Chapter 1

Extrapolation to zero

In this short chapter we will describe shortly the concept of *extrapolation to zero* and how we can apply it.

1.1 Motivation

Let $T :]0, \varepsilon[\to \mathbb{R}$ be function and assume that we have

$$T(h) = T_0 + ah^n + O(h^{n+1}). \tag{1.1}$$

for $h \to 0$. We are interested in computing $T_0 = \lim_{h\to 0} T(h)$ up to some desired accurracy. In order to do that we might have to compute $T(h)$ for very small h. That might not be feasible since $T(h)$ might be very expensive to compute for small h or even impossible due to numerical instabilities. Hence we would like to somehow accelerate the convergence of T to 0. A nice way to do that is the *Richardson extrapolation scheme* which goes as follows: Let $0 < r < 1$. Plug rh into (1.1). Then we get

$$T(rh) = T_0 + ar^n h^n + O(h^{n+1}). \tag{1.2}$$

Now multiply (1.1) by r^n, subtract it from (1.2) and divide the result by $1 - r^n$. Then we get:

$$R(h) = T_0 + O(h^{n+1})$$

where

$$R(h) := \frac{T(rh) - r^n T(h)}{1 - r^n}.$$

Note that $R(h)$ has $O(h^{n+1})$ convergence to T_0 while $T(h)$ has $O(h^n)$, i.e. $R(h)$ converges asymptotically faster. But what did we actually do? We took the linear polynomial in t^n which goes through $(rh, T(rh))$ and $(h, T(h))$ and let $R(h)$ be its value at 0, i.e. we interpolated the points and then evaluated the interpolation polynomial outside the interval; hence the term *extrapolation*. This should serve as a motivation for the sequel.

1.2 The extrapolation table

We always think of T as arising from some numerical scheme e.g. the trapezoidal rule and then T_0 is the integral of some function. Thus we do not require that T is necessarily defined for all values near 0, but only on set which has 0 as an accumulation point. In what follows, we will thus refer to T as a *method* for computing T_0.

Definition 1.1. Let T be a method for computing T_0. We say that T has an asymptotic expansion in h^p up to order pm if there exist constants $\tau_p, \tau_{2p}, \ldots, \tau_{mp} \in \mathbb{R}$ such that

$$T(h) = T_0 + \tau_p h^p + \tau_{2p} h^{2p} + \cdots \tau_{mp} h^{mp} + O(h^{(m+1)p}) \tag{1.3}$$

for $h \to 0$.

Let $(x_1, y_1), \ldots, (x_k, y_k)$ be a collection of points such that $x_1, \ldots, x_k$ are distinct. Then there exists a polynomial P which interpolates the points, i.e. $P(x_i) = y_i$ for all i. We say that P is *the interpolation polynomial* for the points if P has the lowest degree among all polynomials which interpolate them. The interpolation polynomial is unique. Let $p > 0$ be an integer and points $(x_1^p, y_1), \ldots, (x_n^p, y_n)$ such that x_i^p are distinct, be given. Let P be the interpolation polynomial for the points. We then call $P(h^p)$ the *interpolation polynomial in p* for the points.

Let T be a method with asymptotic expansion in p up to pm. The extrapolation process works as follows: We compute $T(h)$ for some points $h_1, h_2, \ldots, h_k$ where $k \leq m$. Then we compute the interpolation polynomial P in h^p which goes through $(h_1, T(h_1)), \ldots, (h_k, T(h_k))$. We then hope that $P(0)$ gives a good approximation T_0.

In order to compute $P(0)$ we use the *Neville scheme*. Let $P_{ij}(h^p) \coloneqq P(h^p; h_{i-j+1}^p, h_i^p)$ be the interpolation polynomial in h^p which interpolates $(h_{i-j+1}^p, T(h_{i-j+1}), \ldots, (h_i^p, T(h_i^p))$ and set $T_{ij} \coloneqq P_{ij}(0)$. Then according to the Neville scheme we can compute T_{ij}, $j \leq i$, in the following recursive way:

1. $T_{i1} \coloneqq T(h_i)$ for $i = 1, \ldots, k$.
2. $T_{ij} \coloneqq T_{i,j-1} + \dfrac{T_{i,j-1} - T_{i-1,j-1}}{r^p - 1} = \dfrac{r^p T_{i,j-1} - T_{i-1,j-1}}{r^p - 1}$ for $1 < j \leq i$ where $r \coloneqq h_{i-j+1}/h_i$.

If we align T_{ij} to a triangular table, we call that the *extrapolation table*.

1.3 Convergence

If we have a numerical method or scheme that has an asymptotic expansion as (1.3), then the error decays polynomially as $h \to 0$. It is known (see e.g. theorem 9.22 in [1]) that T_{ij} has faster polynomial decay of higher degree, as $h \to 0$, then T. Let $\varepsilon_k \coloneqq |T_{kk} - T|$. We want to analyze how ε_k behaves as $k \to +\infty$, i.e. how ε_k behaves when we increse the number of extrapolation steps. Let $N_n k$ be some measure of the effort needed to compute T_{kk}. In what follows we will test numerically the qualitative hypothesis that the error converges exponentially with the computational effort i.e.

$$\varepsilon_k \sim A \exp(-c N_k^q) \tag{1.4}$$

for constants A, c, q. Note that if $\varepsilon_k = A \exp(-c N_k^q)$ then $\ln \varepsilon_k = b - c N_k^q$ so in order to test the hypothesis we will do the following: Assume that we have the error ε_k for $k = 1, \ldots, n$. Then we will compute

$$(b, c, q) \coloneqq \arg\min \left\{ \sum_{k=1}^{n} |\ln \varepsilon_k - (b - c N_k^q)|^2 \right\} \tag{1.5}$$

and see whether the points $(N_k, \ln \varepsilon_k)$ fit well to the graph of $t \mapsto b - ct^q$.

We will also test the hypothesis that the error converges exponentially with the number of extrapolation steps, i.e. whether

$$\varepsilon_k \sim A \exp(-ck^q) \tag{1.6}$$

for constants A, c, q.

In order to validate the estimated parameters b, c, q we will do a simple "cross validation" by fitting the model to subsets of the data and see whether the parameters vary a lot. If they vary a lot, we conclude that the fitting is unstable. If they are almost the same we will be more confident in that the model is actually appropriate.

1.4 Code

The following Python mehtod computes the extrapolation table for some scheme which has an asymptotic expansion in h^p.

```
#sc (Scheme): The scheme to extrapolate
#prob: The problem to apply the scheme to. We assume that sch is an
#      implementation of Scheme which can be applied to prob.
#seq (Sequence): The sequence to use in the extrapolation
#hp (bool): Indicates whether to use high precision arithmetic (true)
#           or standard double precision (false).
#returns: The extrapolation table as a list of lists.
def extrapolate(sc, prob, seq, hp):
  n = len(seq)
  X = [[0 for j in range(i + 1)] for i in range(n)]

  #X[i][j] = T_ij
  for i in range(n):
    X[i][0] = sc.apply(prob, seq[i])
    for j in range(1, i + 1):
      #r = h_{i-j} / h_i = seq[i] / seq[i-j]
      #rp = r^p.
      #Must cast the elements of seq to hp numbers if in hp mode.
      rp = ((mpf('1') * seq[i]) / (mpf('1') * seq[i-j]) if hp else seq[i] / seq[i-j]) ** sc.p
      X[i][j] = (rp * X[i][j-1] - X[i-1][j-1]) / (rp - 1)

  return X
```

Chapter 2

Romberg quadrature

2.1 The algorithm

Let $f : [a, b] \to \mathbb{R}$ be a function and $I := \int_a^b f(x)dx$. The *trapezoidal rule* is a method for approaching I which works as follows: Let $a = t_0 < t_1 < \cdots < t_n = b$ be a subdivision of $[a, b]$. On each of the intervals $[t_{i-1}, t_i]$ we approximate $\int_{t_{i-1}}^{t_i} f(x)dx$ by the area of a trapezoid with verticies $(t_{i-1}, 0)$, $(t_{i-1}, f(t_{i-1}))$, $(t_i, f(t_i))$, $(t_i, 0)$ i.e. by $\frac{1}{2}(t_i - t_{i-1})(f(t_{i-1}) + f(t_i))$. Hence we approximate I by

$$I = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} f(x)dx \approx \sum_{i=1}^{n} \frac{1}{2}(t_i - t_{i-1})(f(t_{i-1}) + f(t_i)).$$

If $t_i - t_{i-1} = \frac{1}{n}(b - a) =: h$ for each i then the above estimate becomes

$$I \approx h \left(\frac{1}{2}(f(a) + f(b)) + \sum_{i=1}^{n-1} f(a + ih) \right) \tag{2.1}$$

We define $T_f(h)$ as the right hand side in (2.1).

Let $F : [0, n] \to \mathbb{R}$ be a $2k + 1$ times continuously differentiable function, n a positive integer. Then by Euler's summation formula (see formula 298 in [2]) we have

$$\sum_{i=0}^{n} F(i) = \int_0^n F(x)dx + \frac{1}{2}(F(0) + F(n)) + \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!}(F^{(2i-1)}(n) - F^{(2i-1)}(0)) + R_k \tag{2.2}$$

where $R_k = \int_0^n P_{2k+1}(x)F^{(2k+1)}(x)dx$, B_m are the *Bernoulli numbers* and P_m the *Bernoulli polynomials*. If let $F(x) := f(a + xh)$ then we get the following asymptotic expansion for the trapezoidal rule:

Theorem 2.1. *Let $f : [a, b] \to \mathbb{R}$ be $2k + 1$ times continuously differentiable and $h := (b - a)/n$. Then*

$$T_f(h) = I + \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!}(f^{(2i-1)}(b) - f^{(2i-1)}(a))h^{2i} + h^{2k+1}R_k(h) \tag{2.3}$$

where

$$R_k(h) = \int_a^b P_{k+1}\left(n\frac{x - a}{b - a}\right) f^{(2k+1)}(x)dx. \tag{2.4}$$

The following code is a trivial implementation of the trapezoidal rule. The *TrapezoidalRule* class in an implementation of the abstract class *Scheme* which represents a numerical scheme or method, which has asymptotic expansion in h^p. The Scheme class has a method named *apply* which takes in a problem to which the scheme is applied to. The argument m in the apply-method is the number of subintervals that should be used.

```
class TrapezoidalRule(Scheme):
    def __init__(self):
        super(TrapezoidalRule, self).__init__(2)

    def apply(self, inte, m):
        (a,b) = inte.interval
        h = (b - a) / m
        I = 0.5 * (inte.f(a) + inte.f(b))
        for i in range(1, m):
            I += inte.f(a + i * h)

        return I * h
```

Assume that we have computed the value of $T_f(h)$ for $h = h_1, \ldots, h_k$ and we want extrapolate to zero, i.e. we want to compute the value at zero of the interpolation polynomial in h^2 for $(h_i^2, T_f(h_i)$, $i = 1, \ldots, k$. Denote by T_{ij} the value at zero of the polynomial in h^2 which goes through $(h_{i-j+1}^2, T(h_{i-j+1}), \ldots, (h_i^2, T(h_i))$. The Neville scheme gives us the following algorithm for computing T_{ij}, $1 \leq j \leq i \leq k$, recursively:

1. $T_{i1} \coloneqq T_f(h_i)$ for $i = 1, \ldots, k$.
2. $T_{ij} \coloneqq T_{i,j-1} + \frac{T_{i,j-1} - T_{i-1,j-1}}{\left(\frac{h_{i-j+1}}{h_i}\right)^2 - 1}$ for $2 \leq j \leq i$.

2.2 Numerical experiments

In this section we are going to apply Romberg quadrature to various functions and also try different sequences. We will analyze how different sequences perform in the sense that we want to measure how many function evaluations we need to attain a prescribed precision.

We will try various functions and the following sequences:

- The harmonic sequence: $a_n = n$, $n \geq 0$.
- The Romberg sequence: $a_n = 2^{n-1}$, $n \geq 1$.
- The Bulirsch sequence: $a_1 = 1$, $a_2 = 2$, $a_3 = 3$ and $a_{n+2} = 2 \cdot a_n$ for $n \geq 2$. Its first elements are

$$1, 2, 3, 4, 6, 8, 12, 16, 24, 32, \ldots$$

Suppose that we are approximating the integral $I \coloneqq \int_a^b f(x)dx$ using Romberg quadrature. We will use the stepsizes $h_k \coloneqq (b-a)/a_k$ for the extrapolation. Let T_{ij}, $i \geq 0$ and $j \leq i$ be the extrapolation table we get and $\varepsilon_k \coloneqq |T_{kk} - I|$ be the error on the diagnoals. Let N_k be the number of function evaluations needed to compute T_{kk}. We will use N_k as the measurement of computational effort as mentioned in section 1.3 and we will try to fit the exponential convergence model introduced there. We will also plot the logarithm of the error against the number of extrapolation steps. Note that $N_k = \sum_{i=1}^{k}(a_i + 1)$ where (a_i)

is our sequence, so in case of the Harmonic sequence, we have $N_n = n(n+3)/2 \approx n^2/2$ for n large. Hence if $\varepsilon_n \sim A\exp(-cN_n^q)$ then

$$\varepsilon_n \sim A\exp(-c/2^q n^{2q})$$

for n large. Thus if the error converges exponentially with the number of function evaluations, it will also converge exponentially with the number of extrapolation steps, and the exponent in the latter fitting will be twice the parameter from the former.

If our sequence is the Romberg sequence then $N_k = \sum_{i=1}^{n}(2^{i-1}+1) = 2^k + k - 1 \approx 2^k$ for k large, so if $\varepsilon_k \sim A\exp(-cN_k^q)$ then

$$\varepsilon_k \sim A\exp(-c2^{kq})$$

for k large, which is not exponential convergence. On the other hand, if the we have exponential convergence in the number of extrapolation steps, i.e.

$$\varepsilon_k \sim A\exp(-ck^q)$$

then since $k \approx \ln N_k/\ln 2$ we get

$$\ln\varepsilon_k \sim \ln A - c(\ln N_k/\ln 2)^q = \ln A - \frac{c}{(\ln 2)^q}(\ln N_k)^q$$

so if we consider the ln-ln plot of the error against the number of function evaluations, then the points should fall on the graph of a function of the form $t \mapsto b - ct^q$. The exponent should be the same as in the fitting for the logarithm of the error against the number of extrapolation steps.

For the model fitting we will thus plot the logarithm of the error agains the number of function evaluations, the number of extrapolation steps and the logarithm of the number of extrapolation steps. We will also consider the plot of the base 10 logarithm of the error against the number of function evaluations.

In order to validate the fitting, we will do "cross validation" in the following way: We will estimate the parameters in the models where we only consider every other point, every third point and then when we only consider a consecutive sequence of half of the points, though never fewer than 10.

We conduct the experiments in Python 3 and use the high precision arithmetic library mpmath for all the computations. The precision will be set to 500 significant digits so will not have to worry about numerical instabilities.

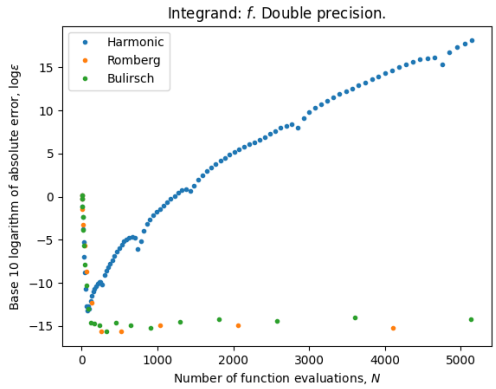
Now we will consider the results of the experiments.

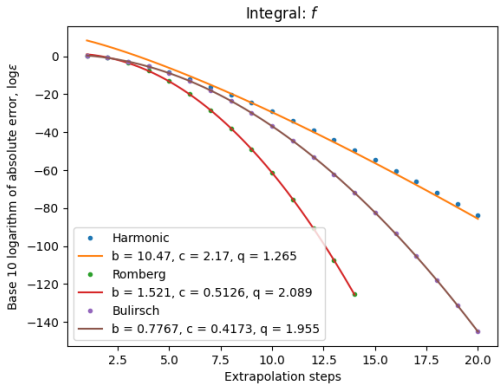
2.2.1 Cosine squared

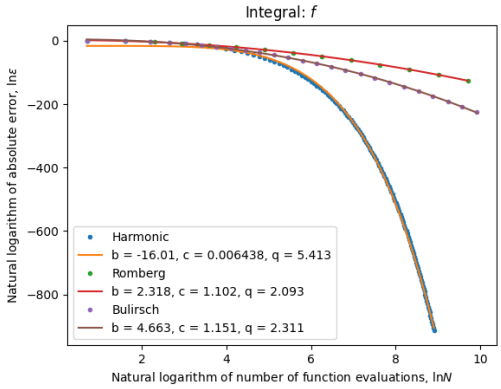
The first function we are going to try is

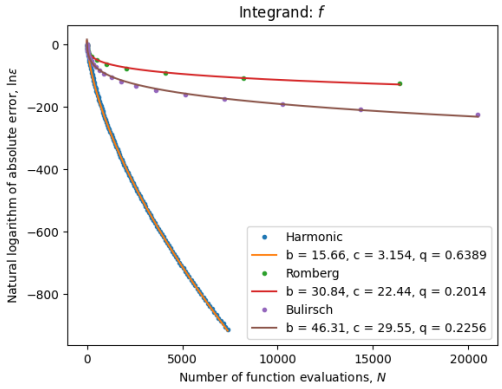
$$f : [0,\pi] \to \mathbb{R}, \quad f(x) \coloneqq \cos^2(x)$$

which is entire.









Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	15.892	0.052543	0.0037803
Romberg	lin-ln evals-error	3.9999	0.10449	0.029386
Bulirsch	lin-ln evals-error	14.911	0.43183	0.20258
Harmonic	lin-ln steps-error	14.477	0.03992	0.0021086
Romberg	lin-ln steps-error	0.066039	0.0010865	$3.8422e-05$
Bulirsch	lin-ln steps-error	0.18524	0.0019423	$5.5812e-05$
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	0.031489	0.00052793	$2.887e-05$
Bulirsch	ln-ln evals-error	2.9654	0.088636	0.0071409

We see that the harmonic sequence performes best, then Bulirsch and then Romberg. In standard double precision arithmetic, we get down to machine level precision using Romberg or Bulirsch, but we are like 2 digits from there, using the harmonic sequence.

For the Romberg and Bulirsch sequence, we can not say that the error converges exponentially with the number of function evaluations since the parameters we get in the cross validation vary a lot. In the case of the harmonic sequence, we seem to have exponential convergence in the number of function evaluations, though that must be verified better, since the b and c parameters vary quite much.

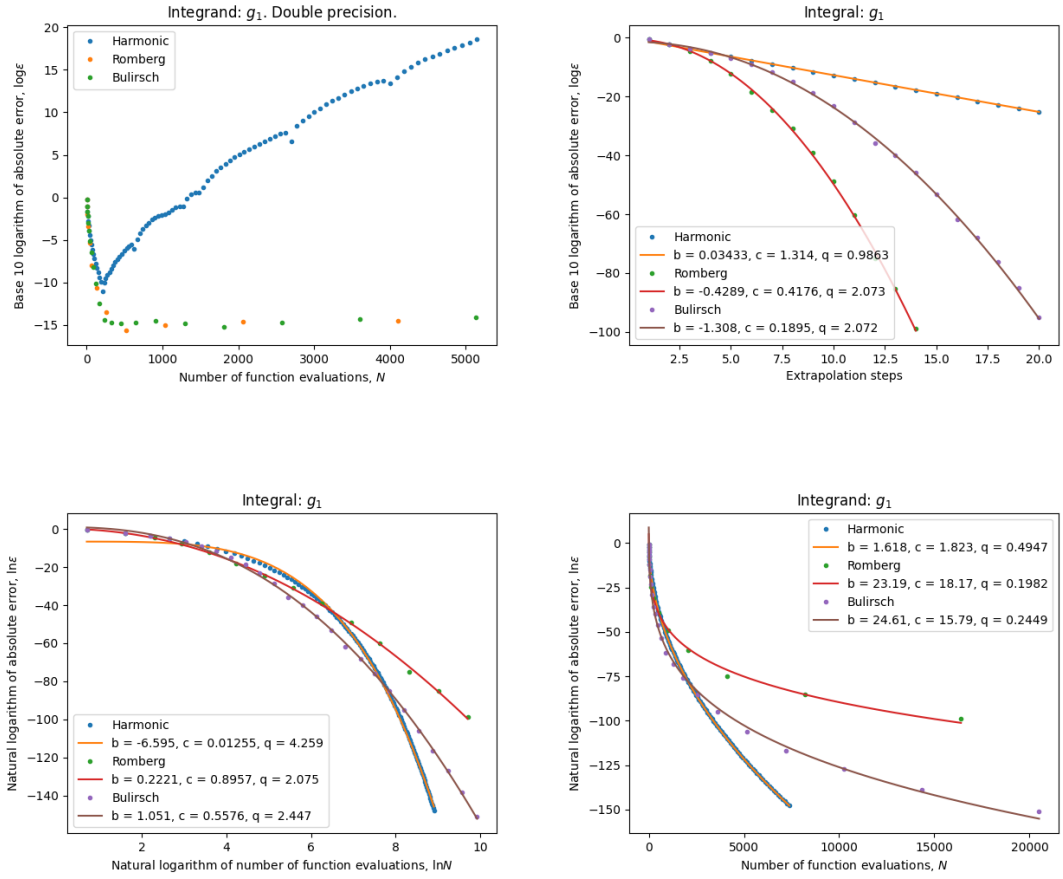
For all sequences the error seems to converge exponentially with the number of extrapolation steps, but again we there is a lot of variance in the b parameter.

As we expect, since the error seems to converge exponentially with the number of extrapolation steps, ln-ln plot for the Romberg and Bulirsch sequence seem to fit quit well on the graph of a function of the form $t \mapsto b - ct^q$. On the other hand, that is not the case for the harmonic sequnce, as we expect.

2.2.2 Function with poles

Now we will consider the following function:

$$g_a : [-1, 1] \to \mathbb{R}, \quad g_a(x) := \frac{1}{a^2 + x^2},\ a > 0$$



Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	0.091387	0.00065694	$3.963e-05$
Romberg	lin-ln evals-error	4	0.33642	0.085159
Bulirsch	lin-ln evals-error	nan	3.2071	0.58712
Harmonic	lin-ln steps-error	0.17361	0.001823	0.00010357
Romberg	lin-ln steps-error	1.8814	0.52416	0.035469
Bulirsch	lin-ln steps-error	15	1.7795	0.099758
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	1.4183	0.45669	0.038901
Bulirsch	ln-ln evals-error	15	1.7737	0.14009

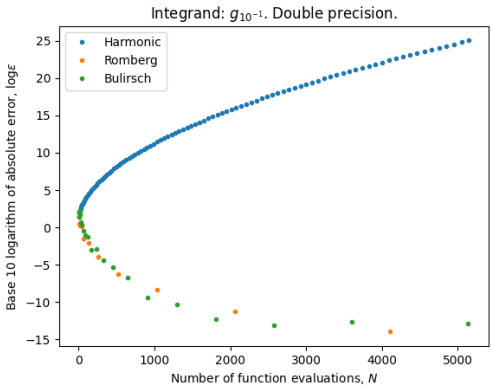
We see that the harmonic sequence performes best, then Bulirsch and then Romberg. In standard double precision arithmetic, we get down to machine level precision using

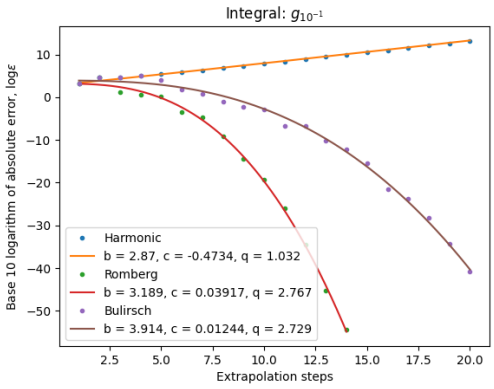
Romberg or Bulirsch, but we are like 5 digits from there, using the harmonic sequence.

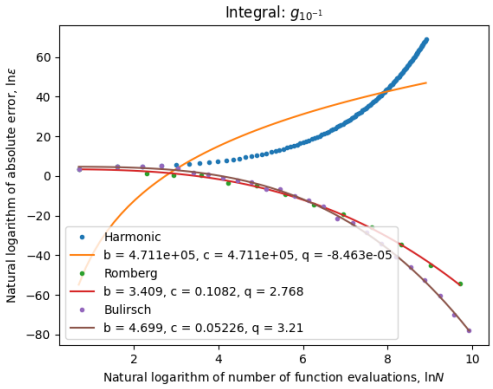
For the Romberg and Bulirsch sequence, we can not say that the error converges exponentially with the number of function evaluations since the parameters we get in the cross validation vary a lot, especially since the exponent q varies a lot. In the case of the harmonic sequence, the model seems to fit very well, since we have very little variance in the parameters.

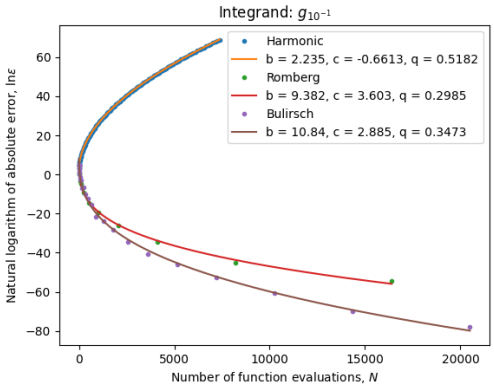
For all sequences the error seems to converge exponentially with the number of extrapolation steps, but again we there is quit a lot of variance in the b parameter. Note that the exponent from the fitting for the Harmonic sequence is twice the parameter we got when considering the number of function evaluations agains the error, as expected.

The model fits quite well to the ln-ln plot in the case of the Romberg sequence. It clearly does not fit for the Harmonic sequnce but fits moderately well for the Bulirsch sequence.





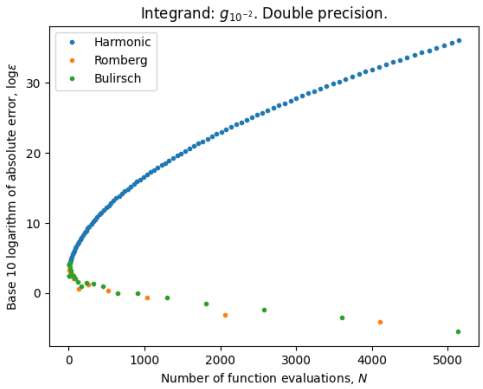


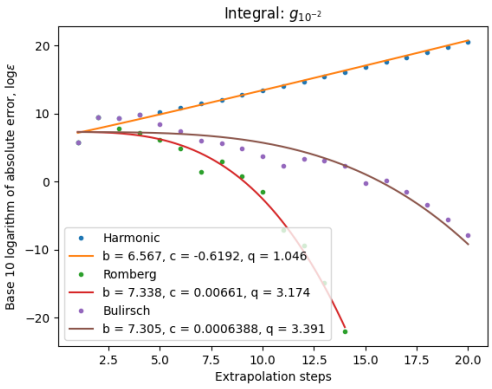


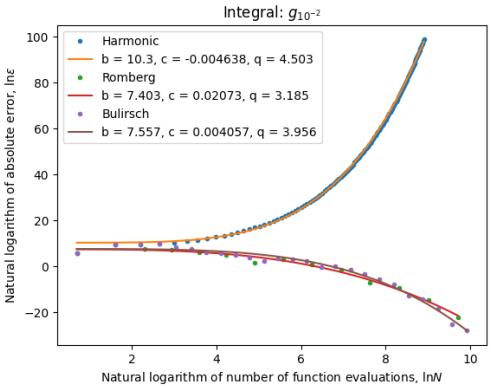
Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	0.66369	0.019182	0.0031665
Romberg	lin-ln evals-error	3.9854	0.30308	0.073011
Bulirsch	lin-ln evals-error	*nan*	14.616	0.74405
Harmonic	lin-ln steps-error	0.29415	0.014971	0.0018903
Romberg	lin-ln steps-error	1.5386	0.49618	0.012829
Bulirsch	lin-ln steps-error	*nan*	14.991	0.29893
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	1.5752	0.4164	0.014402
Bulirsch	ln-ln evals-error	*nan*	14.981	0.33583

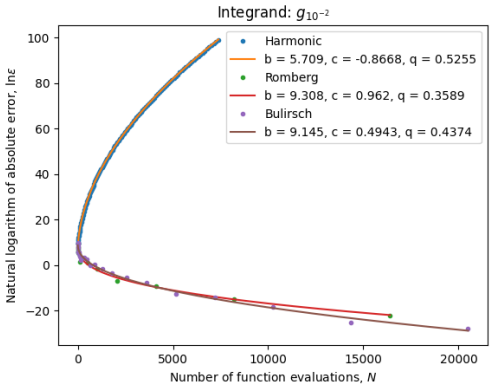
Here we get divergence for the harmonic sequence, but convergence for the other sequences, fastest for Bulirsch. In standard double precision arithmetic, we get down to machine level precision using Romberg or Bulirsch.

For the models, in case of convergence, they do not fit very well in any case. The best fitting is when we consider the logarithm of the error against the number of extrapolation steps and the logarithm of number of function evaluations, for the Romberg sequence. There is though quite a lot of variance in the b and c parameters.









Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	5.0593	0.042405	0.0071056
Romberg	lin-ln evals-error	*nan*	2.7999	1.0815
Bulirsch	lin-ln evals-error	*nan*	6.3194	1.1937
Harmonic	lin-ln steps-error	*nan*	111.94	0.012047
Romberg	lin-ln steps-error	4	3.1912	0.62642
Bulirsch	lin-ln steps-error	*nan*	3.4957	1.7296
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	4	3.6997	0.68554
Bulirsch	ln-ln evals-error	*nan*	3.6555	1.8702

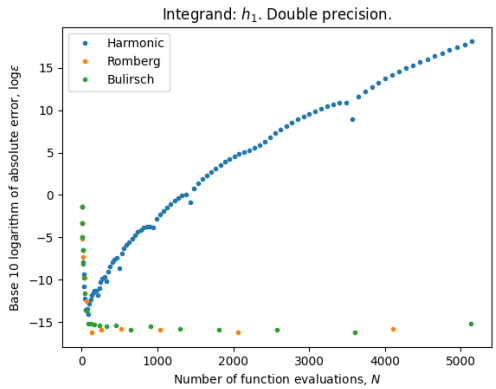
Here the same comments apply as for $a = 10^{-1}$, except that now the Romberg sequence performes better than the Bulirsch sequence and the model fitting is worse.

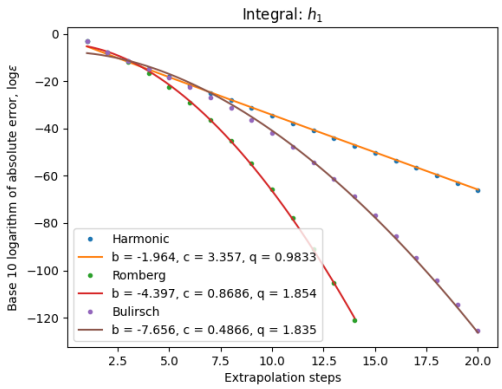
2.2.3 Logarithm

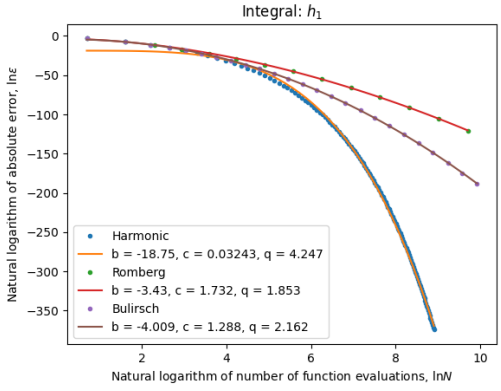
Now we will consider the following function

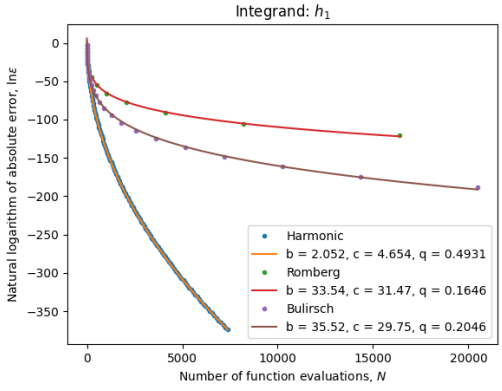
$$h_a : [0, 1] \to \mathbb{R}, \quad h_a(x) \coloneqq \ln(a + x),\ a > 0.$$

This function is analytic on neighbourhood about the interval but we have a singularity at the horizontal ray from $-a$ to $-\infty$.







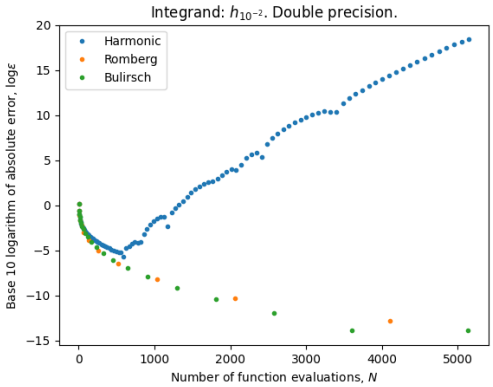


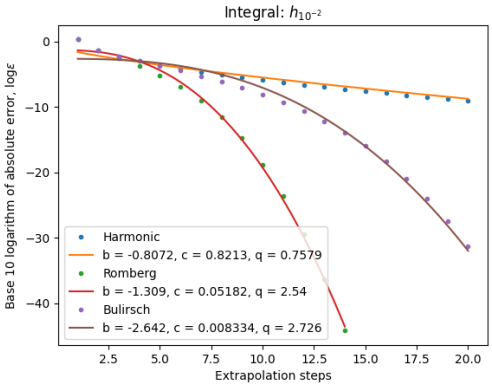
Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	1.6275	0.001334	$8.4531e-05$
Romberg	lin-ln evals-error	3.9961	0.034675	0.0095088
Bulirsch	lin-ln evals-error	13.729	0.23963	0.069978
Harmonic	lin-ln steps-error	3.3305	0.0028975	0.00016396
Romberg	lin-ln steps-error	0.94544	0.018617	0.00067321
Bulirsch	lin-ln steps-error	8.3957	0.32107	0.0068979
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	1.1892	0.019677	0.0010134
Bulirsch	ln-ln evals-error	0.36829	0.0038072	0.00015789

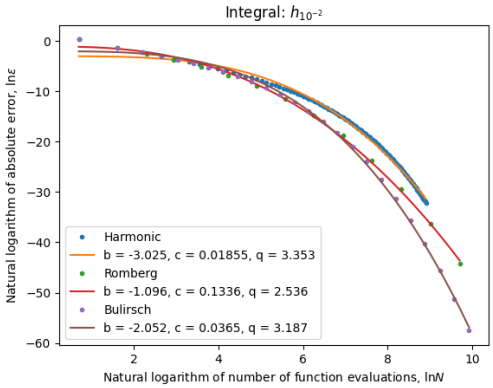
We see that the harmonic sequence performes best, then Bulirsch and then Romberg. In standard double precision arithmetic, we get down to machine level precision using Romberg or Bulirsch, but we are like 2 digits from there, using the harmonic sequence.

