Numerical Calculus

Part-14

MA2103 - 2023

Basic Calculus such as differentiation and integration are important in science and engineering. Here we see how these basic operations can be done numerically and apply for solving some of the science and engineering problems

Functions, f(x), we mean a discreet samples of $f(x_i)$ at regular interval $x_i = x_0 + i \times h$, where $h = \Delta x$ is the sampling interval. We have sample of function at regular interval $x = \{x_0, x_1, x_2, \cdots x_N\}$

It Usually denoted by, $f_0 = f(x_0)$, $f_1 = f(x_1)$, $\dots f_i = f(x_0 + ih)$, \dots , $f_N = f(x_N)$

h should be sufficiently small to avoid loss of data.

h should not be too small, to avoid the computation burden.

Our goal is to do the calculus with discreet samples!

Taylor Series

We use idea of Taylor series for doing calculus on discreetly sampled data.

If we have a smooth function f(x) in the interval $[a = x_0, b = x_N]$, we can express the points f(x) in terms of Taylor series as,

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \dots + \frac{(x - x_0)^n}{n!}f^{(n)}(x_0) + \dots$$

If we fix $(x - x_0) = h$ then we can write a discreet sample $f(x_0 + h) = f_1$, as

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) \implies f_1 = f_0 + hf'_0 + \frac{h^2}{2!}f''_0$$

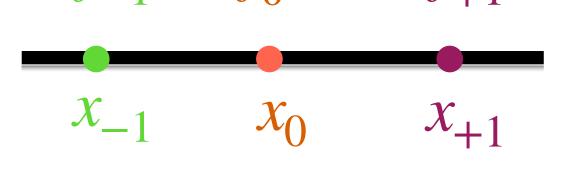
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$$f''_0$$

Same way we can write,
$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2!}f''(x_0)$$

$$f_{\pm 1} \equiv f_0 \pm h f_0' + \frac{h^2}{2} f_0'' \pm \frac{h^3}{6} f_0''' + \mathcal{O}(h^4)$$



Further more

$$f_{\pm 2} \equiv f_0 \pm 2hf_0' + 2f_0'' \pm \frac{4h^3}{3}f_0''' + \mathcal{O}(h^4)$$

We us these equation to separate f_0', f_0'', f_0''' in terms of $f_0, f_{\pm 1}, f_{\pm 2}$

Numerical differentiation

The basic definition of differentiation is

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

we can rewrite as

$$f_0' \approx \frac{\left(f_1 - f_0\right)}{h}$$

This is called forward divided difference and accurate to $\mathcal{O}(h)$

One can also have the backward divided difference by setting h
ightarrow - h

$$f_0' \approx \frac{\left(f_0 - f_1\right)}{h}$$

Above are also called 2-point formula.

How to Improve the accuracy

One way to increase accuracy is by decreasing h. That can not be carried on arbitrary because of machine-level inaccuracy.

In the Taylor series, replacing h by -h and subtracting we get

$$f_0' = \frac{f_{-1} - f_1}{2h}$$

This is called central difference approximation or 3-point formula and accurate up to $\mathcal{O}(h^2)$

Higher order formula

One can get higher order correction from Taylor series, accordingly adding more points to evaluate the differential

