Unit 6.1 – Numerical Differentiation

To fully appreciate the usefulness of numerical differentiation, we should start by considering the mathematical definition of a derivative.

$$\frac{df}{dx} = \lim_{\epsilon \to 0} \frac{f(x_0+\epsilon)-f(x_0)}{\epsilon} \qquad (6.1\text{-}1)$$

It's easy to show, for example how to do this for a polynomial, say

$$f(x) = ax^2 + bx + c$$

$$\frac{df}{dx} = \lim_{\epsilon \to 0} \frac{a(x+\epsilon)^2+b(x+\epsilon)+c \; - (ax^2+bx+c)}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{a(x^2+2x\epsilon+\epsilon^2)+b(x+\epsilon)+c}{\epsilon} - \frac{(ax^2+bx+c)}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{2ax\epsilon+\epsilon^2+b\epsilon}{\epsilon}$$

$$= \lim_{\epsilon \to 0} 2ax+\epsilon+b$$

$$\frac{df}{dx} = 2ax + b \qquad (6.1\text{-}2)$$

But what about for a more complicated case like the Prandtl-Meyer function from the exam?

$$\nu(M) = \sqrt{\frac{\gamma+1}{\gamma-1}}\tan^{-1}\sqrt{\frac{\gamma-1}{\gamma+1}(M^2-1)} - \tan^{-1}\sqrt{M^2-1}$$

Options:

1. Do by hand
2. Use Wolfram
3. Perform a numerical differentiation

derivative of PM function

$$\nu(M)=\sqrt{\frac{\gamma+1}{\gamma-1}}\tan^{-1}\sqrt{\frac{\gamma-1}{\gamma+1}(M^2-1)}-\tan^{-1}\sqrt{M^2-1}$$

let $\sqrt{\frac{\gamma-1}{\gamma+1}}=a$

$$\nu(M)=\frac{1}{a}\tan^{-1}\left(a\sqrt{M^2-1}\right)-\tan^{-1}\sqrt{M^2-1}$$

$$\frac{d\nu}{dM}=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left\{\frac{1}{a}\left[\tan^{-1}\left(a\sqrt{(M+\epsilon)^2-1}\right)-\tan^{-1}\left(a\sqrt{M^2-1}\right)\right]-\left[\tan^{-1}\sqrt{(M+\epsilon)^2-1}-\tan^{-1}\sqrt{M^2-1}\right]\right\}$$

using

$\tan^{-1}(u)\pm\tan^{-1}(v)=\tan^{-1}\left(\frac{u\pm v}{1\mp uv}\right)$ gives

$$\frac{d\nu}{dM}=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left\{\frac{1}{a}\tan^{-1}\left(\frac{a\sqrt{(M+\epsilon)^2-1}-a\sqrt{M^2-1}}{1+a^2\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}}\right)-\tan^{-1}\left(\frac{\sqrt{(M+\epsilon)^2-1}-\sqrt{M^2-1}}{1+\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}}\right)\right\}$$

?

but $\tan^{-1}(z)=z-\frac{z^3}{3}+\frac{z^5}{5}+\cdots=\sum_{n=0}^{\infty}\frac{(-1)^n z^{2n+1}}{2n+1}$

we get z term

$$\frac{d\nu}{dM}=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left[\frac{1}{\cancel{a}}\left(\frac{\cancel{a}\sqrt{(M+\epsilon)^2-1}-\cancel{a}\sqrt{M^2-1}}{1+a^2\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}}\right)-\left[\frac{\sqrt{(M+\epsilon)^2-1}-\sqrt{M^2-1}}{1+\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}}\right]\right]$$

$$=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left[\frac{\left(\sqrt{(M+\epsilon)^2-1}-\sqrt{M^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}{\left(1+a^2\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}-\frac{\left(\sqrt{(M+\epsilon)^2-1}-\sqrt{M^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}{\left(1+\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}\right]$$

$$=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left[\frac{(M+\epsilon)^2-1-(M^2-1)}{\left(1+a^2\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}-\frac{(M+\epsilon)^2-1-(M^2-1)}{\left(1+\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}\right]$$

$$=\lim_{\epsilon\to0}\frac{1}{\cancel{\epsilon}}\left[\frac{\cancel{M^2}+2M\cancel{\epsilon}+\epsilon^{\cancel{2}}-\cancel{1}-\cancel{M^2}+\cancel{1}}{\left(1+a^2\sqrt{M^2-1}\sqrt{(M+\cancel{\epsilon})^2-1}\right)\left(\sqrt{(M+\cancel{\epsilon})^2-1}+\sqrt{M^2-1}\right)}-\frac{\left(M^2+2M\cancel{\epsilon}+\epsilon^2-\cancel{1}-M^2+\cancel{1}\right)}{\left(1+\sqrt{M^2-1}\sqrt{(M+\cancel{\epsilon})^2-1}\right)\left(\sqrt{(M+\cancel{\epsilon})^2-1}+\sqrt{M^2-1}\right)}\right]$$