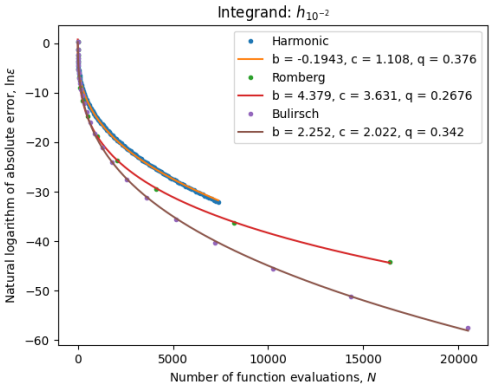
For the Romberg and Bulirsch sequence, we can not say that the error converges exponentially with the number of function evaluations. In the case of the harmonic sequence, the model seems to fit very well, since we have very little variance in the parameters.

For the harmonic sequence the error clearly seems to converge exponentially with the number of extrapolation steps, as we expect, since it seems to converge exponentially with the number of function evaluations. The exponent is approximately two the one from the former fitting as expected. The model, on the other hand, the fitting is rather unstable for the Romberg and Bulirsch sequence though, and hence also when considering the logarithm of the error against the logarithm of the number of function evaluations.





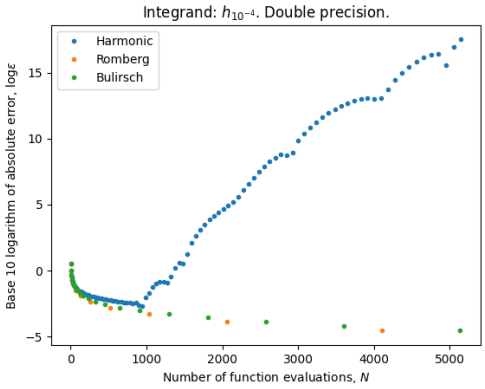


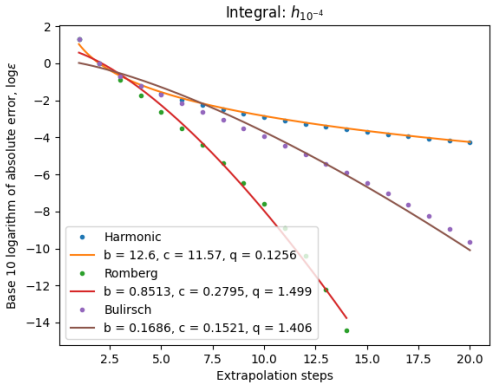


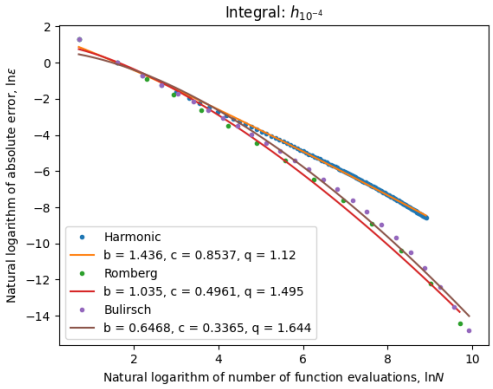
Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	75.169	1.4423	0.030506
Romberg	lin-ln evals-error	1.9659	0.02769	0.002777
Bulirsch	lin-ln evals-error	10.207	0.15642	0.012213
Harmonic	lin-ln steps-error	26.823	1.0482	0.02436
Romberg	lin-ln steps-error	0.5511	0.3681	0.0061046
Bulirsch	lin-ln steps-error	2.8679	3.5395	0.047691
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	0.62271	0.26181	0.0063053
Bulirsch	ln-ln evals-error	1.9572	1.649	0.028369

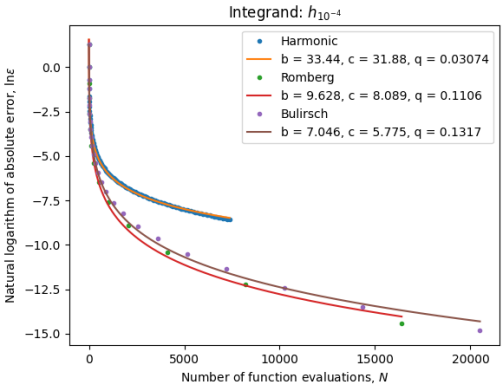
We see that we can not attain high precision using the harmonic sequence and standard double precision. It is hard to tell which sequence performes best in the long run, though we can say that Bulirsch performes better than Romberg.

Here, none of our models seems to fit well.









Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln evals-error	3.9998	0.58702	0.20654
Bulirsch	lin-ln evals-error	3.8706	0.53846	0.31338
Harmonic	lin-ln steps-error	.	.	.
Romberg	lin-ln steps-error	0.79452	0.67424	0.054336
Bulirsch	lin-ln steps-error	1.3261	1.3702	0.15695
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	1.0455	0.61797	0.065037
Bulirsch	ln-ln evals-error	1.0172	0.76715	0.15282

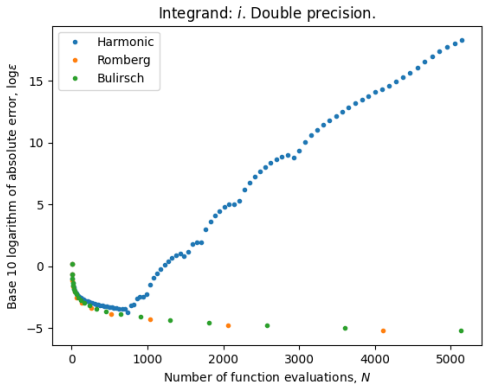
Here again, we do not attain high precision when using the Harmonic sequence in double precision arithmetic. It is hard to say which sequence performes best. None of our models fits.

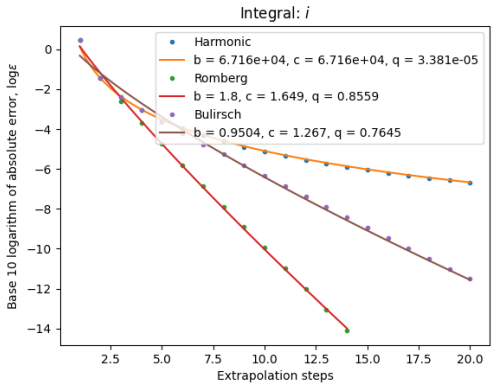
2.2.4 Area of half circle

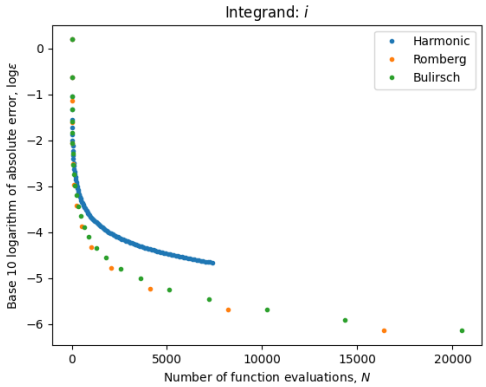
Now we will try the following function:

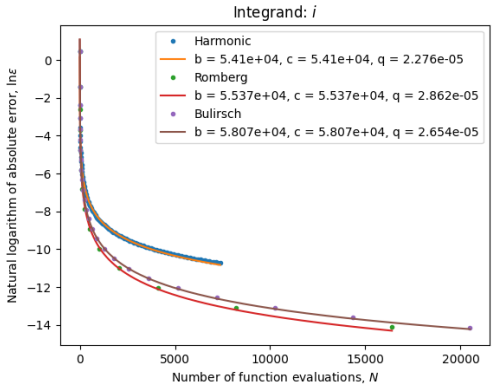
$$i : [-1, 1] \to \mathbb{R}, \quad i(x) := \sqrt{1 - x^2}.$$

This function is analytic inside the interval of definition but not at the endpoints. Its derivative has singularities at the endpoints.









Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln evals-error	nan	0.00074987	0.0010457
Bulirsch	lin-ln evals-error	.	.	.
Harmonic	lin-ln steps-error	.	.	.
Romberg	lin-ln steps-error	0.0017773	0.00025637	$2.7817e-05$
Bulirsch	lin-ln steps-error	0.16248	0.0448	0.003052
Harmonic	ln-ln evals-error	0.66509	0.035037	0.0039765
Romberg	ln-ln evals-error	0.11181	0.0085994	0.001262
Bulirsch	ln-ln evals-error	0.059168	0.0077593	0.001453

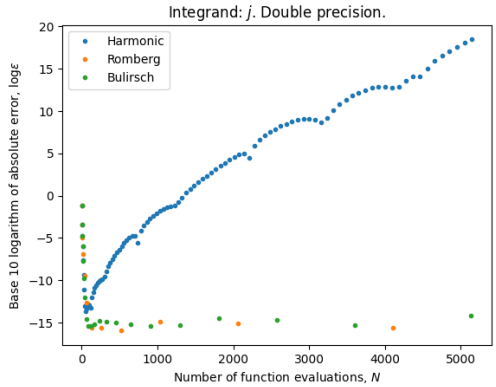
We see that we do not get high precision using double precision arithmetic, independent of sequence. The Romberg and Bulirsch sequence seem to perform similarly well but the harmonic sequence seems to be slowest.

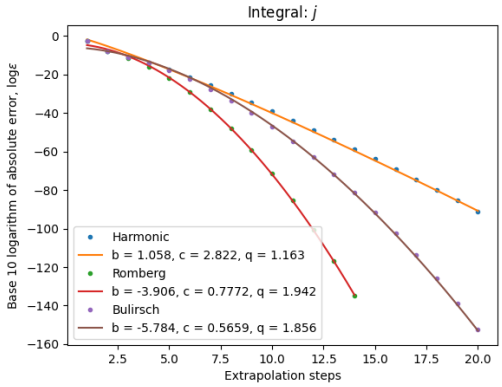
For the harmonic sequence, the error neither converges exponentally with the number of function evaluations nor the number of extrapolation steps. For the Bulirsch none of the models fits well, but for Romberg, model seems to fit moderately well when considering the logarithm of the error against the number of extrapolation steps or the logarithm of the number of function evaluations.

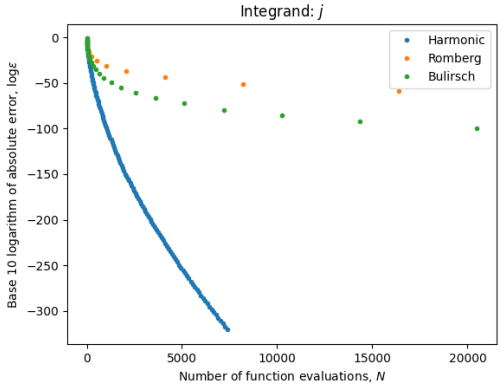
2.2.5 Gaussian

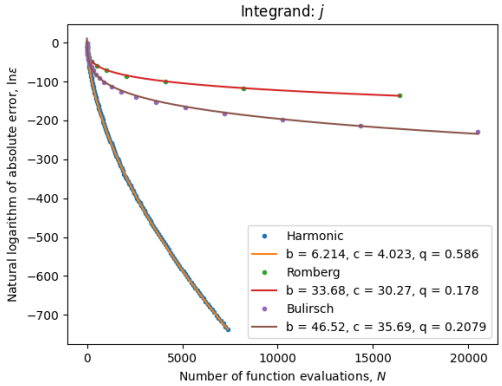
Finally we will consider the Gaussian function

$$j : [0, 1] \to \mathbb{R}, \quad k(x) := \frac{2}{\sqrt{\pi}} e^{-x^2}.$$









Sequence	Plot	A-variance	c-variance	q-variance
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln evals-error	3.9999	0.075546	0.02295
Bulirsch	lin-ln evals-error	nan	2.7536	0.17572
Harmonic	lin-ln steps-error	.	.	.
Romberg	lin-ln steps-error	0.023038	0.00025761	$8.9728e-06$
Bulirsch	lin-ln steps-error	15	1.1721	0.0087318
Harmonic	ln-ln evals-error	.	.	.
Romberg	ln-ln evals-error	0.16893	0.0015778	$7.6206e-05$
Bulirsch	ln-ln evals-error	15	1.4218	0.011922

In double precision arithmetic we get down to machine level precision using Romberg or Bulirsch, but we get down to like 2 digits from there, using the harmonic sequence. The harmonic sequence performes best, then Bulirsch and then Romberg.

For the harmonic sequence, the error seems to converge exponentially with the number of extrapolation steps (and hence also with the number of extrapolation steps), but we though must note that there is quite a lot of variance in the b parameter and the c parameter. For the Romberg sequence, model fits moderately well when considering the logarithm of the error agains the number of extrapolation steps or the logarithm of the number of function evaluations. For the Bulirsch seqeunce, none of the models fits.

The values of the optimal parameters in the curve fitting of evaluations against the logarithm of the error are:

Integrand	Sequence	b	c	q
f	Harmonic	15.66	3.1537	0.63887
f	Romberg	30.844	22.442	0.2014
f	Bulirsch	46.309	29.549	0.22556
$g_{10^{-2}}$	Harmonic	5.7088	-0.8668	0.52546
$g_{10^{-2}}$	Romberg	9.3083	0.96199	0.35893
$g_{10^{-2}}$	Bulirsch	9.1445	0.49433	0.43743
$g_{10^{-1}}$	Harmonic	2.2352	-0.66129	0.51817
$g_{10^{-1}}$	Romberg	9.3824	3.6029	0.29851
$g_{10^{-1}}$	Bulirsch	10.844	2.8849	0.34731
g_1	Harmonic	1.6178	1.823	0.49467
g_1	Romberg	23.192	18.171	0.19817
g_1	Bulirsch	24.613	15.795	0.24492
$h_{10^{-4}}$	Harmonic	33.436	31.879	0.030738
$h_{10^{-4}}$	Romberg	9.6285	8.0889	0.1106
$h_{10^{-4}}$	Bulirsch	7.0462	5.7755	0.13169
$h_{10^{-2}}$	Harmonic	-0.19426	1.1078	0.37602
$h_{10^{-2}}$	Romberg	4.3792	3.631	0.26761
$h_{10^{-2}}$	Bulirsch	2.2519	2.0217	0.34203
h_1	Harmonic	2.052	4.6543	0.4931
h_1	Romberg	33.542	31.468	0.16462
h_1	Bulirsch	35.525	29.752	0.20461
i	Harmonic	54099	54099	$2.2756 \cdot 10^{-5}$
i	Romberg	55368	55367	$2.8621 \cdot 10^{-5}$
i	Bulirsch	58074	58073	$2.6538 \cdot 10^{-5}$
j	Harmonic	6.2138	4.0228	0.58595
j	Romberg	33.68	30.265	0.17797
j	Bulirsch	46.521	35.69	0.20788

Table 2.1: Optimal parameters by test case

The values of the optimal parameters in the curve fitting of extrapolation steps against the logarithm of the error are:

Integrand	Sequence	b	c	q
f	Harmonic	10.466	2.1696	1.2654
f	Romberg	1.5206	0.51255	2.089
f	Bulirsch	0.77673	0.41734	1.9549
$g_{10^{-2}}$	Harmonic	6.5675	−0.61916	1.0458
$g_{10^{-2}}$	Romberg	7.3378	0.0066103	3.1744
$g_{10^{-2}}$	Bulirsch	7.3047	0.00063882	3.3913
$g_{10^{-1}}$	Harmonic	2.8699	−0.47343	1.0317
$g_{10^{-1}}$	Romberg	3.1888	0.039167	2.7667
$g_{10^{-1}}$	Bulirsch	3.9142	0.012441	2.7293
g_1	Harmonic	0.034332	1.3144	0.98632
g_1	Romberg	−0.4289	0.41763	2.0726
g_1	Bulirsch	−1.3077	0.18952	2.0725
$h_{10^{-4}}$	Harmonic	12.604	11.571	0.12559
$h_{10^{-4}}$	Romberg	0.85129	0.27953	1.4991
$h_{10^{-4}}$	Bulirsch	0.16861	0.15206	1.4061
$h_{10^{-2}}$	Harmonic	−0.80722	0.82135	0.75792
$h_{10^{-2}}$	Romberg	−1.309	0.051824	2.5402
$h_{10^{-2}}$	Bulirsch	−2.6424	0.0083341	2.7259
h_1	Harmonic	−1.9642	3.3575	0.98328
h_1	Romberg	−4.397	0.86863	1.8535
h_1	Bulirsch	−7.6558	0.48664	1.8348
i	Harmonic	67160	67160	$3.3808 \cdot 10^{-5}$
i	Romberg	1.8004	1.6494	0.85593
i	Bulirsch	0.95043	1.2669	0.7645
j	Harmonic	1.0579	2.8215	1.1626
j	Romberg	−3.906	0.77717	1.9416
j	Bulirsch	−5.7837	0.56594	1.8564

