Error of numerical derivation

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} = f'(x) + \frac{1}{2!} f''(x)\Delta x + \frac{1}{3!} f^{(3)}(x)\Delta x^2 + \dots$$

Let $\left(D_{\Delta x} F\right)(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x}$,

then $error(\Delta x) = \left| (D_{\Delta x} f)(x) - f'(x) \right|$. We expect $error(\Delta x) = O(\Delta x^1)$.

big Oh: $c_2 \Delta x \leq error(\Delta x) < c_1 \Delta x$, $c_1, c_2 > 0$, for sufficientli small Δx

Error of the linear approximation:

$$\left| f(x+\Delta x) - [f(x) + f'(x)\Delta x] \right| \leq \frac{1}{2} \Delta x^2 \max_{s \in [x, x+\Delta x]} \| f''(s) \|$$

So $error(\Delta x) \leq \frac{1}{2} \Delta x \max_{s \in [x, x+\Delta x]} \| f''(s) \| = O(\Delta x^1)$

Numerical measurement of the exponent 1 in $O(\Delta x^1)$

Set $\Delta x_n = \frac{1}{2^n}$ (or to any $\Delta x_n \to 0$ sequence; preferably $\Delta x_n > 0$)

If $error(\Delta x) = C \cdot \Delta x^\alpha$, then

$$\ln error(\Delta x) = \ln C \cdot \Delta x_n^\alpha = \ln C + \alpha \cdot \ln \Delta x_n = \ln C + \alpha \cdot \ln 2^{-n} = \ln C + \alpha \cdot \ln 2 \cdot (-n)$$

So plot the points $(n, \ln(error(\Delta x_n)))$, fit a straight line to it (this is called linear regression), find its slope m then $\alpha = -\frac{m}{\ln 2}$. *

This is a log-log plot: similar to $\ln \Delta x \leftrightarrow \ln(error(\Delta x))$.

Numerial computation: assume Float = 32 bit numbers.

Δx smaller $\to$ error is better. But: what if $\Delta x = 2^{-30}$?

Then $\frac{f(x+\Delta x) - f(x)}{\Delta x} \sim \frac{\sim 0 \dots 00100}{\underbrace{00 \dots \underbrace{0100}_{\text{2 or 3 nonzero digits}}}_{\text{32 digits}}}$ $\sim$ error's order $\sim 2^{-3} \sim 10\%$, bad.

Conclusion: pick n large enough, so $\Delta x_n = \frac{1}{2^n}$ is small enough, but do not pick too large n.

* Probably it is better to make a $\ln \Delta x_n \leftrightarrow \ln error(\Delta x_n)$ plot, so there will be no $\ln 2$ factor.

Exercises:

(1) Firstly check the type of the floating point number used by your computer. Set $f(x) = \sin x$, $x = 1$, comput $(D_{\Delta x} f)(1)$ for $\Delta x = \frac{1}{2}, \frac{1}{4}, \dots \frac{1}{2^{30}}$ or $\frac{1}{2^{60}}$.
Plot $(n, \ln(\text{error}(\Delta x_n)))$, and measure α in $\text{error}(\Delta x) \sim \Delta x^{\alpha}$.

(2) Repeat this for $F(x) = \sin(x)$, $x = 0$. Explain your result!

(3) Let $(\tilde{D}_{\Delta x} f)(x) = \dfrac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$.

Use the error bound

$$|F(x+\Delta x) - T_n(x+\Delta x)| \le \frac{1}{(n+1)!} \Delta x^{n+1} \cdot \max_{s \in [x, x+\Delta x]} |f^{(n+1)}(s)|$$

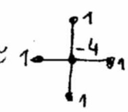
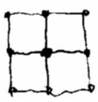
of the Taylor series $T_n(x+\Delta x) = f(x) + f'(x)\Delta x + \dots + \dfrac{F^{(n)}(x)}{n!} \Delta x^n$ to estimate the value α in $\text{error}(\Delta x) \sim \Delta x^{\alpha}$.
Repeat the numerical calculatons of (1) for $\tilde{D}$!

(4) All these cam be dome for higher derivatives, too. $\frac{d^2}{dx^2} \sim (D_{\Delta x})^2$.
What is $(D_{\Delta x})^2$? Repeat (1) for $(D_{\Delta x})^2$!

(5) $\tilde{D}_{\Delta x}$ of (3) is a better approximation of $\frac{d}{dx}$ then $D_{\Delta x}$.
Find a better approximation of $\frac{d^2}{dx^2}$ then $(D_{\Delta x})^2$!
Demonstrate the superiority of your approximation by numerical experiments!

