PolyMath version 1.0 and beyond

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Current Status of PolyMath

- A generic computation framework for Pharo
- MIT Licence
- PolyMath 1.0 release
- https://github.com/PolyMathOrg/PolyMath
- 806 green unit tests, 1034 commits, 100 stars on github (9th Pharo project on github)

Since last year

- Release 1.0 version + new logo
- Clean the code (All PM prefix classes), add more unit tests
- GSOC students implement : PCA and t-SNE
- Random Numbers cleaning (Hemal)
- Automatic Differentiation package cleaning (Serge)
- Data Transformer hierarchy (PMStandardizationScaler) like in scikit-learn
- Trunk-based development since 1.0 (all code is committed to master branch + one release branch)
- Add a contributing guide and code of conduct

Contributors

- Thank you !

[PolyMath]

Moose analysis

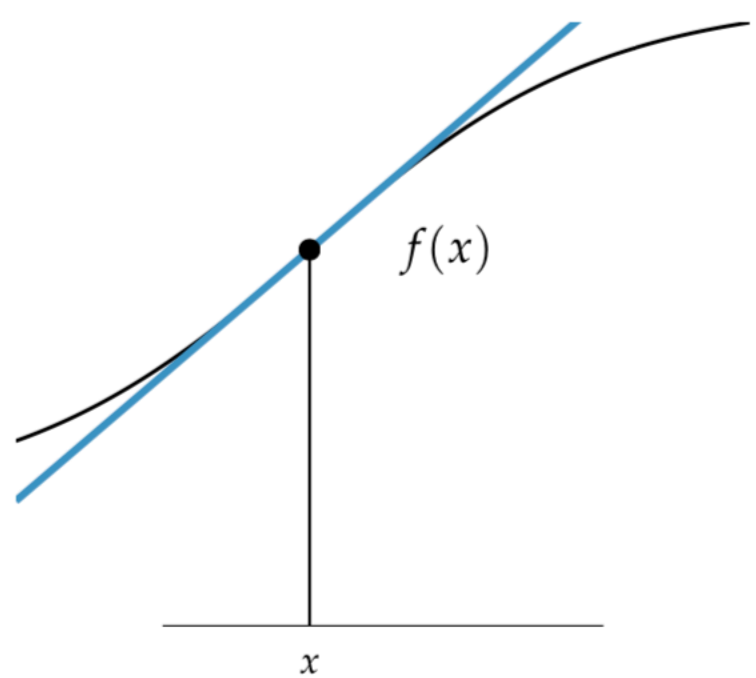
DEMO

Automatic Differentiation

- Explain why this topic is interesting especially in the context of Machine Learning

Derivatives

- The derivatives f'(x) of a function of a single variable x is the rate at which the value of f changes at x.
- How to compute derivatives numerically ?



$$f'(x) = \frac{\Delta f(x)}{\Delta x}$$

Numerical differentiation by using finite difference

$$f'(x) \approx \underbrace{\frac{f(x+h)-f(x)}{h}}_{\text{forward difference}} \approx \underbrace{\frac{f(x+h/2)-f(x-h/2)}{h}}_{\text{central difference}} \approx \underbrace{\frac{f(x)-f(x-h)}{h}}_{\text{backward difference}}$$

- Theoretically, the smaller the h is, the better the derivative estimates
- Practically very small value of h can result in numerical cancellation errors …

```
f := [ :x| x sin ].
x := 1/2.
errorDiffForward := [:h| ((((f value: (x+h)) - (f value: x)) / h) - (x cos)) abs ].

errorDiffForward value: 0.1.
```

Numerical differentiation by the Complex Step Method

- The Complex Step Method bypass the subtractive errors, by using only one single function evaluation (but more complex).

- Taylor expansion for an imaginary step is:

$$f(x+ih) = f(x) + ihf'(x) - h^2\frac{f''(x)}{2!} - ih^3\frac{f'''(x)}{3!} + \cdots$$