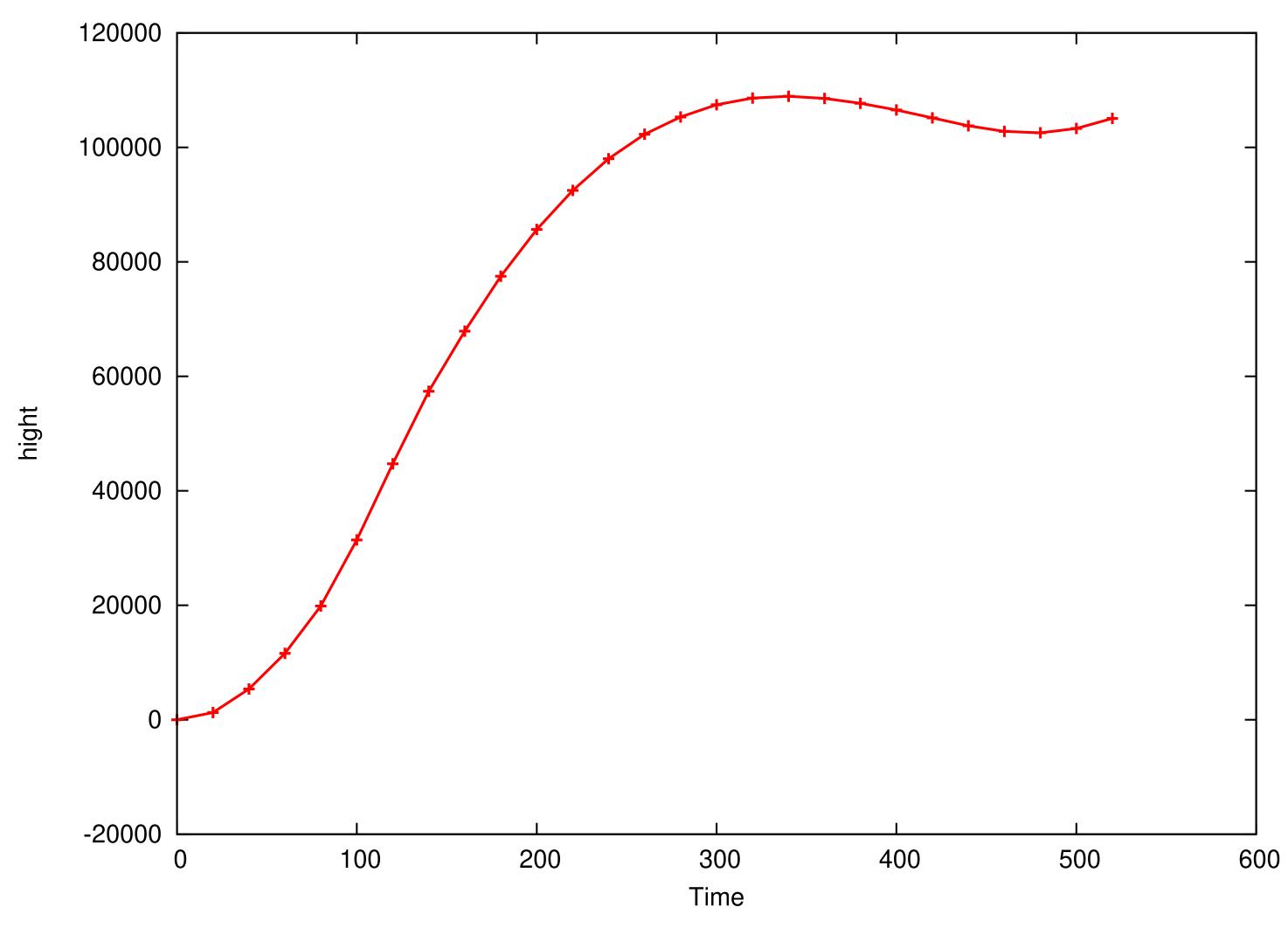
It is possible to improve on 3-point formula by taking more points, For example, using Taylor expansion, it is easy to show that the 5-point formula

$$f_0' = \frac{1}{12h} \left[f_{-2} - 8f_{-1} + 8f_1 - f_2 \right] + \mathcal{O}(h^4)$$