Table 2.2: Optimal parameters by test case

Chapter 3

Extrapolation of difference quotients

3.1 The algorithm

Let $a \in \mathbb{R}$, $\varepsilon > 0$ and $f :]a-\varepsilon, a+\varepsilon[\to \mathbb{R}$ be differentiable at a. We are interested in estimating $f'(a)$. Assume that f is $2k+1$ times differentiable at a. Then by Taylor's theorem we have

$$f(a+h) = f(a) + f'(a)h + \frac{f''(a)}{2}h^2 + \cdots + \frac{f^{(2k)}(a)}{(2k)!}h^{2k} + \frac{f^{(2k+1)}(\xi)}{(2k+1)!}h^{2k+1} \tag{3.1}$$

where $a < \xi < a+h$. Now plug $-h$ instead of h in (3.1):

$$f(a-h) = f(a) - f'(a)h + \frac{f''(a)}{2}h^2 - \cdots + \frac{f^{(2k)}(a)}{(2k)!}h^{2k} - \frac{f^{(2k+1)}(\eta)}{(2k+1)!}h^{2k+1} \tag{3.2}$$

where $a-h < \eta < a$. If we subtract (3.2) from (3.1) and divide by $2h$ we get:

$$f'(a) = D_f(h) + \frac{f'''(a)}{3!}h^2 + \cdots + \frac{f^{(2k-1)}(a)}{(2k-1)!}h^{2k-2} + \frac{f^{(2k+1)}(\xi) + f^{(2k+1)}(\eta)}{2\cdot(2k+1)!}h^{2k} \tag{3.3}$$

where

$$D_f(h) \coloneqq \frac{f(a+h) - f(a-h)}{2h} \tag{3.4}$$

is the *symmetric difference quotient* of f at a. Note that $\frac{1}{2}(f^{(2k+1)}(\xi) + f^{(2k+1)}(\eta))$ is in the image of $f^{(2k+1)}$ so we can rewrite (3.3) as

$$f'(a) = D_f(h) + \frac{f'''(a)}{3!}h^2 + \cdots + \frac{f^{(2k-1)}(a)}{(2k-1)!}h^{2k-2} + \frac{f^{(2k+1)}(\zeta)}{(2k+1)!}h^{2k} \tag{3.5}$$

where $a-h < \zeta < a+h$. Formula (3.5) tells us that the symmetric difference quotient method has asymptotic expansion in h^2 of order $2k-2$ if f is $2k+1$ times differentiable. Thus we can use the following scheme to extrapolate the symmetric difference quotient method:

1. $D_{i1} \coloneqq D_f(h_i)$ for $i = 1, \ldots, k$.

2. $D_{ij} \coloneqq D_{i,j-1} + \frac{D_{i,j-1} - D_{i-1,j-1}}{\left(\frac{h_{i-j+1}}{h_i}\right)^2 - 1}$ for $2 \le j \le i$.

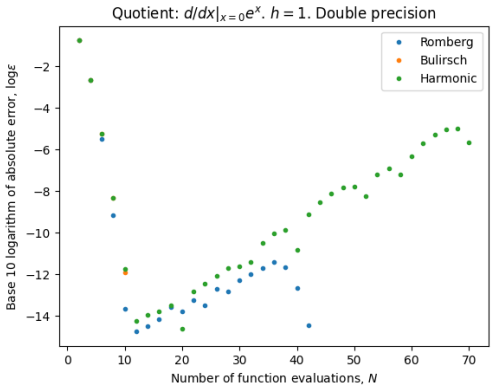
3.2 Numerical experiments

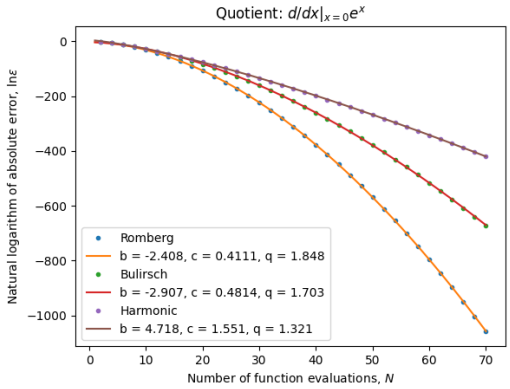
In this section we are going to extrapolate the symmetric difference quotient for approximating the derivative of a function at a given point. Let $h > 0$ be some number, $f :]a-\varepsilon, a+\varepsilon[\to \mathbb{R}$ a function differentiable at a and $n_1 < n_2 < \cdots$ a sequence of integers. Let $h_i := h/n_i$. Let D_{ij} be the extrapolation table that we get from extrapolating in h^2 using the points $(h_1^2, D_f(h_1)), (h_2^2, D_f(h_2)), \ldots$, as we described in the first chapter. We let $\varepsilon_i := |X_{ii} - f'(a)|$. We want to analyze how ε_i as i increases and we also want to do similar efficiency analyzis as in the chapter on Romberg quadrature and check whether we have exponential convergence. We will do the computations with precision up to 500 significant digits and also using standard double precision arithmetic.

Now we will consider the results of the experiments.

3.2.1 The exponential function

We begin by considering the derivative of the exponential function at zero.





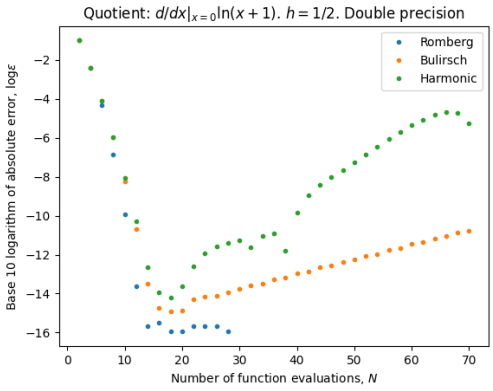
Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3.5085	0.01413	0.00024927
Bulirsch	lin-ln evals-error	4.7628	0.041094	0.00080863
Harmonic	lin-ln evals-error	6.4992	0.022905	0.00090196

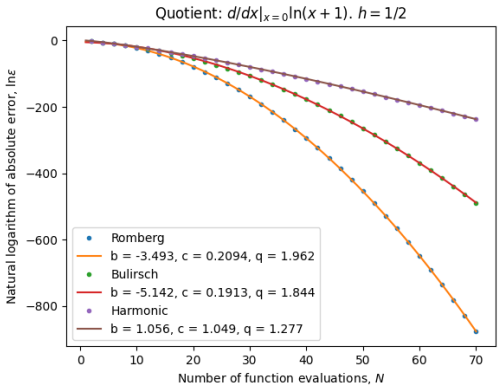
In standard floating point arithmetic, we get down to machine level precision using any sequence. The Romberg sequence works best, then Bulirsch and then the harmonic. The model fits moderately well for the Bulirsch and harmonic sequence but quite well for the Romberg sequence.

3.2.2 Logarithm

Now we will consider the dervative at zero of the function

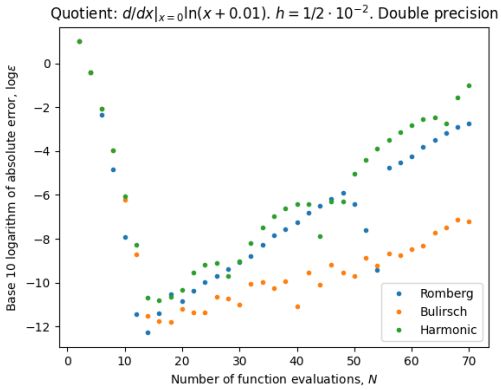
$$g_a(x) := \ln(x+a), \quad a > 0.$$

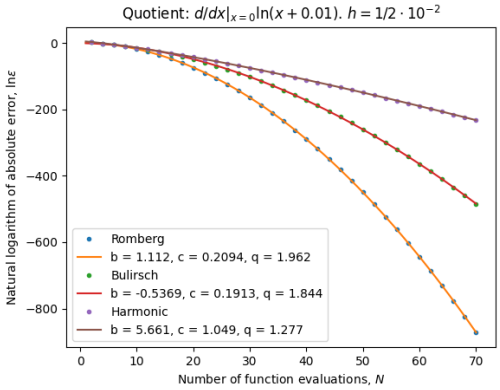




Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.4426	0.0072424	0.00012303
Bulirsch	lin-ln evals-error	6.2746	0.083792	0.0013152
Harmonic	lin-ln evals-error	2.3311	0.010922	0.00041763

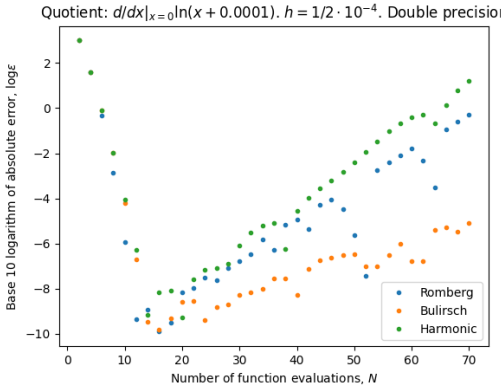
We get down to machine level precision using any sequence, Romberg performes best, then Bulirsch and then the Harmonic one. The model fits quite well for the Romberg sequence and the Harmonic one, but not so well for Bulirsch.

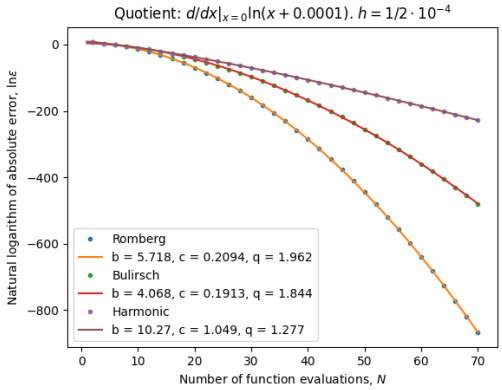




Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.4426	0.0072424	0.00012303
Bulirsch	lin-ln evals-error	6.2746	0.083792	0.0013152
Harmonic	lin-ln evals-error	2.3311	0.010922	0.00041763

Here the same comments apply as for $a = 1$.





Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.4426	0.0072424	0.00012303
Bulirsch	lin-ln evals-error	6.2746	0.083792	0.0013152
Harmonic	lin-ln evals-error	2.3311	0.010922	0.00041763

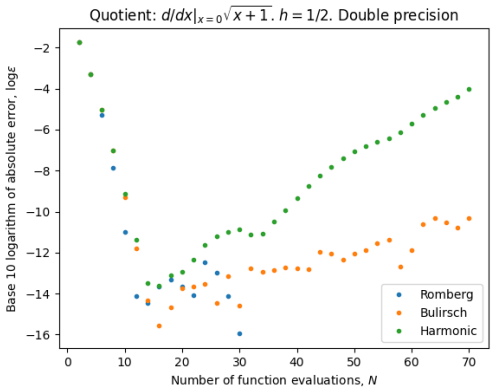
Here the same comments apply as for $a = 1, 10^{-2}$.

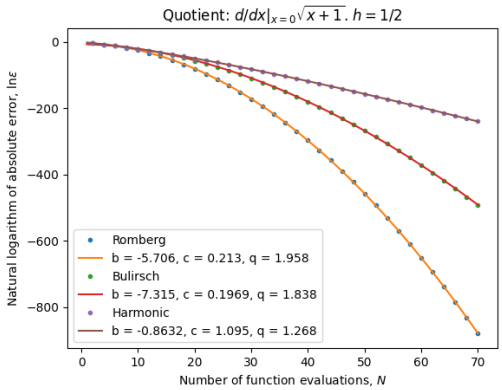
Note that the c and q parameters are independent of a.

3.2.3 Square root

Now we shall consider the derivative at zero of the following function:

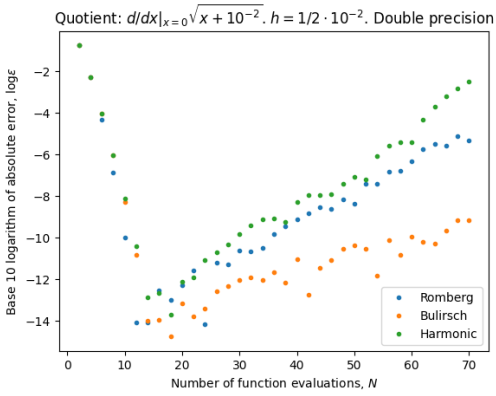
$$h_a(x) := \sqrt{a+x}, \quad a > 0.$$

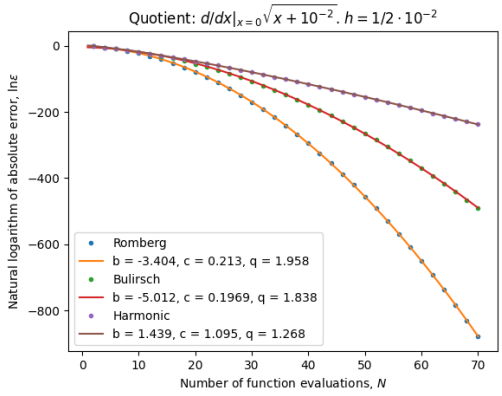




Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3.1845	0.0098756	0.00016602
Bulirsch	lin-ln evals-error	7.1859	0.098014	0.0015128
Harmonic	lin-ln evals-error	2.1015	0.0081581	0.0003023

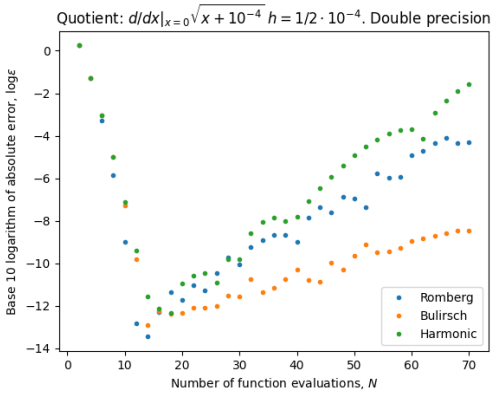
In standard double precision floating point arithmetic we get down to machine level precision using any sequence. The model fits quite well for the Romberg and the Harmonic sequence but not as well for the Bulirsch sequence.

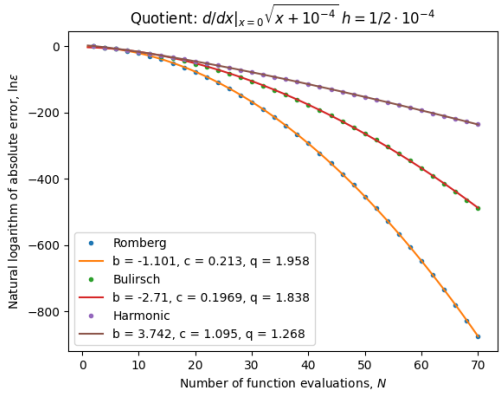




Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3.1845	0.0098756	0.00016602
Bulirsch	lin-ln evals-error	7.1859	0.098014	0.0015128
Harmonic	lin-ln evals-error	2.1015	0.0081581	0.0003023

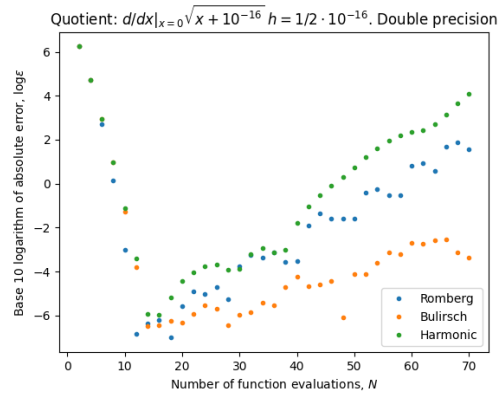
Here the same comments apply as for $a = 1$.

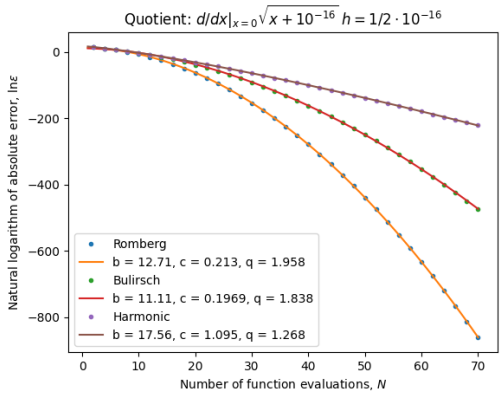




Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3.1845	0.0098756	0.00016602
Bulirsch	lin-ln evals-error	7.1859	0.098014	0.0015128
Harmonic	lin-ln evals-error	2.1015	0.0081581	0.0003023

Here also the same comments apply.





Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3.1845	0.0098756	0.00016602
Bulirsch	lin-ln evals-error	7.1859	0.098014	0.0015128
Harmonic	lin-ln evals-error	2.1015	0.0081581	0.0003023

And they also apply here.

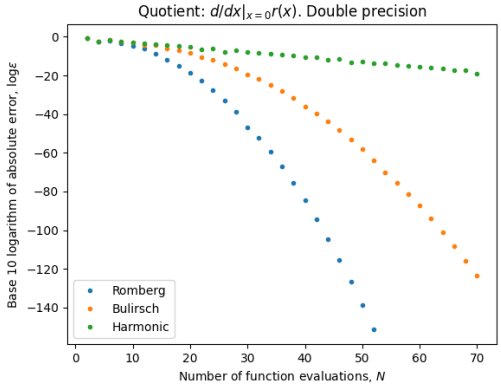
Note that the c and q parameters are independent of a.

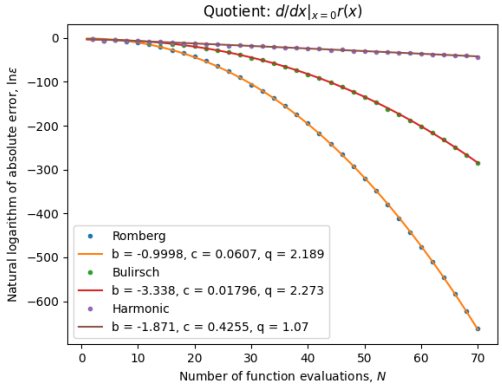
3.2.4 Smooth but not analytic function

Now we will consider the derivate at zero of the following function:

$$r(x) := \begin{cases} e^{-1/x} & \text{if } x > 0 \\ 0 & \text{else} \end{cases}$$

which is smooth but not analytic.





Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	25	2.6439	0.027089
Bulirsch	lin-ln evals-error	25	5.9135	0.075286
Harmonic	lin-ln evals-error	.	.	.

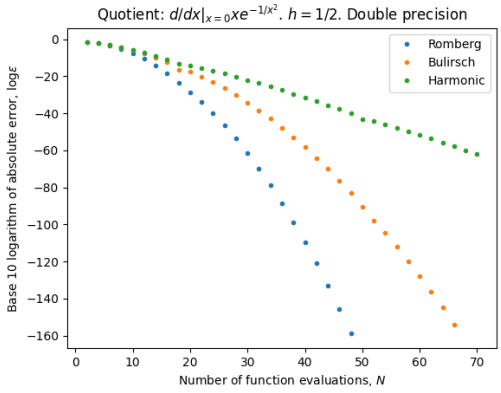
Here the model fits moderately well in the case of the Romberg sequence and the Bulirsch sequence but not in the case of the harmonic sequence.

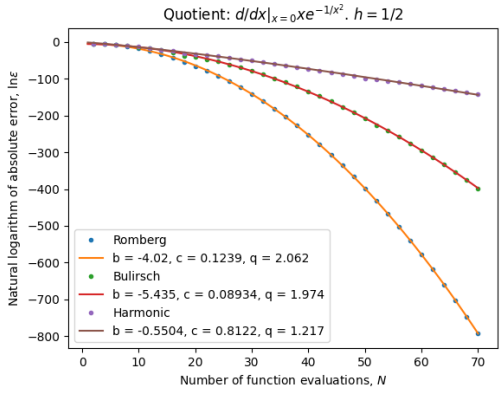
3.2.5 Another smooth but not analytic function

Now we will consider the derivative at zero of the following function:

$$i(x) := \begin{cases} xe^{-1/x^2} & \text{if } x \neq 0 \\ 0 & \text{else} \end{cases}$$

which is smooth but not analytic.





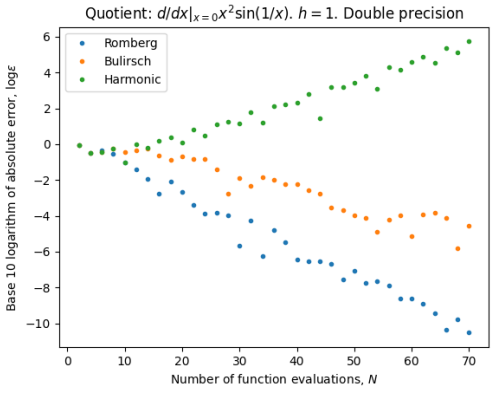
Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	24.394	0.62692	0.0044816
Bulirsch	lin-ln evals-error	25	7.8984	0.082446
Harmonic	lin-ln evals-error	.	.	.

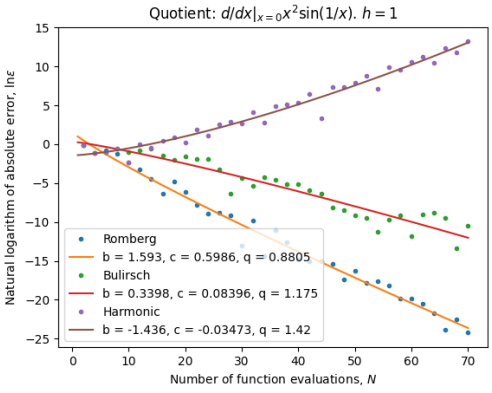
Here the model fits fine in the case of the Romberg sequence but not in the other cases.

3.2.6 Only once differentiable function

Finally we will consider the derivate at zero of the following function which is only once differentiable at that point:

$$j(x) := \begin{cases} x^2 \sin \frac{1}{x} & \text{if } x \neq 0 \\ 0 & \text{else} \end{cases}.$$





Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	*nan*	2.2825	3.9235
Bulirsch	lin-ln evals-error	.	.	.
Harmonic	lin-ln evals-error	.	.	.

Here the model simply does not fit. Note that we do not have the asymptotic expansion for the derivate here, since the function is only once differentiable.

The parameters from the fitting are:

Derivative	Sequence	b	c	q
$d/dx\|_{x=0} r(x)$	Romberg	-0.99982	0.060703	2.189
$d/dx\|_{x=0} r(x)$	Bulirsch	-3.3384	0.017962	2.2735
$d/dx\|_{x=0} r(x)$	Harmonic	-1.8705	0.42555	1.0695
$d/dx\|_{x=0} xe^{-1/x^2}$. $h = 1/2$	Romberg	-4.0202	0.12391	2.0616
$d/dx\|_{x=0} xe^{-1/x^2}$. $h = 1/2$	Bulirsch	-5.4352	0.089335	1.9741
$d/dx\|_{x=0} xe^{-1/x^2}$. $h = 1/2$	Harmonic	-0.55045	0.81216	1.2174
$d/dx\|_{x=0} \sin x$. $h = 1/2$	Romberg	-5.3663	0.51067	1.8066
$d/dx\|_{x=0} \sin x$. $h = 1/2$	Bulirsch	-5.1899	0.64124	1.651
$d/dx\|_{x=0} \sin x$. $h = 1/2$	Harmonic	3.912	1.9876	1.2878
$d/dx\|_{x=0} \ln(x + 0.0001)$. $h = 1/2 \cdot 10^{-4}$	Romberg	5.7177	0.20942	1.9619
$d/dx\|_{x=0} \ln(x + 0.0001)$. $h = 1/2 \cdot 10^{-4}$	Bulirsch	4.0682	0.19126	1.8443
$d/dx\|_{x=0} \ln(x + 0.0001)$. $h = 1/2 \cdot 10^{-4}$	Harmonic	10.266	1.0494	1.2768
$d/dx\|_{x=0} \ln(x + 0.01)$. $h = 1/2 \cdot 10^{-2}$	Romberg	1.1125	0.20942	1.9619
$d/dx\|_{x=0} \ln(x + 0.01)$. $h = 1/2 \cdot 10^{-2}$	Bulirsch	-0.53694	0.19126	1.8443
$d/dx\|_{x=0} \ln(x + 0.01)$. $h = 1/2 \cdot 10^{-2}$	Harmonic	5.6607	1.0494	1.2768
$d/dx\|_{x=0} \ln(x + 1)$. $h = 1/2$	Romberg	-3.4927	0.20942	1.9619
$d/dx\|_{x=0} \ln(x + 1)$. $h = 1/2$	Bulirsch	-5.1421	0.19126	1.8443
$d/dx\|_{x=0} \ln(x + 1)$. $h = 1/2$	Harmonic	1.0555	1.0494	1.2768
$d/dx\|_{x=0} x^2 \sin(1/x)$. $h = 1$	Romberg	1.5925	0.59863	0.88054
$d/dx\|_{x=0} x^2 \sin(1/x)$. $h = 1$	Bulirsch	0.33976	0.083956	1.1751
$d/dx\|_{x=0} x^2 \sin(1/x)$. $h = 1$	Harmonic	-1.436	-0.034733	1.4204
$d/dx\|_{x=0} \sqrt{x + 1}$. $h = 1/2$	Romberg	-5.7063	0.21299	1.9582
$d/dx\|_{x=0} \sqrt{x + 1}$. $h = 1/2$	Bulirsch	-7.315	0.19691	1.8379
$d/dx\|_{x=0} \sqrt{x + 1}$. $h = 1/2$	Harmonic	-0.86323	1.0951	1.2682
$d/dx\|_{x=0} \sqrt{x + 10^{-2}}$. $h = 1/2 \cdot 10^{-2}$	Romberg	-3.4037	0.21299	1.9582
$d/dx\|_{x=0} \sqrt{x + 10^{-2}}$. $h = 1/2 \cdot 10^{-2}$	Bulirsch	-5.0125	0.19691	1.8379
$d/dx\|_{x=0} \sqrt{x + 10^{-2}}$. $h = 1/2 \cdot 10^{-2}$	Harmonic	1.4394	1.0951	1.2682
$d/dx\|_{x=0} \sqrt{x + 10^{-4}}$ $h = 1/2 \cdot 10^{-4}$	Romberg	-1.1011	0.21299	1.9582
$d/dx\|_{x=0} \sqrt{x + 10^{-4}}$ $h = 1/2 \cdot 10^{-4}$	Bulirsch	-2.7099	0.19691	1.8379
$d/dx\|_{x=0} \sqrt{x + 10^{-4}}$ $h = 1/2 \cdot 10^{-4}$	Harmonic	3.7419	1.0951	1.2682
$d/dx\|_{x=0} \sqrt{x + 10^{-16}}$ $h = 1/2 \cdot 10^{-16}$	Romberg	12.714	0.21299	1.9582
$d/dx\|_{x=0} \sqrt{x + 10^{-16}}$ $h = 1/2 \cdot 10^{-16}$	Bulirsch	11.106	0.19691	1.8379
$d/dx\|_{x=0} \sqrt{x + 10^{-16}}$ $h = 1/2 \cdot 10^{-16}$	Harmonic	17.557	1.0951	1.2682
$d/dx\|_{x=0} e^x$	Romberg	-2.408	0.41106	1.8479
$d/dx\|_{x=0} e^x$	Bulirsch	-2.9068	0.48137	1.703
$d/dx\|_{x=0} e^x$	Harmonic	4.7175	1.5509	1.3212

Table 3.1: Optimal parameters by test case

Excluding the computation of $d/dx|_{x=0} x^2 \sin 1/x$, the model fits exceptionally. We always get fast convergence except when computing $d/dx|_{x=0} x \sin 1/x$ and extrapolation with the harmonic sequence. Excluding this case, we always get almost down to machine level precision when using double precision arithmetic, using any extrapolation sequence. It is worth noting that $x \sin 1/x$ is only once differentiable at 0 so we do not have the asymptotic expansion for its derivative at 0. The Romberg sequence performes best and the harmonic sequence worst, in all cases.

Chapter 4

Initial Value Problems

4.1 The explicit midpoint rule

Let $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ be a smooth mapping and consider the initial value problem

$$y'(t) = f(t, y(t)), \quad y(a) = y_a, \quad t \in [a, b]. \tag{4.1}$$

The explicit midpoint methods is a method for computing an approximation to the solution of (4.1), and it goes as follows: Let $n \geq 1$ be an integer and $h := (b - a)/2n$. We then define recursively

$$\xi_h(a) := y_a, \quad \xi_h(a + h) := \xi_h(a) + hf(a, \xi_h(a))$$

and

$$\xi_h(a + (i + 1)h) := \xi_h(a + (i - 1)h) + 2hf(a + ih, \xi(a + ih)).$$

Then ξ_h is an approximate solution to (4.1) defined at $a, a + h, \ldots, b$. We are interested in the value $X_f(h) := \xi_h(b)$. It is possible to show that $X_f(h)$ has an asymptotic expansion in h^2. We have the following implementation in Python of the explicit midpoint rule for computing $X_f(h)$.

```
class ExplicitMidpointRule(Scheme):

  def __init__(self):
    super(ExplicitMidpointRule, self).__init__(2)

  def apply(self, ivp, n):
    h = (ivp.b - ivp.a) / (2 * n)
    y_sl = ivp.y0
    y_l = ivp.y0 + h * ivp.f(ivp.a, ivp.y0)

    for i in range(1, 2 * n):
      tmp = y_l
      y_l = y_sl + 2 * h * ivp.f(ivp.a + i * h, y_l)
      y_sl = tmp

    return y_l
```

4.2 Numerical experiments

In this section we are going to extrapolate the explicit midpoint rule and analyze the convergence of the approximations as we extrapolate more often. Consider the initial value

problem (4.1). Let $n_1 < n_2 < \cdots$ be some sequence of integers and $h_i := (b-a)/n_i$. Let X_{ij} the extrapolation table which we get from extrapolating in h^2, using the points $(h_i, X_f(h_i))$. Let $\varepsilon_i := |X_{ii} - y(b)|$ be the absolute error. We are going to do the same convergence and efficency analysis as in the two previous chapters. We will both do the computations using high precision arithmetic with 500 correct digits and also in standard double precision.

In those cases where we do not have an analytic solution to the equations, we computed a reference solution up to 500 significant digits. We did that by using extrapolation with the harmonic sequence and estimating the error as the difference between successive terms in the sequence of approximations.

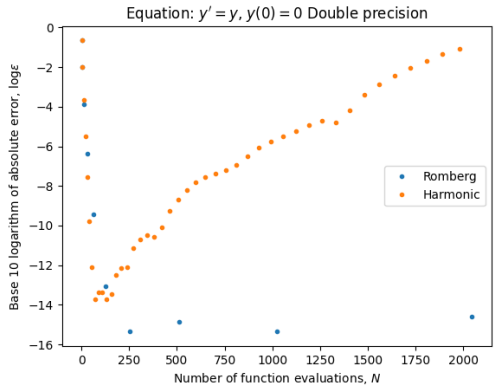
Now we will consider the results of the experiments.

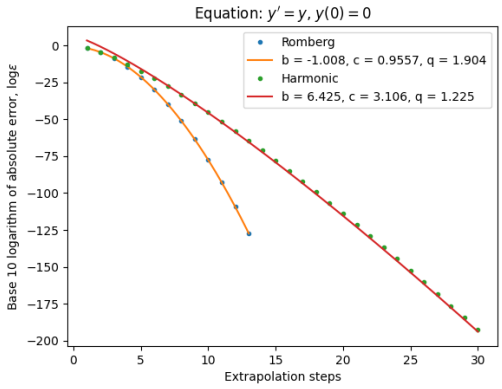
4.2.1 Exponential growth

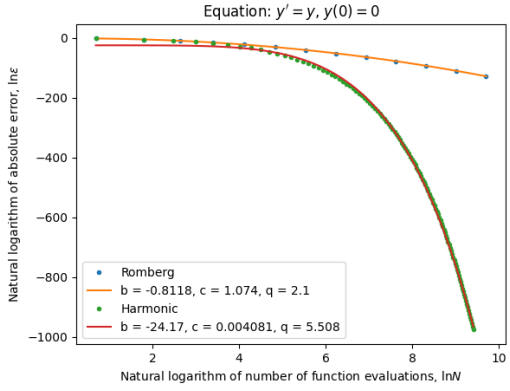
First we will consider the following initial value problem:

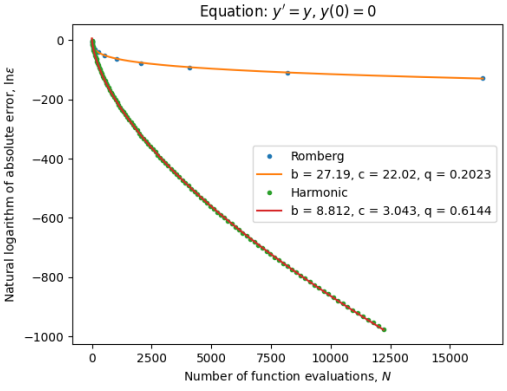
$$y'(x) = y(x), \quad y(0) = 0, \quad x \in [0, 1] \tag{4.2}$$

whose solution is the analytic function $y(x) = e^x$.









Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3	0.085281	0.021208
Harmonic	lin-ln evals-error	12.161	0.021332	0.001013
Romberg	lin-ln steps-error	0.077032	0.0008956	$3.583e-05$
Harmonic	lin-ln steps-error	11.697	0.017508	0.00078485
Romberg	ln-ln evals-error	0.18082	0.0019753	$8.8653e-05$
Harmonic	ln-ln evals-error	.	.	.

Here we have exponential convergence in all cases. The harmonic sequence performes better than Romberg. In standard floating point arithmetic, we get down to maching level error using either sequence.