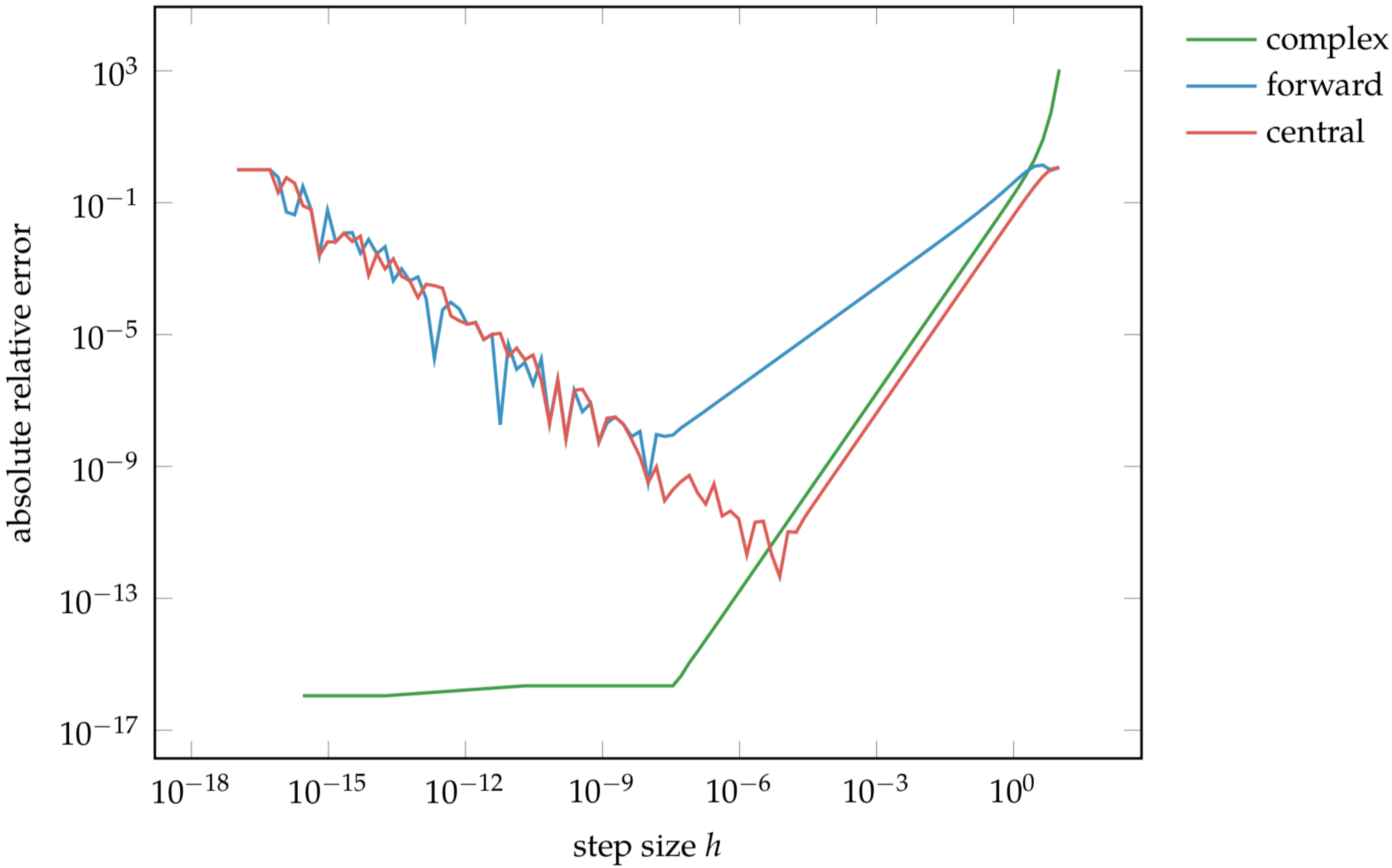
$$\mathrm{Im}(f(x+ih)) = hf'(x) - h^3\frac{f'''(x)}{3!} + \cdots$$

$$\begin{aligned}\Rightarrow f'(x) &= \frac{\mathrm{Im}(f(x+ih))}{h} + h^2\frac{f'''(x)}{3!} - \cdots \\ &= \frac{\mathrm{Im}(f(x+ih))}{h} + O(h^2) \text{ as } h \to 0\end{aligned}$$

Consider $f(x) = \sin(x^2)$. The function value at $x = \pi/2$ is approximately 0.624266 and the derivative is $\pi\cos(\pi^2/4) \approx -2.45425$. We can arrive at this using the complex step method:

```
f := [ :x| (x*x) sin ].
pi := Float pi.
x := pi /2.
h := 0.001.
((f value: (h*1i +x )) imaginary) / h.

pi * ((pi*pi/4) cos)
```



absolute relative error
10^{3}
10^{-1}
10^{-5}
10^{-9}
10^{-13}
10^{-17}
10^{-18}
10^{-15}
10^{-12}
10^{-9}
10^{-6}
10^{-3}
10^{0}
step size h
complex
forward
central

Automatic Differentiation

- Introduce DualNumber library in PolyMath
- Give an example

t-SNE

- Introduce what is t-SNE (dimensionality reduction)
- Demo of Atharva
- Demo of Oleks to include here

Future of PolyMath

- ActivePapers (1 slide)
- Domains (1 slide)
- Towards Scientific AI (1 slide)
- Fundings (1 slide)