Example

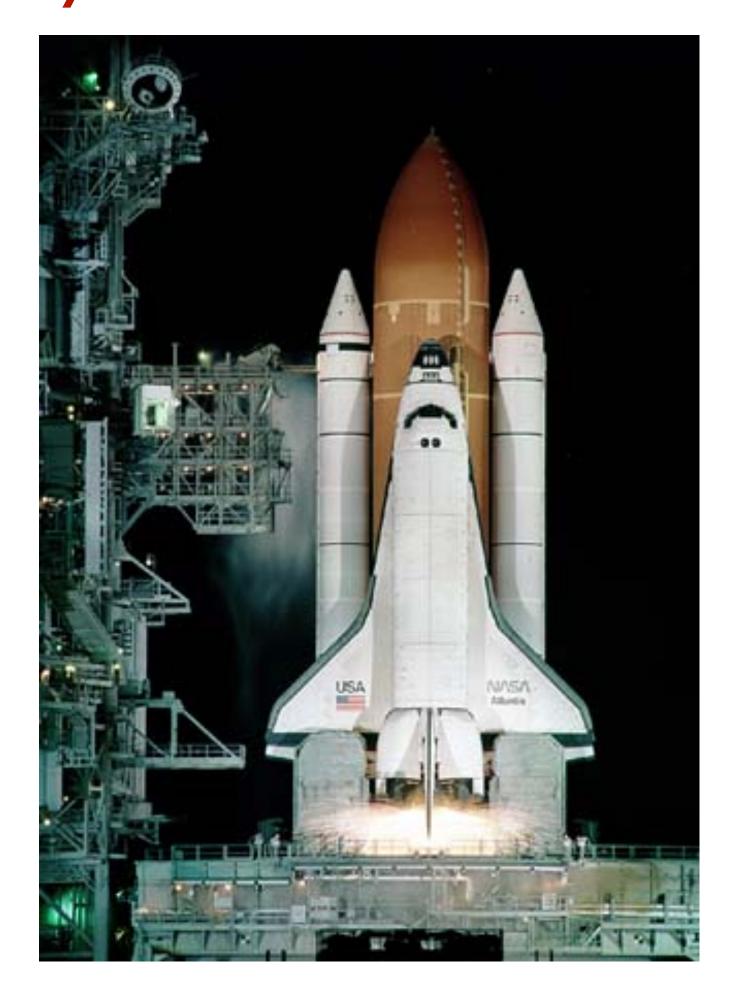
Telemetry data from Space-shuttle mission STS-121 Ascent-data, Determine vertical velocity.