4.2.2 Logistic curve

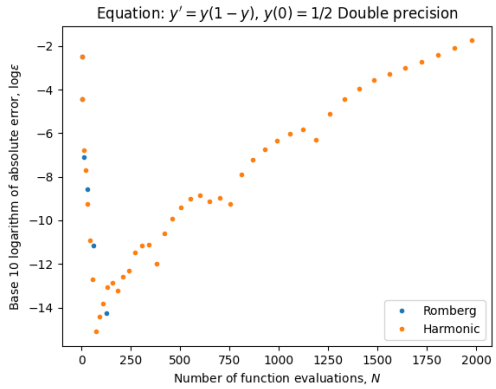
Then we will consider the following initial value problem

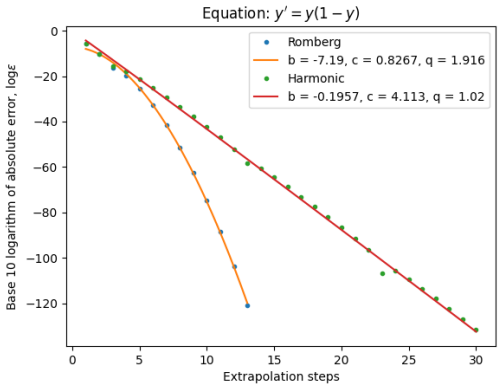
$$y'(x) = y(x)(1 - y(x)), \quad y(0) = 1/2, \quad x \in [0, 1] \tag{4.3}$$

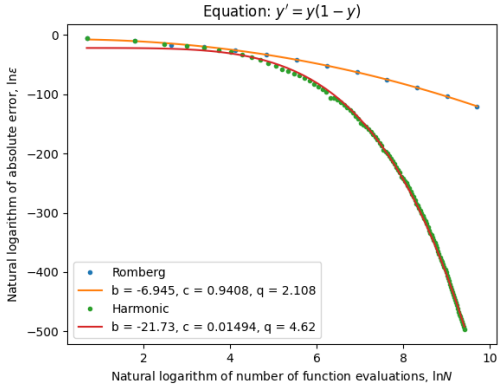
whose solution is the sigmoid function

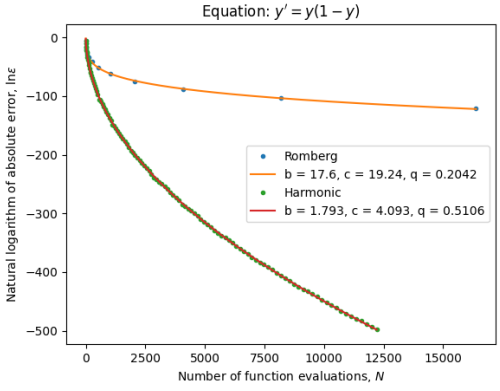
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

which is analytic.









Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.9992	0.083333	0.020783
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	0.10654	0.0019686	$7.2672e-05$
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	0.10079	0.002435	0.00011182
Harmonic	ln-ln evals-error	.	.	.

Here the model also fits very well, the Harmonic sequence performes better and we get down to machine level precision using either sequence in standard floating point arithmetic.

4.2.3 Tangens

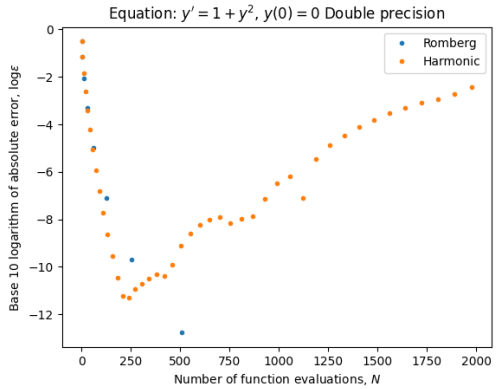
Now we will consider the following equation

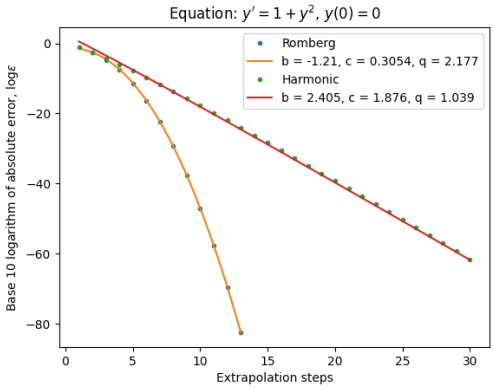
$$y'(x) = 1 + y(x)^2, \quad y(0) = 0, \quad x \in [0, 1] \tag{4.4}$$

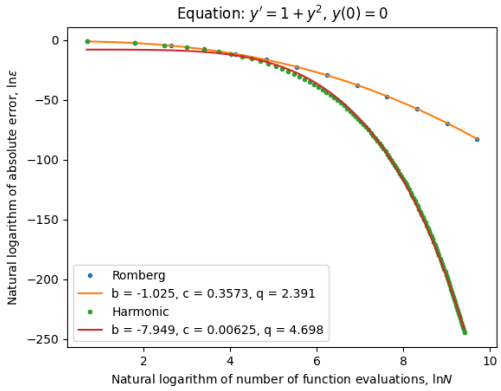
whose solution is

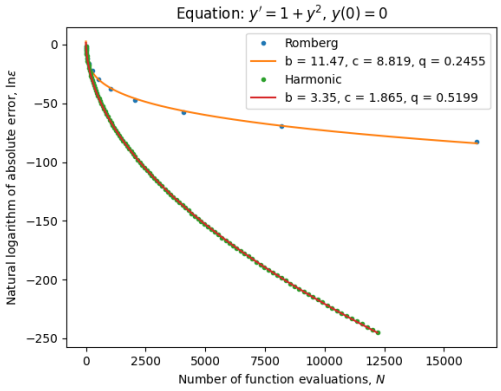
$$y(x) \coloneqq \tan(x)$$

which is meromorphic and we are quite far from singularites.









Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.9973	0.1255	0.024015
Harmonic	lin-ln evals-error	0.97512	0.014263	0.0011377
Romberg	lin-ln steps-error	0.0052197	0.00017853	$5.4868e-06$
Harmonic	lin-ln steps-error	0.94149	0.012584	0.00097006
Romberg	ln-ln evals-error	0.2211	0.0081118	0.0002882
Harmonic	ln-ln evals-error	.	.	.

Here we also have exponential convergence in all cases. The harmonic sequence performes better than Romberg. In standard floating point arithmetic, we get down to maching level error using either sequence.

4.2.4 Equation with singularity

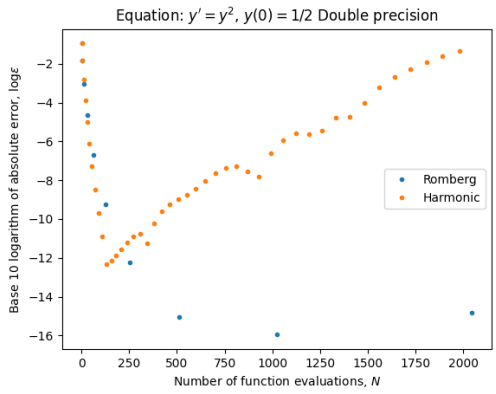
Now we will consider the following initial value problem:

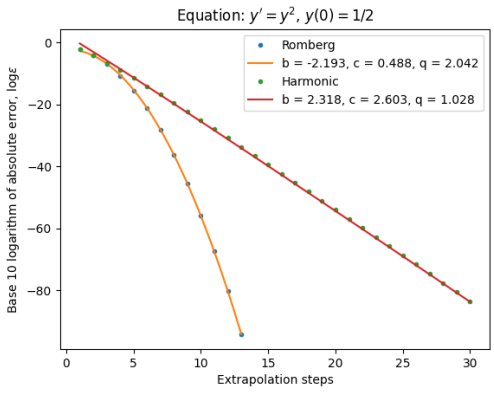
$$y'(t) = y^2(t), \quad y(0) = 1/(1+a), \quad t \in [0,1] \tag{4.5}$$

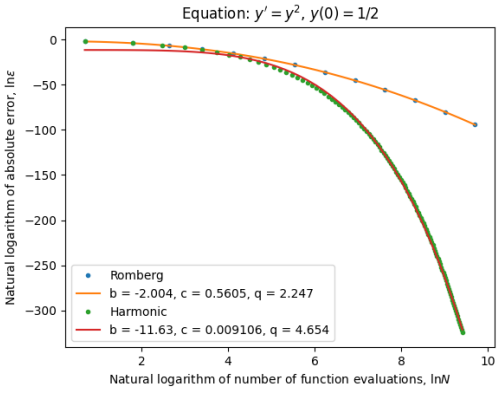
whose solution is

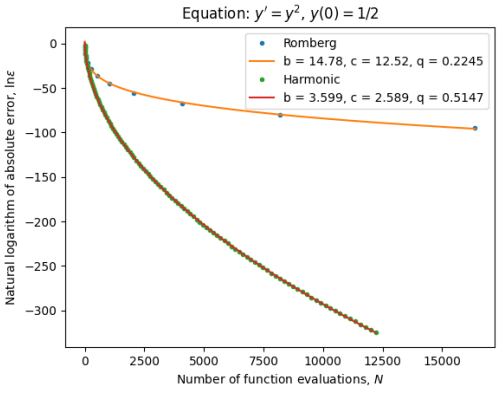
$$y(t) = \frac{1}{1-(t-a)}.$$

The solution is meromorphic with a pole at $1+a$.

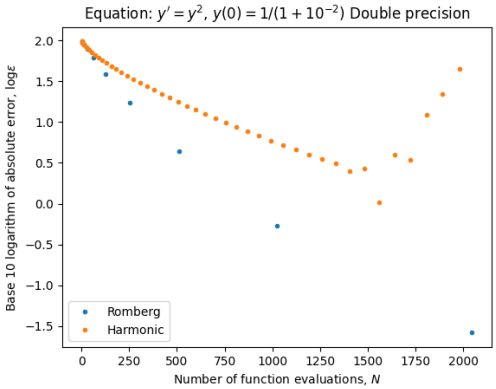


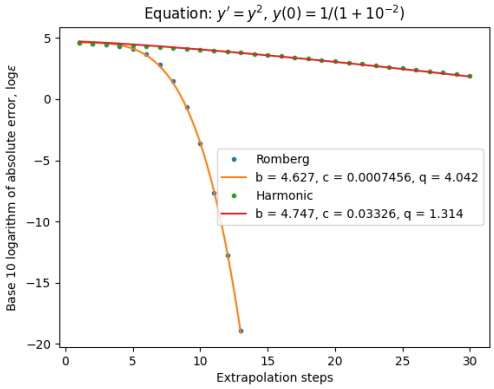


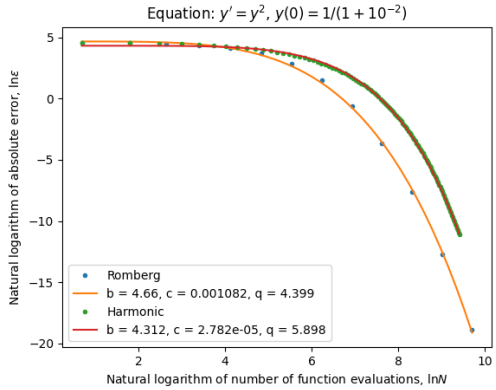


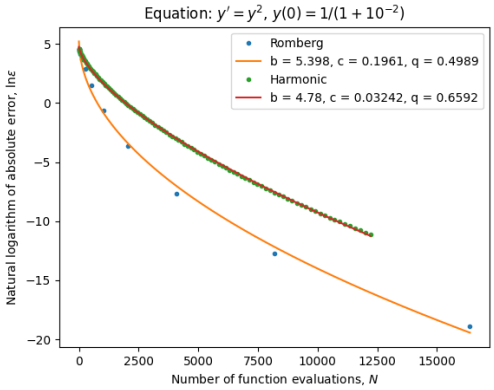


Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.999	0.097019	0.020639
Harmonic	lin-ln evals-error	0.91848	0.0079606	0.00061987
Romberg	lin-ln steps-error	0.029451	0.00085321	$3.0385e-05$
Harmonic	lin-ln steps-error	0.88236	0.0068517	0.00051693
Romberg	ln-ln evals-error	0.095823	0.0022727	$8.8823e-05$
Harmonic	ln-ln evals-error	.	.	.

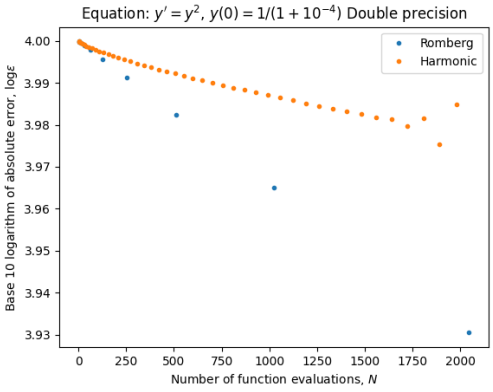


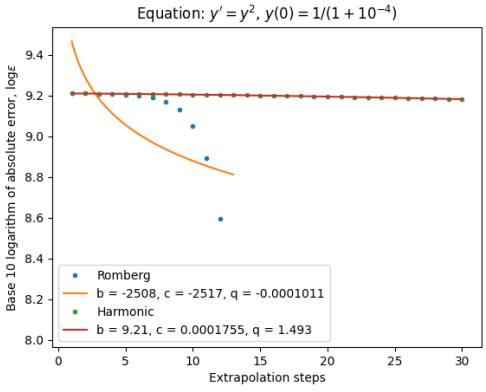


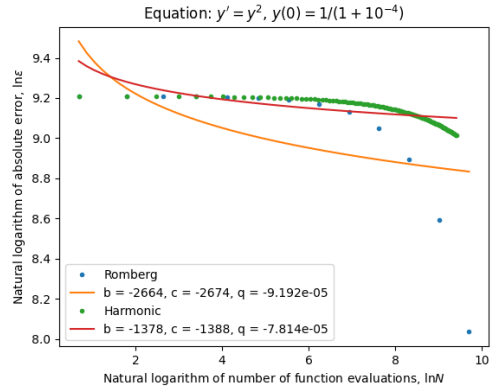


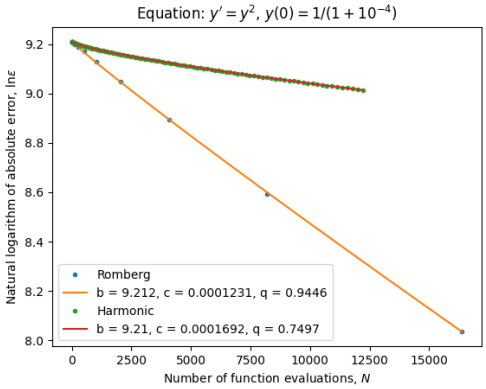


Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	1.1426	0.70222	0.036614
Harmonic	lin-ln evals-error	0.43372	0.23731	0.0075673
Romberg	lin-ln steps-error	0.054061	0.33189	0.0027716
Harmonic	lin-ln steps-error	0.43591	51.961	0.027035
Romberg	ln-ln evals-error	0.082011	0.43662	0.0041259
Harmonic	ln-ln evals-error	.	.	.





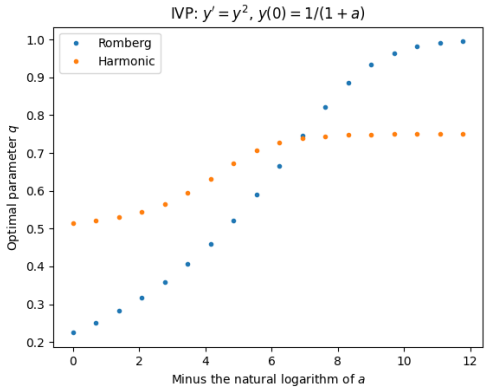




Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	$9.0721e-07$	0.011092	0.00016407
Harmonic	lin-ln evals-error	$2.5283e-08$	0.00028227	$7.3639e-06$
Romberg	lin-ln steps-error	0.33335	3	0.3392
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	1	1.2321	1.0023
Harmonic	ln-ln evals-error	.	.	.

The model fits well for large a, and then the Harmonic sequence works better. But for small a we get a very poor fitting, and extremely slow convergence towards the solution. For $a = 10^{-4}$, when considering the number of function evaluations agains the error, we can not say that we have exponential convergence because the values on the vertical axis are on much smaller scale then the ones on the horizontal axis. The fitting fails entirely when considering the number of extrapolation steps against the error with the Romberg sequence and $a = 10^{-4}$.

