Introduction to Computational Physics

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(Additional discussion on Friday, 20.6. and Monday, 23.6.)

EXERCISE 6.1: **Romberg Integration**

My implementation of the Romberg algorithm in Mathematica can be found in `Ex6.1.m` which represents my solution to exercise 6.1. The results of the first investigation can be printed with `PrintRombergf1`. As one observes, even for the highest parameters $m = 10$ and $k = 3$, the accuracy is only about $3 \cdot 10^{-5}$.

The slow convergence can be traced back to the fact that the ratio R_m for $m = 1, \ldots, 5$ is around 2.8, far away from the expected ratio of 4. This result can be displayed with `PrintRombergf1R`. The deviation from 4 in turn is due to the divergence of the derivatives at the end-points.

After the substitution, one has to calculate the integral

$$I \;=\; \int\limits_0^\pi \sin^2\theta \, d\theta \,.$$

Now the situation is completely opposite. All derivatives at the end-points vanish identically, and thus the trapezoidal rule yields the exact result independent of the number of intervals for the integration. This can be shown with `PrintRombergf2`. Bye the way this leads to the following result for a sum over $\sin^2\theta$:

$$\sum_{k=1}^{n-1} \sin^2 \frac{k\pi}{n} \;=\; \frac{n}{2} \,.$$

EXERCISE 6.2: **Improper Integrals**

My implementation of this exercise can be found in `Ex6.2.m`. My suggested substitution would be $t = (1/z-1)^2$ which yields the integral:

$$\Gamma(1/2) \;=\; 2\int\limits_0^1 \frac{dz}{z^2}\, e^{-(1/z-1)^2} \;=\; \sqrt{\pi} \,.$$

This substitution solves the problem with the square-root singularity and the infinite integration range. There is still a numerical problem at $z = 0$, which, however, can be solved by simply omitting the lower boundary. Romberg integration with for example $m = 7$ and $k = 1$ then gives the desired accuracy.

EXERCISE 6.3: **Elliptic Integrals**

My implementation of this exercise can be found in `Ex6.3.m`. Apart from the point $\theta_0 = \pi$, where the integral diverges ($T = \infty$ - metastable point), with $m = 8$ and $k = 1$ the elliptic integral can be obtained with roughly machine precision. (See `PrintRombergf`.) A plot of the function can be obtained with `PlotEllipticK`.