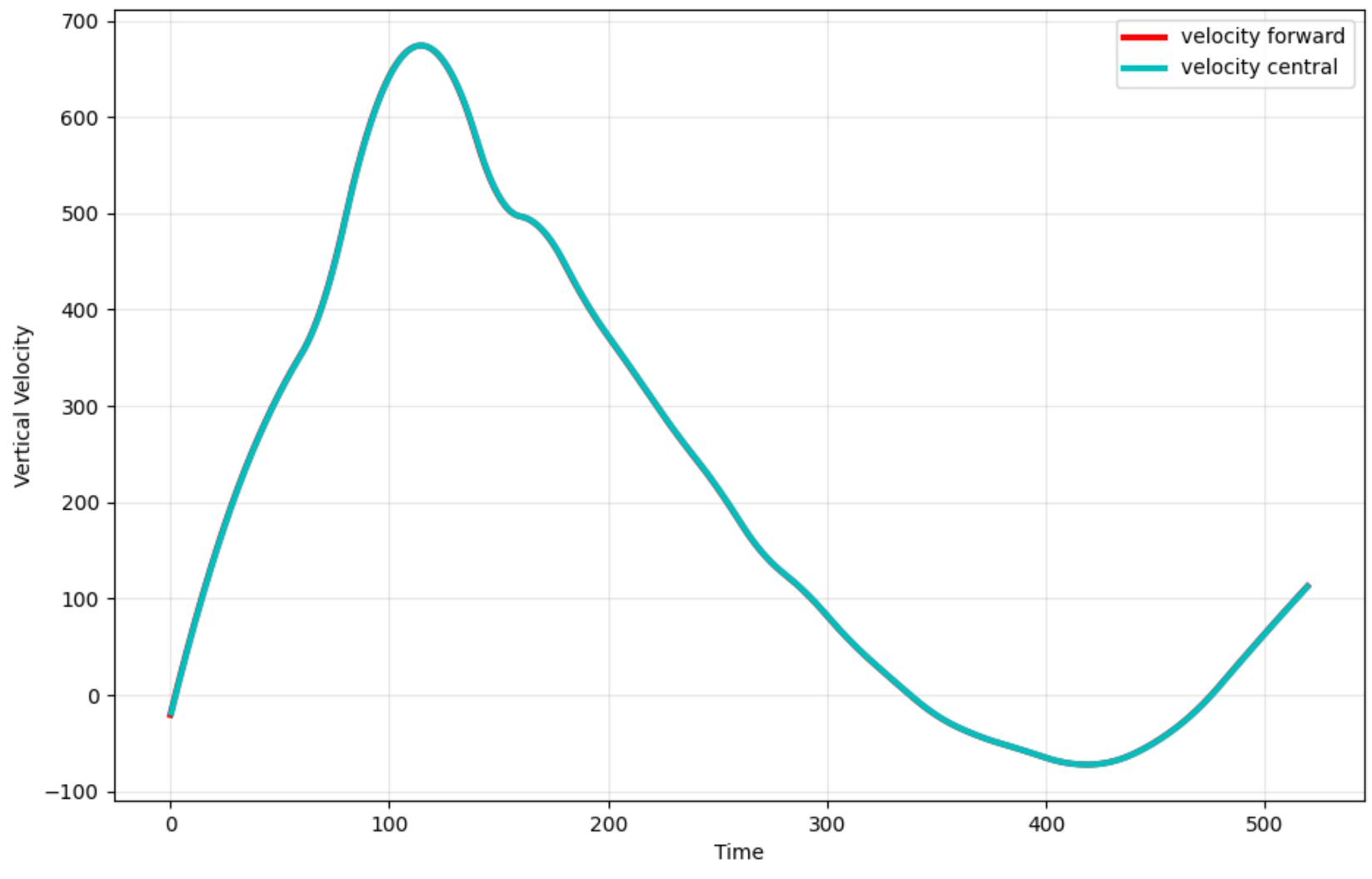




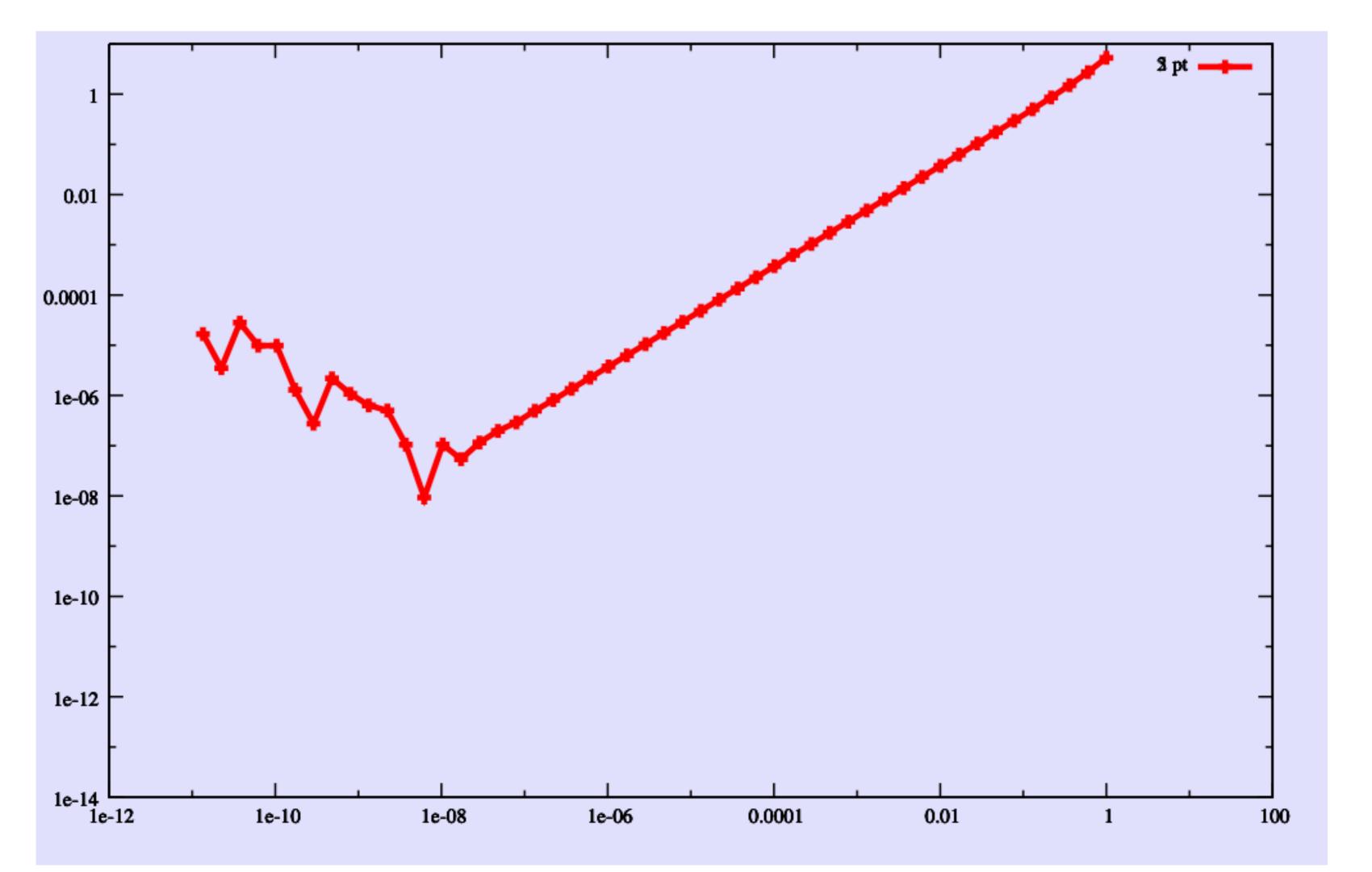