The plot of q against a is as follows:



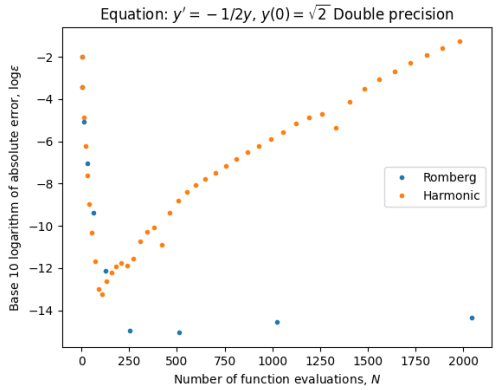
4.2.5 Equation with moderate singularity

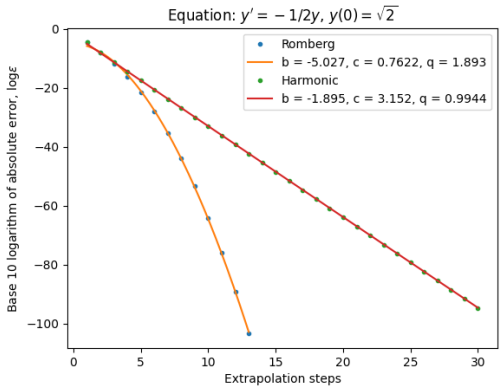
Now we will consider the following initial value problem

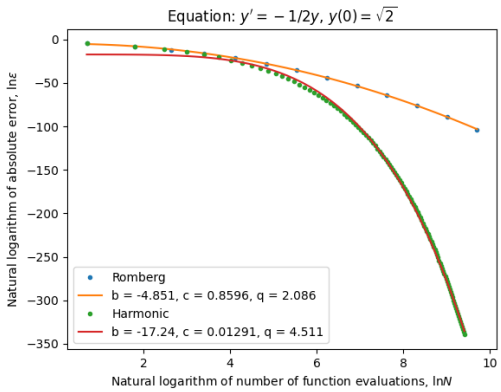
$$y'(t) = -\frac{1}{2y}, \quad y(0) = \sqrt{1+a}, \quad t \in [0,1] \tag{4.6}$$

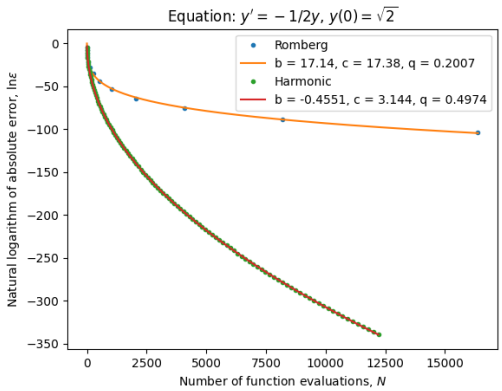
whose solution is

$$y(t) = \sqrt{1-(t-a)}$$

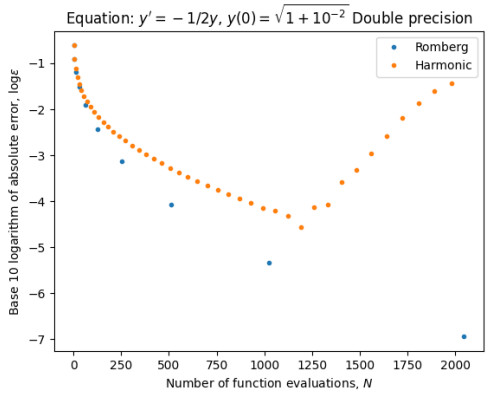


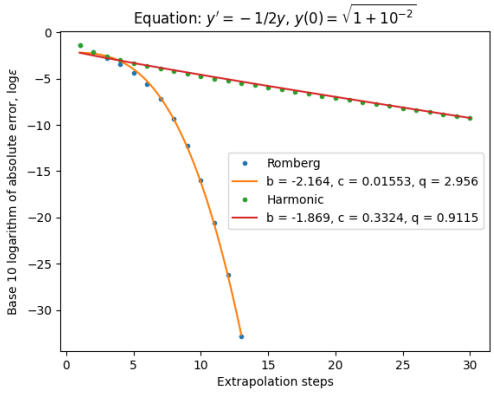


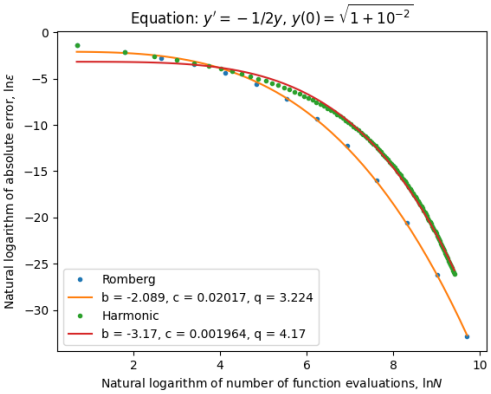


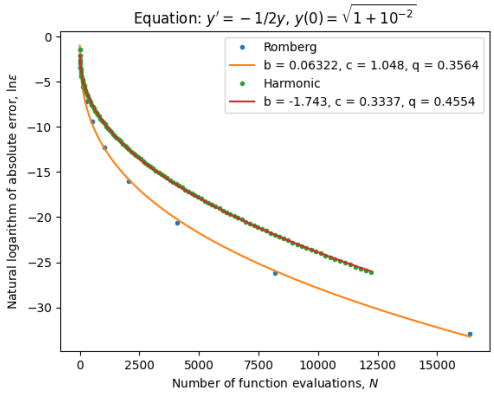


Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.9986	0.063649	0.014426
Harmonic	lin-ln evals-error	0.11952	0.00020154	$1.1402e-05$
Romberg	lin-ln steps-error	0.39967	0.0092624	0.0003485
Harmonic	lin-ln steps-error	0.14404	0.00026111	$1.552e-05$
Romberg	ln-ln evals-error	0.019547	0.0003673	$1.5503e-05$
Harmonic	ln-ln evals-error	.	.	.

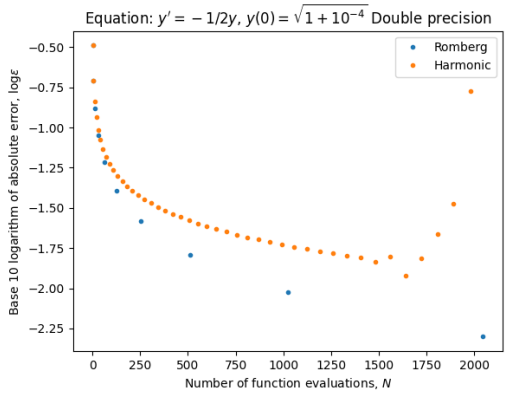


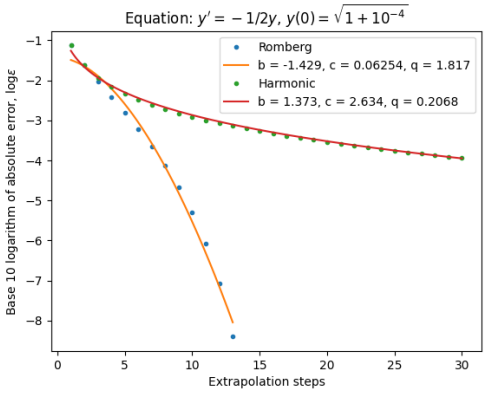


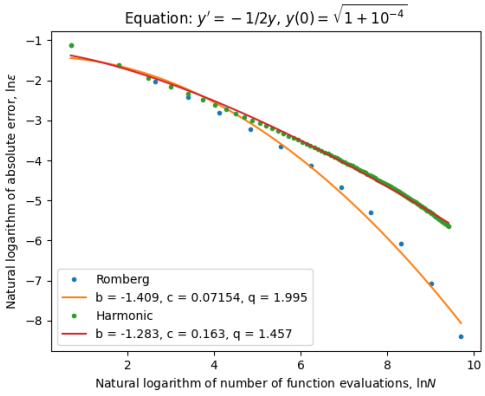


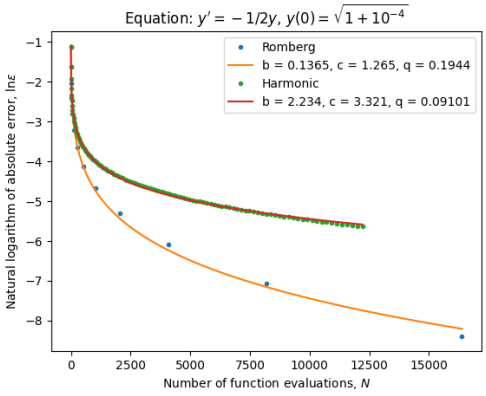


Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	1.2766	0.12651	0.0091735
Harmonic	lin-ln evals-error	0.94084	0.26912	0.0072616
Romberg	lin-ln steps-error	0.040437	0.084713	0.0012532
Harmonic	lin-ln steps-error	0.65386	0.22155	0.0065738
Romberg	ln-ln evals-error	0.018924	0.037351	0.00063283
Harmonic	ln-ln evals-error	.	.	.



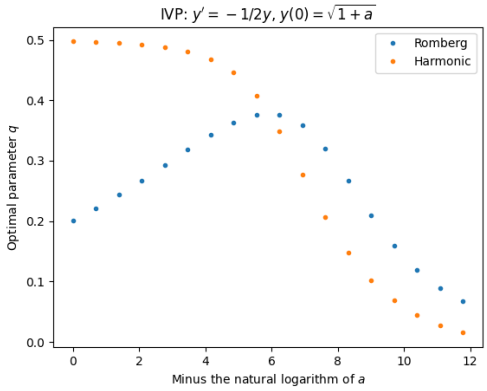






Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	1.0475	0.33656	0.080763
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	0.19193	0.85108	0.055949
Harmonic	lin-ln steps-error	18.031	1.0619	0.12319
Romberg	ln-ln evals-error	0.19211	0.75886	0.052841
Harmonic	ln-ln evals-error	.	.	.

The plot of q against a is as follows:



4.2.6 Circular rotation

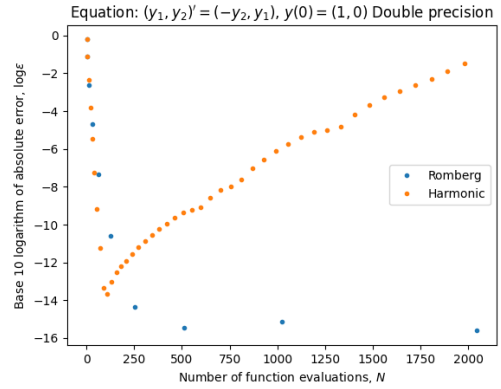
Now we will consider the following system of equations:

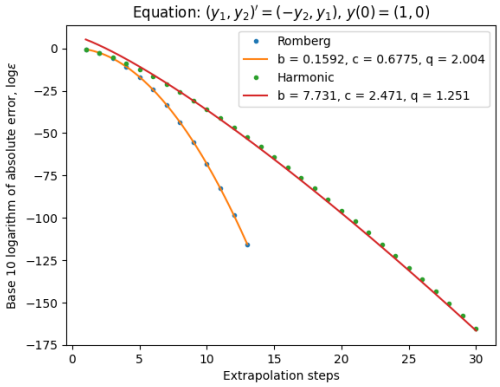
$$(y_1(t), y_2(t))' = (-y_2(t), y_1(t)), \quad y(0) = (1, 0), \quad t \in [0, \pi/2] \tag{4.7}$$

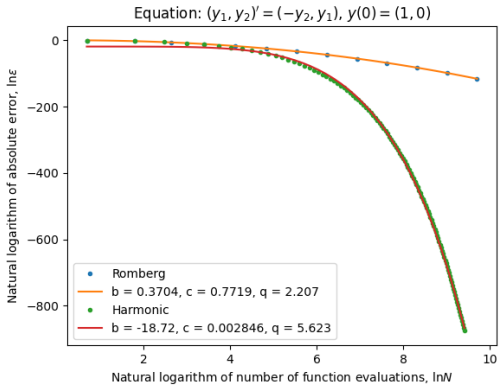
whose solution is

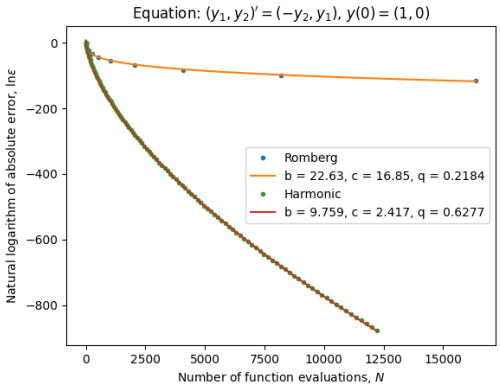
$$(y_1(t), y_2(t)) = (\cos t, \sin t)$$

which is entire.









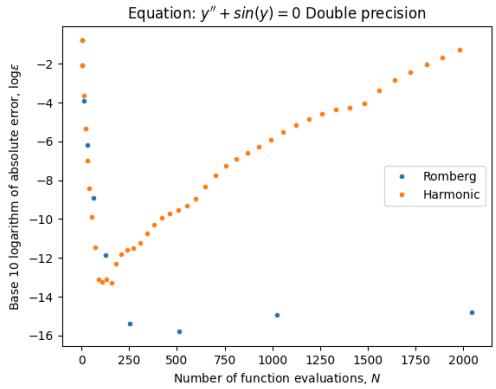
Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3	0.10301	0.023866
Harmonic	lin-ln evals-error	12.976	0.0327	0.0016544
Romberg	lin-ln steps-error	0.00036387	$6.2232e-06$	$2.3974e-07$
Harmonic	lin-ln steps-error	12.521	0.027616	0.0013176
Romberg	ln-ln evals-error	0.34845	0.0052258	0.00022025
Harmonic	ln-ln evals-error	.	.	.

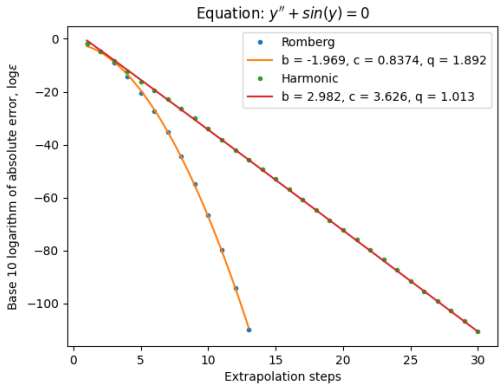
The harmonic sequence works better then Romberg and we get down to machine level precision using either sequence when using standard floating point arithmetic.

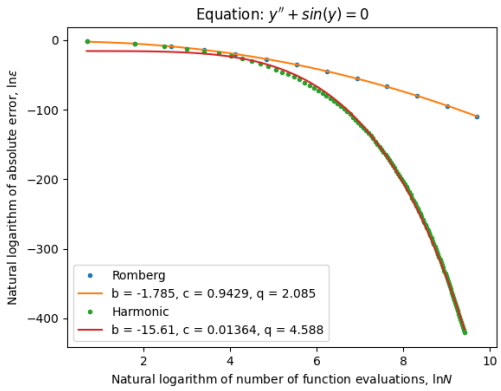
4.2.7 Mathematical pendulum

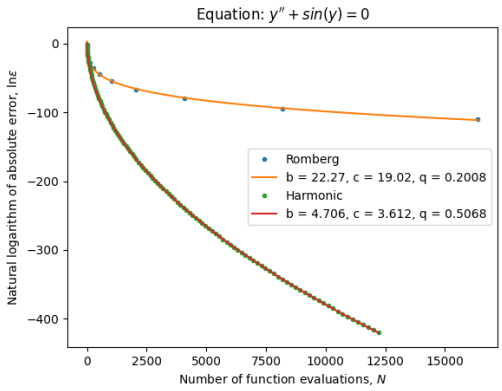
Now we will consider the mathematical pendulum equation:

$$y''(t) + \sin y(t) = 0, \quad y(0) = 0,\ y'(0) = 1, \quad t \in [0, 1]. \tag{4.8}$$









Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	3	0.062258	0.011024
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	1.6709	0.035263	0.001162
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	0.74493	0.014052	0.00055219
Harmonic	ln-ln evals-error	.	.	.

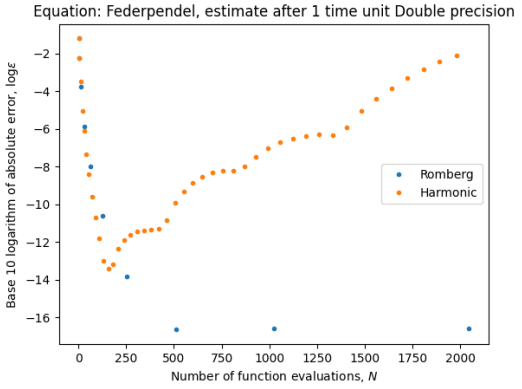
Here the model also fits very well, the harmonic sequence works better and we get down to machine level precision in standard floating point arithmetic, using either sequence.

