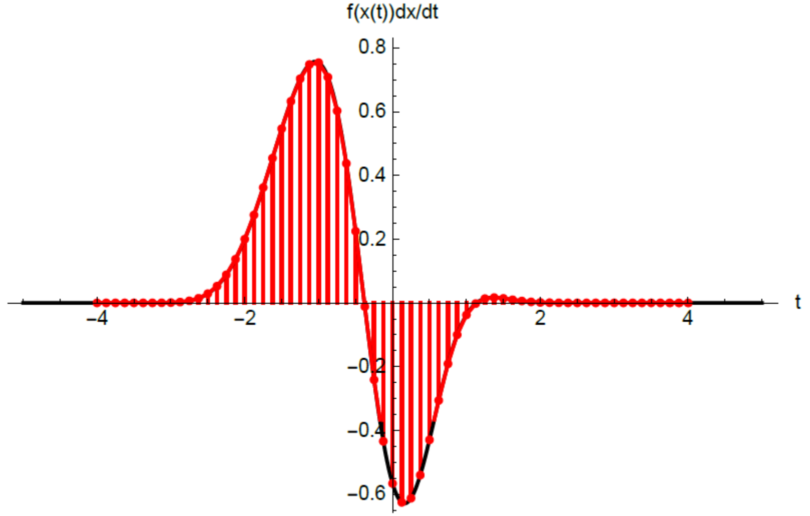
$\{1.11022 \times 10^{-16},\ 0.\}$

```
Plot[Legended[F[t] dxdt, "F[t]dx/dt"], {t, -5, 5}, PlotRange → All]
```



And just apply the Trapezoidal method on F(t) using e.g. the truncation -5<=t<=5





i	A(hi)	A(hi-1)-A(hi)	A(hi)-A	#f-computations
2.	-0.158428	-0.97456	-0.526627	3.
3.	0.0464992	-0.204927	-0.3217	7.
4.	0.15013	-0.10363	-0.21807	15.
5.	0.216014	-0.0658842	-0.152185	31.
6.	0.261042	-0.0450283	-0.107157	63.
7.	0.292533	-0.031491	-0.075666	127.
8.	0.31472	-0.022187	-0.0534789	255.
9.	0.33039	-0.0156696	-0.0378093	511.
10.	0.341466	-0.0110755	-0.0267338	1023.

Standard midpoint method

i	A(hi)	A(hi-1)-A(hi)	A(hi)-A	e_d=Exp[-Pi^2/h]	Antal f-ber.
1.	-2.43592	*	-2.80412	0.100736	3.
2.	-0.945831	-1.49009	-1.31403	0.0101476	5.
3.	0.324935	-1.27077	-0.0432644	0.000102975	9.
4.	0.368189	-0.0432539	-0.0000104809	1.06038×10^{-8}	17.
5.	0.368199	-0.0000104809	-1.40632×10^{-12}	1.1244×10^{-16}	33.

DE-rule

Notice that the error estimate e_d is very inaccurate, but convergence is much faster.

Summary on methods for numerical integration

- Newton-Cotes quadratures (Midpoint, Trapezoidal, Simpson):
  - Errors accurately estimated by Richardson (remember to check order first)
  - Simpson recommended
  - Convergence can be improved for ”nice” integrands using automated Richardson Extrapolation (Romberg Integration). Not part of NM

- DE-rule
  - Fast convergence
  - Mandatory if there are singularities. If the singularity is at an interior point c ($a<c<b$), split the integral into (a;c) and (c;b) and apply DE-rule to each of them.
  - Also excellent even for integrands without singularities
  - Richardson cannot be used, but more than compensated

Exercises

- Same as last time, but now with DE-rule.
- 3rd Mandatory Exercise will be handed out later today. Due April, 22nd at 23:59.