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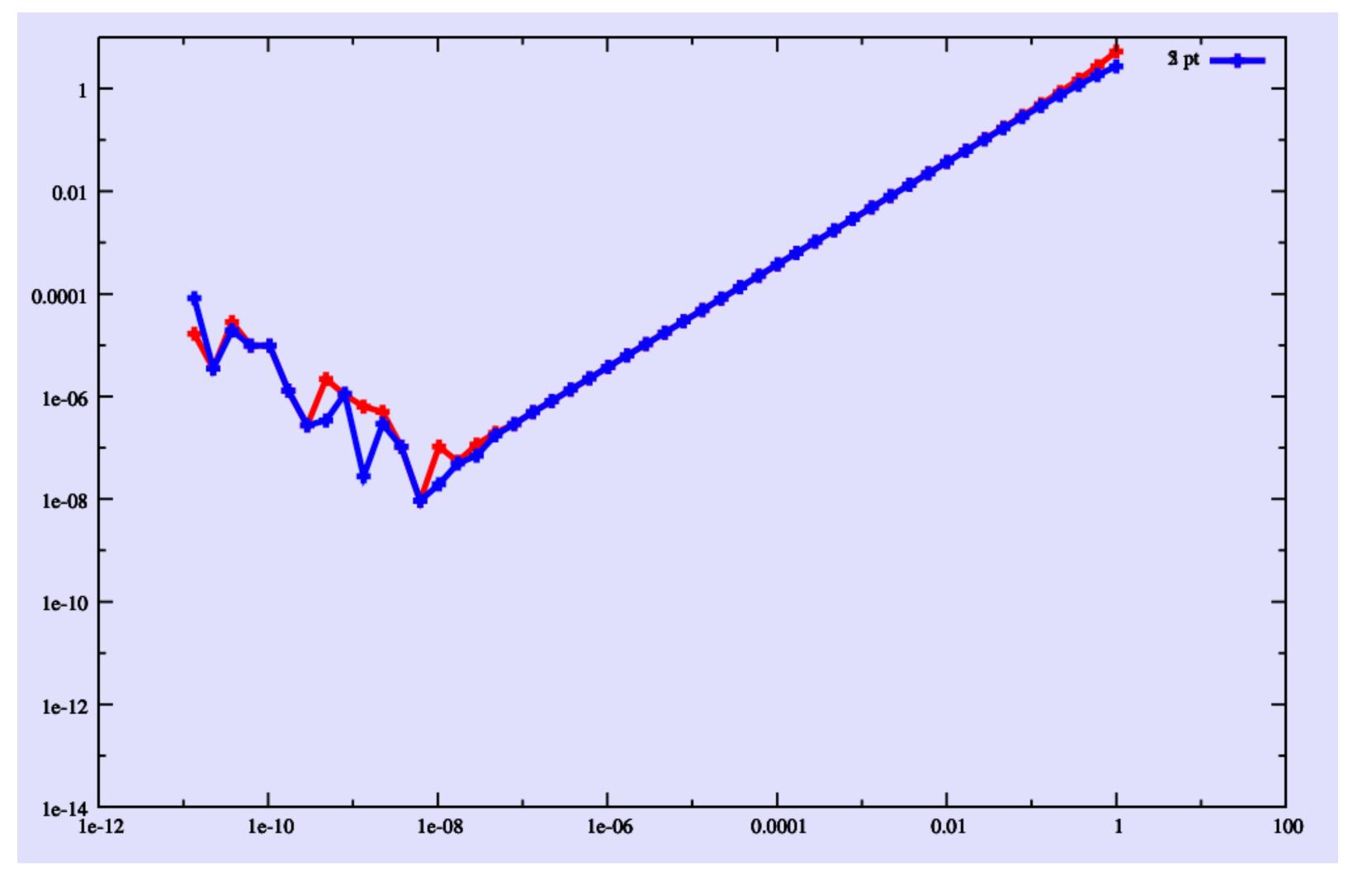




