Excercise to Discretization I
Practical in Numerical Astronomy SS 2010

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1 Excercises in short

- Define the quality of the numerical differentials of the function $f(t) = Sin(t)$ using forward and centered differencing depending on the stepzie h and the type of variables being used (*single precision*, *double precision*)
- Prove that
$$f_{xy}(x, y) \approx \frac{f(x+h, y+h) - f(x+h, y-h) - f(x-h, y+h) + f(x-h, y-h)}{4h^2}$$
by using the right combinations of Taylor Series developments of $f(x, y)$ at $f(x+h, y+h), f(x+h, y), f(x-h, y-h), \ldots$
- Generate an Euler's integration scheme for the simple harmonic oscillator.

1.1 Numerical differentiation

Let $f : \mathbb{R} \to \mathbb{R}$, where we denote $h = t - t_0$ as being the so-called 'stepsize', $\{t, t_0, h\} \in \mathbb{R}$. Combining the fundamental theorem of calculus and the mean value theorem as well as forming the limit $h \to 0$ one arrives at the equation for the differential-quotient (Wikipedia Proof 1, 2009):

$$\lim_{h \to 0} \frac{f(t_0 + h) - f(t_0)}{h} = \dot{f}(t_0)$$

Since we are dealing with finite precision numbers, we have to neglect the limit $h \to 0$ and accept that, from this point onward, we are dealing with approximations. of $\dot{f}(t)$, the so-called 'difference-quotients'.

$$\frac{f(t_0 + h) - f(t_0)}{h} \simeq \dot{f}(t_0) \tag{1}$$

The functions' values $f(t_0 + h), f(t_0)$ as well as the stepsize h are now being representable by discrete numbers. Furthermore, equation 1 can be reformulated to resemble a Taylor-series approximation of $f(t_0 + h)$ up to the first order in h

$$f(t_0 + h) = f(t_0) + \dot{f}(t_0) \cdot h + O(h^2)$$

Adding similar Taylor-expansions of $f(t_0+h)$ and $f(t_0-h)$ will allow us to gain a better approximation of the first derivative:

$$\frac{f(t_0 + h) - f(t_0 - h)}{2h} \simeq \dot{f}(t_0) \tag{2}$$

Latter method is called 'centered-difference' for it produces the estimated derivative of f, $\frac{df(t)}{dt}$, at position t_0, yet it uses the function's values at $t_0 + h$ and $t_0 - h$.

1.2 Numerical integration

Having a proper look at equation (1) one could also discover a way to integrate ordinary differential equations of fist order. Integration in this sense can be set equal to propagation along a parameter (e.g. time t). Rearranging equation (1) produces once again Taylor's approximation:

$$f(t_0 + h) \simeq f(t_0) + h \cdot \dot{f}(t_0) \tag{3}$$

and that's it! Given the initial conditions $f(t_0)$ and a way to evaluate the first derivative $\dot{f}(t_0)$ at that t_0 one can calculate the value of $f(t_0 + h)$ at $t_0 + h$. Truncating Taylor's series after the first dericative and using it like that is called Euler's integration scheme, since it is said to have been introduced by Leonhard Euler (1707-1783).

2 Exercises in detail

2.1 Quality control

Of which order $O(h), O(h^2), O(h^3)$... in stepsize h is the approximation to $\frac{df(t)}{dt}$ in equation (1)? Try to find the Taylor-expansions that will result in equation (2) for yourself. Of which order $O(h), O(h^2), O(h^3)$... is the approximation to $\frac{df(t)}{dt}$ in equation (2)? Is it actually better? Reason your answer! Show the dependency of the numerical approximations to an analytical derivative (equations (1) and (2)) on the stepsize h using the function $f(t) = Sin(t)$.
In order to achieve that, compare $\dot{f}(t_0)_{analytical}$ to $\dot{f}(t_0)_{numerical}$ and calculate the relative deviation $r(h)$:

$$r(h) = log_{10}|\frac{\dot{f}(t_0)_{analytical} - \dot{f}(t_0)_{numerical}}{\dot{f}(t_0)_{analytical}}| \tag{4}$$

at $t_0 = 5$ for at least 100 different stepsizes h between 1 and 10^{-6} for single precision (using Fortran90: *real* variables) and h between 1 and 10^{-15} for double precision (using Fortran90: *real*8* variables). Plot the results!. How does the stepsize h influcence the results? What happens when h becomes very small?

2.2 Mixed second derivatives

Use combinations of multidimensional Taylor series expansions around the point $f(x, y)$ for $f(x + h, y + h), f(x + h, y), f(x - h, y - h), \ldots$ and so on (no terms $+2h$ should be required) in order to prove the approximative relation:

$$f_{xy}(x, y) \approx \frac{f(x + h, y + h) - f(x + h, y - h) - f(x - h, y + h) + f(x - h, y - h)}{4h^2}$$

2.3 Euler's Method

Try to find a way to formulate the second order differential equation of the simple harmonic oszillator in terms of Euler's method.

$$x'' = -kx$$

Just write it down please!

3 Requirements

One protokoll containing

- an introduction to the problems posed.
- answers to *each and every* question.
- *no source code!* Latter shall be sent to *siegfried.eggl@univie.ac.at* in form of a *compilable* textfile.

Please send the protocol as a PDF file to *siegfried.eggl@univie.ac.at*

References

Wikipedia, *Fundamental theorem of calculus*, `http://en.wikipedia.org/wiki/Fundamental_theorem_of_calculus` (2009)