Introduction to Computational Physics

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(Additional discussion on Friday, 16.5. and Monday, 19.5.)

EXERCISE 1.1: **Numerical accuracy**

Due to rounding errors, the difference quotient has a relative precision of $\sim \epsilon f/(hf')$, where ϵ is the machine precision. On the other hand, from the Taylor expansion, the next terms are of order hf''/f' and $h^2 f'''/f'$, respectively. (Neglecting factors of 2 etc.) For the optimal h, both uncertainties should be of the same order. This yields for the first formula:

$$h_{\rm opt} \;\sim\; \epsilon^{1/2}\,; \quad \delta f'/f' \;\sim\; \epsilon^{1/2}\,,$$

and for the improved symmetrical formula:

$$h_{\rm opt} \;\sim\; \epsilon^{1/3}\,; \quad \delta f'/f' \;\sim\; \epsilon^{2/3}\,,$$

where function values and derivatives are assumed to be of $\mathcal{O}(1)$. In the cases at hand, these estimates work remarkably well!

EXERCISE 1.2: **Numerical stability**

In the Mathematica program, the exact result for p_n with $n = 1\ldots 20$ is given in the table `pTable`. Since for larger n, the result is of the form *large number* minus *large number times e* which almost cancel, discuss the problems when one just calculates `N[pTable]`, and compare with `N[pTable,40]` (which is correct up to ~20 digits). Discuss that the original recursion relation (`precTable`) breaks down for larger n, because a small deviation ϵ is blown up with $n!$. On the contrary, for the inverse recursion relation (`pinvTable`), a deviation is damped with $1/n!$, and thus even taking an arbitrary initial value p_{30}, p_{20} is already very close to the exact result.