$$\frac{d\nu}{dM}=\frac{2M}{\left(1+a^2(M^2-1)\right)2\sqrt{M^2-1}}-\frac{2M}{\left(1+M^2-1\right)2\sqrt{M^2-1}}$$

$$=\frac{M}{(a^2M^2-a^2+1)\sqrt{M^2-1}}-\frac{M}{M^2\sqrt{M^2-1}}$$

$$=\frac{M^2-(a^2M^2-a^2+1)}{M(a^2M^2-a^2+1)\sqrt{M^2-1}}$$

$$=\frac{M^2(1-a^2)+a^2-1}{M(a^2M^2-a^2+1)\sqrt{M^2-1}}$$

$$=\frac{(M^2-1)(1-a^2)}{M(a^2M^2-a^2+1)\sqrt{M^2-1}}$$

$$\boxed{\frac{d\nu}{dM}=\frac{(1-a^2)\sqrt{M^2-1}}{a^2M(M^2-1)+M}}$$

What about the z^3 term?

$$=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left[\frac{1}{a}\left(\frac{a\sqrt{(M+\epsilon)^2-1}-a\sqrt{M^2-1}}{1+a^2\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}}\right)^3-\left(\frac{\sqrt{(M+\epsilon)^2-1}-\sqrt{M^2-1}}{1+\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}}\right)^3\right]$$