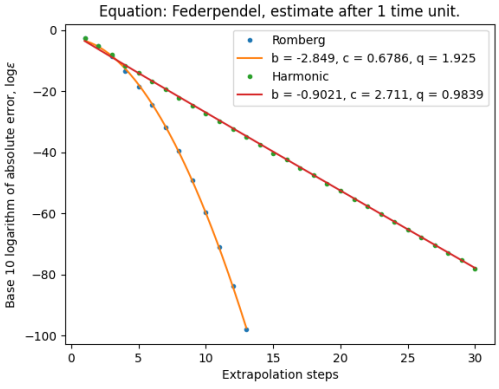
4.2.8 Federpendel

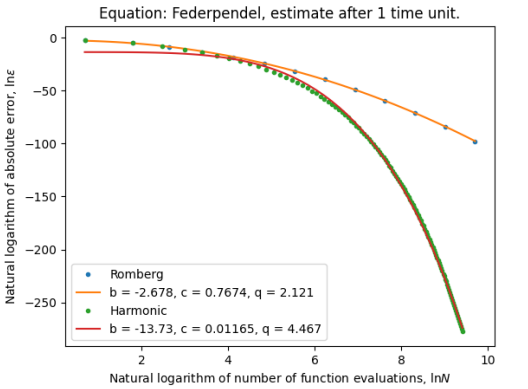
Now we will consider the equation of motion for das Federpendel or the spring pendulum:

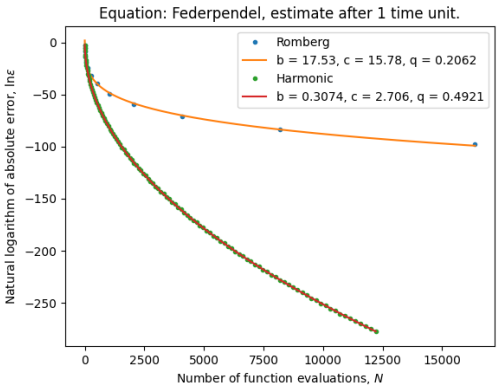
$$\mathbf{p}' = -(|\mathbf{q}| - 1)\frac{\mathbf{q}}{|\mathbf{q}|} - \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{q}' = \mathbf{p}$$

where $\mathbf{p}$ and $\mathbf{q}$ are two dimensional vectors. We will consider it with the initial condition $\mathbf{q}(0) = (1, 0)$ and $\mathbf{p}(0) = (0, 1)$ and try to both estimate the solution at time $t = 1$ and time $t = 2$.

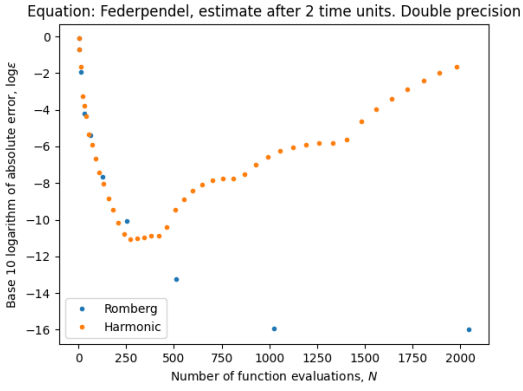


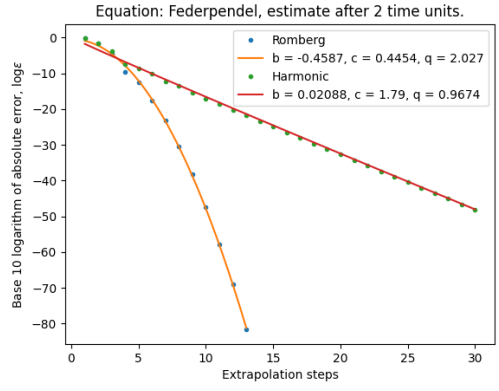


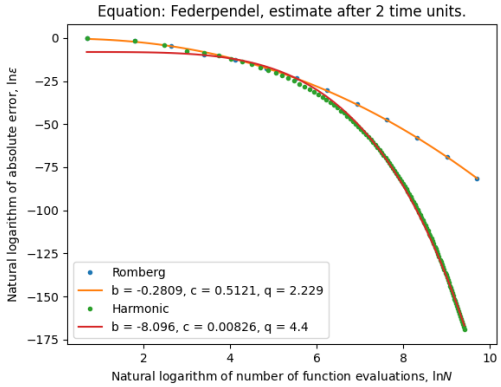


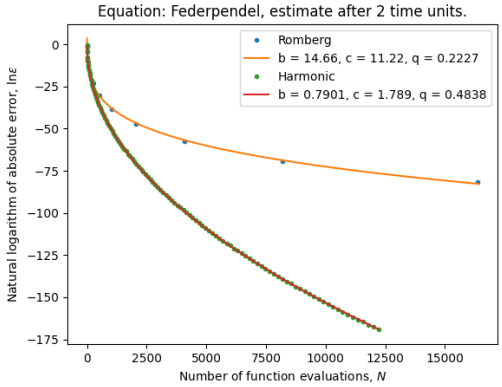


Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.8972	0.073866	0.017293
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	0.22658	0.0077523	0.00028806
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	0.2334	0.0030672	0.00011101
Harmonic	ln-ln evals-error	.	.	.









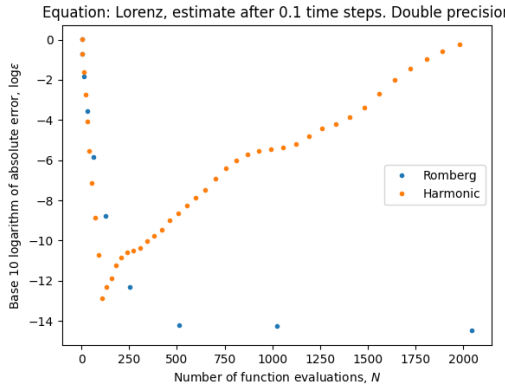
Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.9999	0.17146	0.043627
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	0.44685	0.040823	0.0016262
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	0.66964	0.058913	0.0028387
Harmonic	ln-ln evals-error	.	.	.

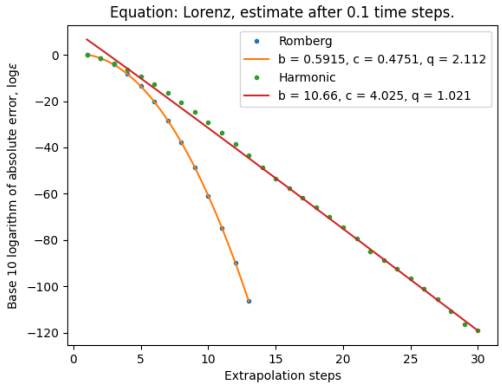
4.2.9 Lorenz equations

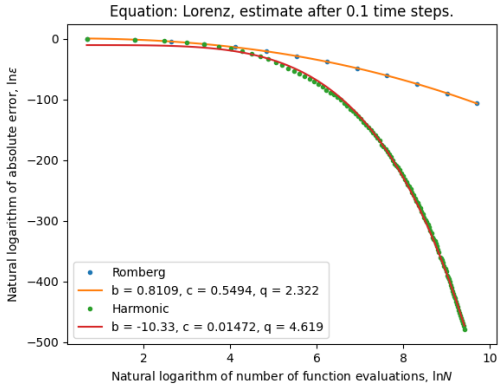
The Lorenz equations are the following system:

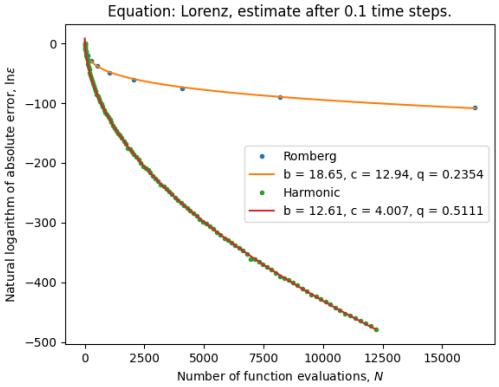
$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = x(\rho - z) - y, \quad \frac{dz}{dt} = xy - \beta z$$

where σ, ρ and β are constants. In our experiment, the constants are set to $\sigma = 10$, $\rho = 28$ and $\beta = 8/3$. The initial condition we will consider is $(x(0), y(0), z(0)) = (1, 1, 1)$.

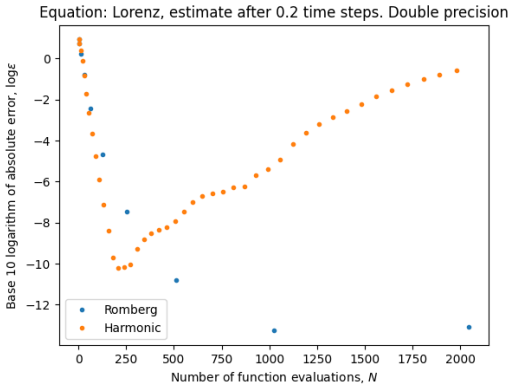


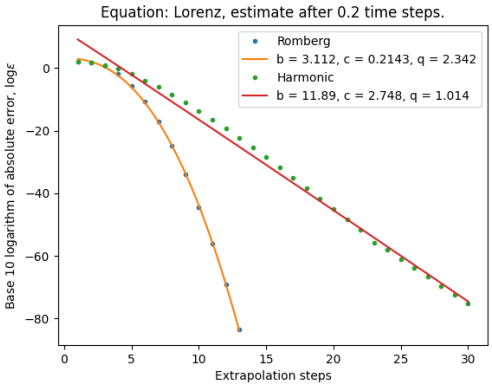


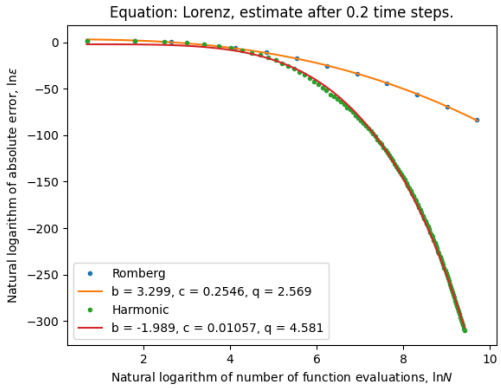


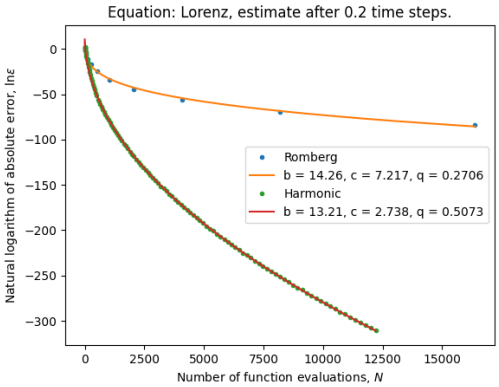


Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.9999	0.12421	0.026917
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	0.040351	0.00096717	$3.4986e-05$
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	0.49281	0.011165	0.00044689
Harmonic	ln-ln evals-error	.	.	.









Sequence	Plot	A-variance	c-variance	q-variance
Romberg	lin-ln evals-error	2.9996	0.18327	0.034985
Harmonic	lin-ln evals-error	.	.	.
Romberg	lin-ln steps-error	0.33224	0.014775	0.00047548
Harmonic	lin-ln steps-error	.	.	.
Romberg	ln-ln evals-error	0.86945	0.038167	0.00137
Harmonic	ln-ln evals-error	.	.	.

The model fits very well in both cases when we consider the number of evaluations against error. The harmonic sequence works better. The fitting is not as nice when considering the number of extrapolation seps against the error. In standard floating point arithmetic, we obtain higher accurracy using the Romberg sequence, though we get high accurracy in both cases.

The values of the optimal parameters in the fitting of the number evaluations against the error, are:

IVP	Sequence	b	c	q
$y' = y$, $y(0) = 0$	Romberg	27.187	22.015	0.20227
$y' = y$, $y(0) = 0$	Harmonic	8.8124	3.0433	0.61436
$y' = y(1-y)$	Romberg	17.604	19.237	0.20418
$y' = y(1-y)$	Harmonic	1.7927	4.0933	0.51064
$y' = 1 + y^2$, $y(0) = 0$	Romberg	11.465	8.8186	0.24549
$y' = 1 + y^2$, $y(0) = 0$	Harmonic	3.3496	1.8647	0.51993
$(y_1, y_2)' = (-y_2, y_1)$, $y(0) = (1, 0)$	Romberg	22.626	16.846	0.2184
$(y_1, y_2)' = (-y_2, y_1)$, $y(0) = (1, 0)$	Harmonic	9.7592	2.4171	0.62765
$y' = y^2$, $y(0) = 1/2$	Romberg	14.78	12.517	0.22455
$y' = y^2$, $y(0) = 1/2$	Harmonic	3.5994	2.5894	0.51472
$y' = y^2$, $y(0) = 1/(1 + 10^{-2})$	Romberg	5.3983	0.1961	0.4989
$y' = y^2$, $y(0) = 1/(1 + 10^{-2})$	Harmonic	4.7796	0.032416	0.6592
$y' = y^2$, $y(0) = 1/(1 + 10^{-4})$	Romberg	9.212	0.00012308	0.94461
$y' = y^2$, $y(0) = 1/(1 + 10^{-4})$	Harmonic	9.2104	0.00016925	0.74975
$y' = -1/2y$, $y(0) = \sqrt{2}$	Romberg	17.142	17.376	0.2007
$y' = -1/2y$, $y(0) = \sqrt{2}$	Harmonic	-0.45512	3.1436	0.49744
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-2}}$	Romberg	0.063222	1.0479	0.35645
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-2}}$	Harmonic	-1.7425	0.33371	0.45544
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-4}}$	Romberg	0.13652	1.2653	0.19436
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-4}}$	Harmonic	2.2343	3.3206	0.091009
$y'' + \sin(y) = 0$	Romberg	22.275	19.017	0.20078
$y'' + \sin(y) = 0$	Harmonic	4.7064	3.6116	0.50678
Federpendel, estimate after 1 time unit.	Romberg	17.532	15.778	0.20624
Federpendel, estimate after 1 time unit.	Harmonic	0.30737	2.706	0.49211
Federpendel, estimate after 2 time units.	Romberg	14.66	11.217	0.22272
Federpendel, estimate after 2 time units.	Harmonic	0.79006	1.789	0.48379
Lorenz, estimate after 0.1 time steps.	Romberg	18.654	12.939	0.2354
Lorenz, estimate after 0.1 time steps.	Harmonic	12.615	4.0068	0.5111
Lorenz, estimate after 0.2 time steps.	Romberg	14.264	7.2173	0.27063
Lorenz, estimate after 0.2 time steps.	Harmonic	13.212	2.7376	0.50732

Table 4.1: Optimal parameters by test case

We note that in those cases where the singularities of the solutions are not very close to our time interval, then q is close to 0.5 for the harmonic sequence and close to 0.2 for the Romberg sequence.

The values of the optimal parameters in the fitting of the number of extrapolation steps against the error, are:

IVP	Sequence	b	c	q
$y' = y$, $y(0) = 0$	Romberg	-1.0083	0.9557	1.904
$y' = y$, $y(0) = 0$	Harmonic	6.425	3.1061	1.225
$y' = y(1 - y)$	Romberg	-7.1901	0.82672	1.916
$y' = y(1 - y)$	Harmonic	-0.19572	4.1127	1.0204
$y' = 1 + y^2$, $y(0) = 0$	Romberg	-1.2103	0.30542	2.1771
$y' = 1 + y^2$, $y(0) = 0$	Harmonic	2.405	1.8763	1.0387
$(y_1, y_2)' = (-y_2, y_1)$, $y(0) = (1, 0)$	Romberg	0.15924	0.67746	2.004
$(y_1, y_2)' = (-y_2, y_1)$, $y(0) = (1, 0)$	Harmonic	7.7307	2.4712	1.2513
$y' = y^2$, $y(0) = 1/2$	Romberg	-2.193	0.48799	2.0424
$y' = y^2$, $y(0) = 1/2$	Harmonic	2.3181	2.6033	1.0284
$y' = y^2$, $y(0) = 1/(1 + 10^{-2})$	Romberg	4.6269	0.00074557	4.042
$y' = y^2$, $y(0) = 1/(1 + 10^{-2})$	Harmonic	4.7474	0.033263	1.3137
$y' = y^2$, $y(0) = 1/(1 + 10^{-4})$	Romberg	-2507.7	-2517.1	-0.00010114
$y' = y^2$, $y(0) = 1/(1 + 10^{-4})$	Harmonic	9.2101	0.00017545	1.4929
$y' = -1/2y$, $y(0) = \sqrt{2}$	Romberg	-5.0269	0.76221	1.8929
$y' = -1/2y$, $y(0) = \sqrt{2}$	Harmonic	-1.8945	3.1518	0.99437
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-2}}$	Romberg	-2.1638	0.015532	2.9565
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-2}}$	Harmonic	-1.8689	0.33241	0.91148
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-4}}$	Romberg	-1.4291	0.062542	1.8173
$y' = -1/2y$, $y(0) = \sqrt{1 + 10^{-4}}$	Harmonic	1.3726	2.6336	0.20682
$y'' + \sin(y) = 0$	Romberg	-1.9686	0.83745	1.8917
$y'' + \sin(y) = 0$	Harmonic	2.9822	3.6265	1.0128
Federpendel, estimate after 1 time unit.	Romberg	-2.8486	0.67856	1.9249
Federpendel, estimate after 1 time unit.	Harmonic	-0.90208	2.7108	0.98385
Federpendel, estimate after 2 time units.	Romberg	-0.45874	0.44537	2.0272
Federpendel, estimate after 2 time units.	Harmonic	0.020877	1.79	0.96743
Lorenz, estimate after 0.1 time steps.	Romberg	0.59151	0.47509	2.112
Lorenz, estimate after 0.1 time steps.	Harmonic	10.659	4.0254	1.0213
Lorenz, estimate after 0.2 time steps.	Romberg	3.1116	0.21429	2.3417
Lorenz, estimate after 0.2 time steps.	Harmonic	11.891	2.7477	1.014

Table 4.2: Optimal parameters by test case

Bibliography

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