(6) Let us repeat all these in two dimensions. Since $f''(x) \approx \frac{1}{\Delta x^2}\left(f(x+\Delta x) - 2f(x) + f(x-\Delta x)\right)$,

$$\Delta f = (\partial_x^2 + \partial_y^2) f(x,y) \approx \frac{1}{\Delta x^2}\Big(f(x+\Delta x, y) + f(x-\Delta x, y) + f(x, y+\Delta x) + f(x, y-\Delta x) - 4f(x,y)\Big).$$

With a picture: $\Delta \approx$  $\cdot \frac{1}{\Delta x^2}$. Pick a function, for example $\sin(3 + xy + x^2)$, and measure the error of $(\Delta f)(0,0) \sim \Delta x^{\alpha}$. Estimate α!
Is it possible to increase the value of α by setting $\Delta \approx \frac{1}{\Delta x^2}$  ?

(7) Find a reasonable approximation for ∂_{xy}!

Estimation of the error of numerical derivatives

$$(D_{\Delta x} f) = \frac{f(x+\Delta x) - f(x)}{\Delta x}, \quad \left|(D_{\Delta x} f)(x) - f'(x)\right| = \text{error}(\Delta x) \sim \Delta x^{\alpha}, \quad \alpha = 1$$

$$(\tilde{D}_{\Delta x} f) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}, \quad \text{error}(\Delta x) \sim \Delta x^{\alpha}, \quad \alpha = 2$$

$D_{\Delta x}$: $\frac{1}{\Delta x} \cdot$ -1 at x, 1 at $x+\Delta x$

$\tilde{D}_{\Delta x}$: $\frac{1}{\Delta x} \cdot$ $-1/2$ at $x-\Delta x$, 0 at x, $1/2$ at $x+\Delta x$

How can we guess α?

① Check the equality $(D_{\Delta x} f)(x) = f'(x)$ for $x = 0$, $f(x) = 1, x, x^2, x^3 \ldots x^n, \ldots$

if $D_{\Delta x}$ is independent on x, then shift $x \to 0$, $f(z) \to f(z+x)$

② Find the smallest n such that the equality fails.

$$(D_{\Delta x} 1)(0) = \frac{1}{\Delta x}(1-1) = 0, \quad \text{same as } 1' \text{ at } x=0$$

$$(D_{\Delta x} x)(0) = \frac{1}{\Delta x}(\Delta x - 0) = 1, \quad \text{same as } x' = 1 \text{ at } x = 0$$

$$(D_{\Delta x} x^2)(0) = \frac{1}{\Delta x}(\Delta x^2 - 0) = \Delta x^1, \quad \underline{\text{not}} \text{ the same as } x^2 = 2x, \text{ which is } 0 \text{ at } x = 0$$

So $\text{error}(\Delta x) \sim \Delta x^1$.

Now do the same for $\tilde{D}_{\Delta x}$!

$$(\tilde{D}_{\Delta x} 1)(0) = \frac{1}{\Delta x}\left(\frac{1}{2}\cdot 1 - \frac{1}{2}\cdot 1\right) = 0 \quad ✓ \quad \text{o.k.}$$

$$(\tilde{D}_{\Delta x} x)(0) = \frac{1}{\Delta x}\left(\frac{1}{2}\cdot\Delta x - \frac{1}{2}(-\Delta x)\right) = 1 \quad ✓ \quad \text{o.k.}$$

$$(\tilde{D}_{\Delta x} x^2)(0) = \frac{1}{\Delta x}\left(\frac{1}{2}\Delta x^2 - \frac{1}{2}(-\Delta x)^2\right) = 0 \quad ✓ \quad \text{o.k.}$$

$$(\tilde{D}_{\Delta x} x^3)(0) = \frac{1}{\Delta x}\left(\frac{1}{2}\Delta x^3 - \frac{1}{2}(-\Delta x)^3\right) = \Delta x^2, \quad \text{not zero: } (x^3)' = 2x^2, \text{ which is } 0 \text{ at } x = 0$$

So $\text{error}(\Delta x) \sim \Delta x^2$

Exercise:

① Repeat this for $\frac{d^3}{dx^3} \approx D_{\Delta x}^3$!

② Repeat this for $\frac{d^3}{dx^3} \approx \tilde{D}_{\Delta x}^3$!