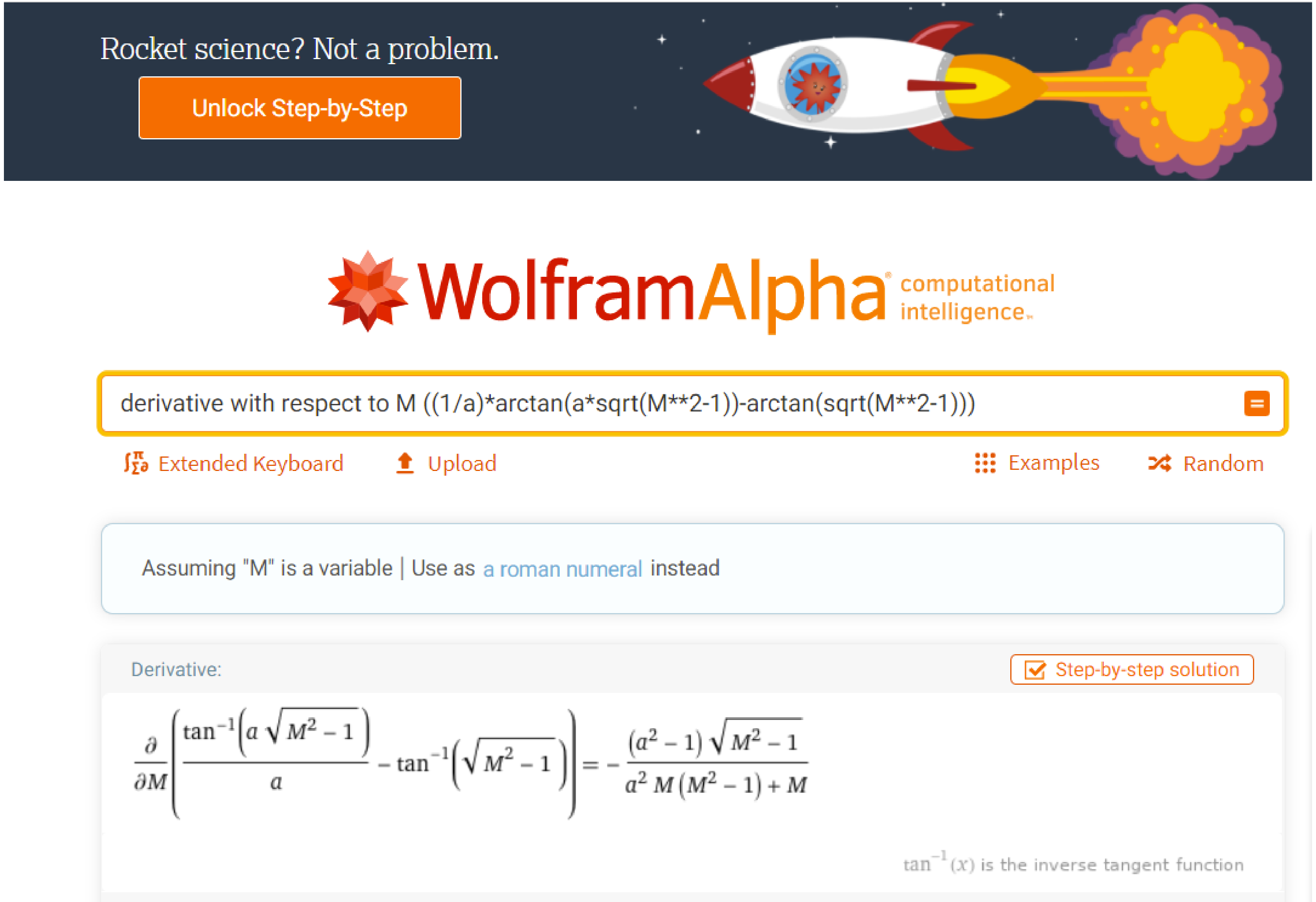
which becomes

$$=\lim_{\epsilon\to0}\frac{1}{\epsilon}\left[a^2\left(\frac{2M\epsilon+\epsilon^2}{\left(1+a^2\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}+\sqrt{M^2-1}\right)}\right)^3-\left(\frac{2M\epsilon+\epsilon^2}{\left(1+\sqrt{M^2-1}\sqrt{(M+\epsilon)^2-1}\right)\left(\sqrt{(M+\epsilon)^2-1}-\sqrt{M^2-1}\right)}\right)^3\right]$$

The lowest order ϵ term in the numerator is ϵ^3

$$\lim_{\epsilon\to0}\frac{1}{\cancel{\epsilon}}\epsilon^{\cancel{3}}[\;]=\epsilon^2[\;]=0$$

So all higher terms in the series [illegible]



Clearly this one can be done, but at what cost and for how much trouble?

The numerical equivalent is found by doing just a little bit more math.

We assume the series converges – terms shrink

Consider the Taylor series approximations:

$$f(x_0+\Delta x) = f(x_0) + \Delta x \frac{df}{dx}(x_0) + \frac{\Delta x^2}{2}\frac{d^2 f}{dx^2}(x_0) + \frac{\Delta x^3}{6}\frac{d^3 f}{dx^3}(x_0) + \cdots + \frac{\Delta x^n}{n!}\frac{d^n f}{dx^n}(x_0) + \cdots \qquad (6.1\text{-}3)$$

$$f(x_0-\Delta x) = f(x_0) - \Delta x \frac{df}{dx}(x_0) + \frac{\Delta x^2}{2}\frac{d^2 f}{dx^2}(x_0) - \frac{\Delta x^3}{6}\frac{d^3 f}{dx^3}(x_0) + (-1)^n\frac{\Delta x^n}{n!}\frac{d^n f}{dx^n}(x_0) + \cdots \qquad (6.1\text{-}4)$$

Subtracting 6.1-4 from 6.1-3 we get:

$$f(x_0+\Delta x) - f(x_0-\Delta x) = 2\Delta x \frac{df}{dx}(x_0) + \frac{\Delta x^3}{3}\frac{d^3 f}{dx^3}(x_0) + \cdots \qquad (6.1\text{-}5)$$

Or rearranging, gives the so-called **first derivative central difference formula**:

$$\frac{df}{dx}(x_0) = \frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x} + \frac{\Delta x^2}{6}\frac{d^3 f}{dx^3}(x_0) + \cdots \qquad (6.1\text{-}6)$$

Or said another way:

$$\frac{df}{dx}(x_0) = \frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2) \qquad (6.1\text{-}7)$$

Similarly, subtracting $f(x_0)$ from 6.1-3 gives the **first derivate forward difference formula**:

$$\frac{df}{dx}(x_0) = \frac{f(x_0+\Delta x)-f(x_0)}{\Delta x} + \mathcal{O}(\Delta x) \qquad (6.1\text{-}8)$$

The $\mathcal{O}(\Delta x)$ and $\mathcal{O}(\Delta x^2)$ terms represent the **truncation error** of the approximation. That is, the error incurred by a finite difference the extra terms are truncated off.

Similarly, subtracting 6.1-4 from $f(x_0)$ gives the **first derivative backward difference formula**:

$$\frac{df}{dx}(x_0) = \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x} + \mathcal{O}(\Delta x) \qquad (6.1\text{-}9)$$

Adding 6.1-3 and 6.1-4 gives

Or rearranging, gives the **second derivative central difference formula**:

$$\frac{d^2 f}{dx^2}(x_0) = \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \qquad (6.1\text{-}10)$$

These so-called finite differences can be constructed at various orders by taking combinations of equations like 6.1-3 and 6.1-4. A full list of central and one-sided differences is given in the text.

Cautions:

- These formulae work so long as Δx is constant.
- Non-uniform grid formulas can also be constructed by using appropriate series and combining terms.
- One needs to determine the "best" Δx by balancing truncation and roundoff error.