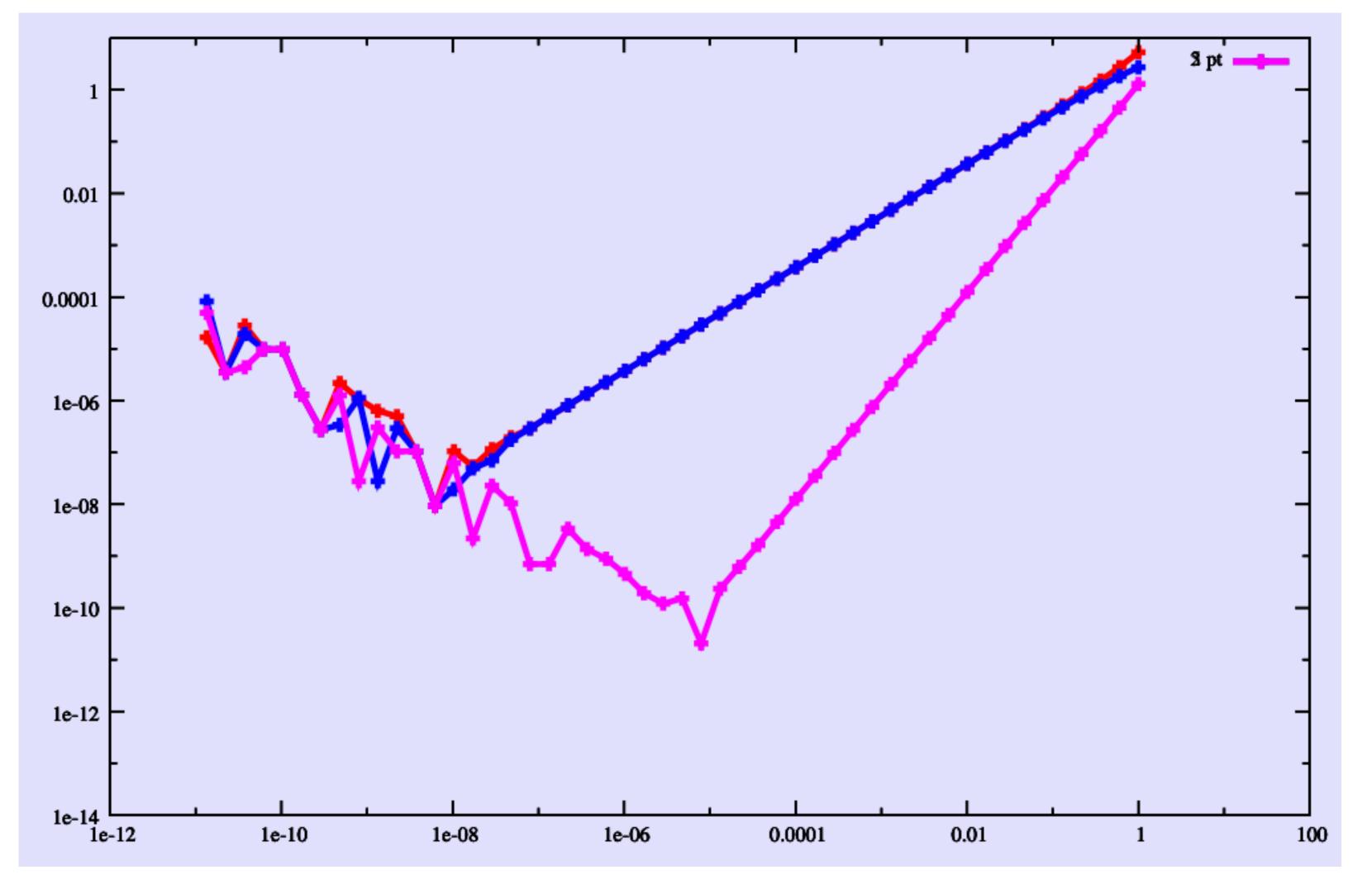
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