Error of numerical solutions, ODE

$$\frac{d}{dt}\vec{y}(t)=\vec{F}(t,\vec{y}(t)),\quad \vec{y}(0)=\vec{y}_0$$

① Euler's method: $t_n = n\cdot\Delta t$, $y(t_n)\approx y_n$

$$y_{n+1}=y_n+f(t_n,y_n)\,\Delta t$$

② Heun's method: $k_1=f(t_n,y_n)$, $k_2=f(\underbrace{t_n+\Delta t}_{t_{n+1}},\overbrace{y_n+f(t_n,y_n)\Delta t}^{\text{Euler's prediction of } y_{n+1}})$

$$y_{n+1}=y_n+\frac{k_1+k_2}{2}\Delta t$$

③ Midpoint method: $k=f(t_n+\frac{\Delta t}{2},\ y_n+f(t_n,y_n)\frac{\Delta t}{2})$

$$y_{n+1}=y_n+k\,\Delta t.$$

Exercise: ⓐ $\frac{d}{dt}y=\cos(t+y)\sin(y)$, $y(0)=2$

ⓑ $\frac{d}{dt}\begin{bmatrix}y_1\\y_2\end{bmatrix}=\begin{bmatrix}y_1-\cos(t)\,y_1y_2\\-y_2+\cos(t)\,y_1y_2\end{bmatrix}$, $\vec{y}(0)=\begin{bmatrix}3\\4\end{bmatrix}$

Pick $\Delta t=\frac{1}{8},\frac{1}{16},\dots\frac{1}{2^N}$, $N=15$. Use Heun's and the midpoint methods, to calculate $y(2)$ and $\vec{y}(2)$. Assume that $\text{error}(\Delta t)\approx C\cdot\Delta t^{\alpha}$. Estimate C and α for these methods. Which one is the better? Repeat this for a pair of other ODE!

Third order Runge-kutta

Exercise: Design a third order Runge-kutta method!

(Hard with OCTAVE!)

Solution: (draft)

$$k_1 = f(t_n, y_n)$$
$$k_2 = f(t_n + \alpha\Delta t,\ y_n + \beta\Delta t\, k_1)$$
$$k_3 = f(t_n + \gamma\Delta t,\ y_n + \delta\,\Delta t\, k_1 + \varepsilon\,\Delta t\, k_2)$$
$$y_{n+1} = y_n + (w_1 k_1 + w_2 k_2 + w_3 k_3)\Delta t$$

Equations for $\alpha, \beta, \gamma, \delta, \varepsilon, w_1, w_2\, w_3$:

① t_n can be set to 0.

② $$f(0+\Delta u,\ y_n + \Delta v) \approx \sum_{\substack{r,s\geq 0\\ r+s\leq 2}} \frac{f^{(r,s)}(0, y_n)}{r!\,s!}\Delta u^r \Delta v^s$$

(Note that it is enough to expand f up to Δt^2, since in y_{n+1} it has an extra Δt multiplier)

③ $$y_{n+1} \approx y(0+\Delta t) \approx y(0) + y'(0)\Delta t + \frac{y''(0)}{2}\Delta t^2 + \frac{y'''(0)}{3}\Delta t^3$$

where $y'(t) = f(t, y)$

$$y''(t) = \left(\frac{\partial}{\partial t} + f(t,y)\frac{\partial}{\partial y}\right) f(t,y)$$
$$y'''(t) = \left(\frac{\partial}{\partial t} + f(t,y)\frac{\partial}{\partial y}\right)^2 f(t,y)$$

④ Compare the predictions of y_{n+1}:

③ and the method should give the same result up to a term $o(\Delta t^4)$

Now we have a system of equations for $\alpha \ldots, w_3$.

⑤ Find a solution of those equations!

⑥ Check your method: Pick a DE, for example $y' = \cos(t+y)\sin(y)$, $y(0) = 2$, and repeat the exercise of page 1_{II}.

Implicit Euler method

$\boxed{3_{II}}$

$$\vec{y}_{n+1} = \vec{y}_n + \Delta t \cdot \vec{f}(t_n+\Delta t, \vec{y}_{n+1})$$ (Compare to the explicit $\vec{y}_{n+1} = \vec{y}_n + \Delta t \cdot \vec{f}(t_n, \vec{y}_n)$)

equation for y_{n+1}. In practice, one solves it only approximately, in this exercise solve it "exactly".

$\Delta t = \frac{1}{2^5}, \frac{1}{2^6}, \ldots \frac{1}{2^{10}}$.

Exercise: Apply the explicit and implicite Euler methods for the following DE:

1. $y' = -y, \quad y(0) = 1, \quad y(2) = ?$
2. $y' = y, \quad y(0) = 1, \quad y(2) = ?$
3. $\frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -1/2 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \vec{y}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \vec{y}(2) = ?$
4. $\frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} -y_1 + (y_1 y_2)^2 \\ +y_2 - (y_1 y_2)^2 \end{bmatrix}, \quad \vec{y}(0) = \begin{bmatrix} 1.5 \\ 1.3 \end{bmatrix}, \quad \vec{y}(2) = ?$

For 1, 2, 3 the equation for $\vec{y}_{n+1}$ can be solved easyly, so smaller Δt can be choosen, let say up to $\Delta t = \frac{1}{2^{15}}$.
In the case of 4, use a numerical solver for the computation of $\vec{y}_{n+1}$.

Which of the implicit and explicit methods is better?