# Numerical integration, convergence and extrapolation

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## Contents



## I. INTRODUCTION

This project deals with numerical evaluation of line integrals involving vector fields. The integrals can be done exactly. The purpose of the exercises is to illustrate the basic concepts and to study convergence properties and convergence acceleration techniques .

### A. What is expected

1. A report submitted by email before the due date, which is to be announced. No pictures of hand-written notes;

2. The report should be a self-contained, intelligible paper;

3. If you cannot get certain assignments to work, describe what you did and where things went wrong;

4. No computer programs.

## II. THE LINE INTEGRAL

### A. Exact calculation

Consider the directed curve $C$ in three-dimensional space consisting of the points

$$\boldsymbol{c}(t) = \cos nt\, \hat{\mathbf{e}}_x + a \sin nt\, \hat{\mathbf{e}}_y + \sin t\, \hat{\mathbf{e}}_z \tag{1}$$

with $a > 0$, integral $n > 0$, and $t$ increases from 0 to $2\pi$.

For visualization you can use Mathematica's `ParametricPlot3D` to plot $c(t)$ with $a = 2$ and $n = 3$, the special case we'll consider.

Define a vector field $\boldsymbol{F}$ by

$$\boldsymbol{F}(x, y, z) = -\frac{y}{r^2}\, \hat{\mathbf{e}}_x + \frac{x}{r^2}\, \hat{\mathbf{e}}_y \tag{2}$$

with

$$r^2 = x^2 + y^2. \tag{3}$$

The problem is to evaluate—both analytically and numerically—the following line integral

$$I(n, a) == \frac{1}{2\pi} \oint_C \boldsymbol{F} \cdot d\boldsymbol{r} \tag{4}$$

for $n = 1, 2, \ldots$ , where $d\boldsymbol{r}$ is tangential to the curve defined in Eq. (1).

**Assignment 1** The function $c(t)$ in Eq. (1) has period $2\pi$, but the period of the integrand in Eq. (4) is $\pi/n$ for integral $n$. Explain this geometrically.

**Assignment 2** Calculate the integral exactly for integral $n$.

**Hint:** use Stokes's Theorem to deform the curve into a combination of simple geometric shapes. What kinds of deformations will leave the line integral unchanged, and why? Also give an example of a deformation of the line that changes the line integral.

### B. Numerical integral

Compute the integral numerically using the trapezoidal rule:

$$I \equiv \int_0^1 w(t)\,dt \approx \frac{1}{N}\left(\frac{1}{2}w(0) + \sum_{i=1}^{N-1} w(\frac{i}{N}) + \frac{1}{2}w(1)\right) \equiv T_N. \tag{5}$$

The approximation improves as the integer $N$ increases, and becomes exact in the limit $N \to \infty$ for "reasonable" functions $w$.

Convergence as $N \to \infty$ of the trapezoidal rule typically is power law convergence, *i.e.*,

$$|I - T_N| \propto \frac{1}{N^p} \tag{6}$$

with $p > 0$. For periodic functions convergence may be exponential, *i.e.*,

$$|I - T_N| \propto e^{-cN}, \tag{7}$$

with $c > 0$. For more on this see this paper. It discusses the theory of convergence of numerical integration for periodic functions.

Let $J$ denote the integral in Eq. (4) normalized so that the integral equals unity when integrate over a full, single period of the integrand. From here on use $a = 2$ and $n = 3$.

**Assignment 3** apply Eq. (5) to a full, single period of the integrand and produce a table successive approximants $T_N$ of $J$ for increasing values of $N$.

**Assignment 4** Calculate the constant $c$ in Eq. (7) applicable to this case.

**Hint:** find the zero of the denominator of the integrand. Sometimes, if you have to solve an equation $f(x) = 0$ for $x$ it's easier to introduce an new variable $y = ix$ and solve for $y$, where $i = \sqrt{-1}$.

**Assignment 5** Make a semi-log plot of $|T_N - J|$, a plot $\log|T_N - J|$ as a function of $N$. For comparison, plot the function $e^{-cx}$ as a function of the continuous variable $x$ in the same plot.

**Hint:** you can make the semi-log plot of the table using `pl1=ListLogPlot[...]`. For the continuous line you can use and `pl2=LogPlot[...]`. Combine the plots with `pl3=Show[pl1,pl2]`. Finally, you export the plot with `Export["plot.jpg",pl3]`

**Assignment 6** From two successive approximants $T_N$ and $T_{N+1}$ you can obtain an estimate of $c_N \approx c$.

1. Produce a table showing $N$, $T_N$, and $c_N$.
2. Explain why the number of significant digits of $c_N$ decreases as $N$ increases.

**Assignment 7** Apply Eq. (5) to $\frac{9}{10}^{\text{th}}$ of a full period of the integrand and produce a table of successive approximants $T_N$ of $J$ for increasing values of $N$.

Note that $J \neq 1$ in this case, but it can still be calculated exactly.

**Assignment 8** Make a log-log plot of $|T_N - J|$, *i.e.,* a plot $\log |T_N - J|$ as a function of $N$. For comparison, plot the function $x^{-p}$ as a function of the continuous variable $x$ in the same plot, where you choose $p$ so as to agree with the expected convergence behavior.

**Hint:** you can make the semi-log plot of the table using `pl1=ListLogLogPlot[...]`. For the continuous line you can use and `pl2=LogLogPlot[...]`.

## III. ACCELERATING CONVERGENCE

To speed up convergence of a sequence $T_1, T_2, \ldots$, you can generate from this sequence a new sequence $T'_1, T'_2, \ldots$ that converges more rapidly. Such acceleration techniques depend on the assumed type of convergence behavior of the original sequence and they can often be applied repeatedly, *i.e.,* iteratively. Acceleration methods can speed up computations tremendously. Round-off errors increase for every iteration and this limit the number of numerically meaningful iterations.

### A. Power-law convergence

If the $T_N$ display power-law convergence, *i.e.,* if asymptotically the following relation holds

$$T_N = T_\infty + aN^{-p}, \tag{8}$$

where $p$ is some known exponent you can obtain $T_\infty$ from two successive values $T_N, T_{N+1}$, by eliminating the unknown amplitude $a$ and solving for $T_\infty$. The latter estimate defines

$$T'_N = T'_N(T_N, T_{N+1}) \tag{9}$$

**Assignment 9** Find $T'_N$ for this acceleration technique. Pretend that you do not know the exact integral and produce a table showing $N$, $T_N$ and $T'_N$.

A table produced by applying this trick repeatedly is called an Aitken-Shanks table; $T'_N$ is called the Aitken-Shanks transform.

### B. Exponential convergence

Likewise, if the $T_N$ converge exponentially,[1] *i.e.,* if asymptotically the following relation holds

$$T_N = T_\infty + ae^{-bN}, \tag{10}$$

one can obtain $T_\infty$ from three successive values $T_N, T_{N+1}, T_{N+2}$ which allows one to define

$$T'_N = T'_N(T_N, T_{N+1}, T_{N+2}) \tag{11}$$

**Assignment 10** Find the expression for $T'_N$ for this exponential acceleration technique, which is known as Aitken extrapolation. Produce a table like the one in the previous assignment.

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[1] In numerical analysis this is called *linear convergence.* This refers to the rate at which the number of correct digits increases with every iteration. There are numerical problems for which algorithms exist with that number increasing quadraticly with the number of iterations.