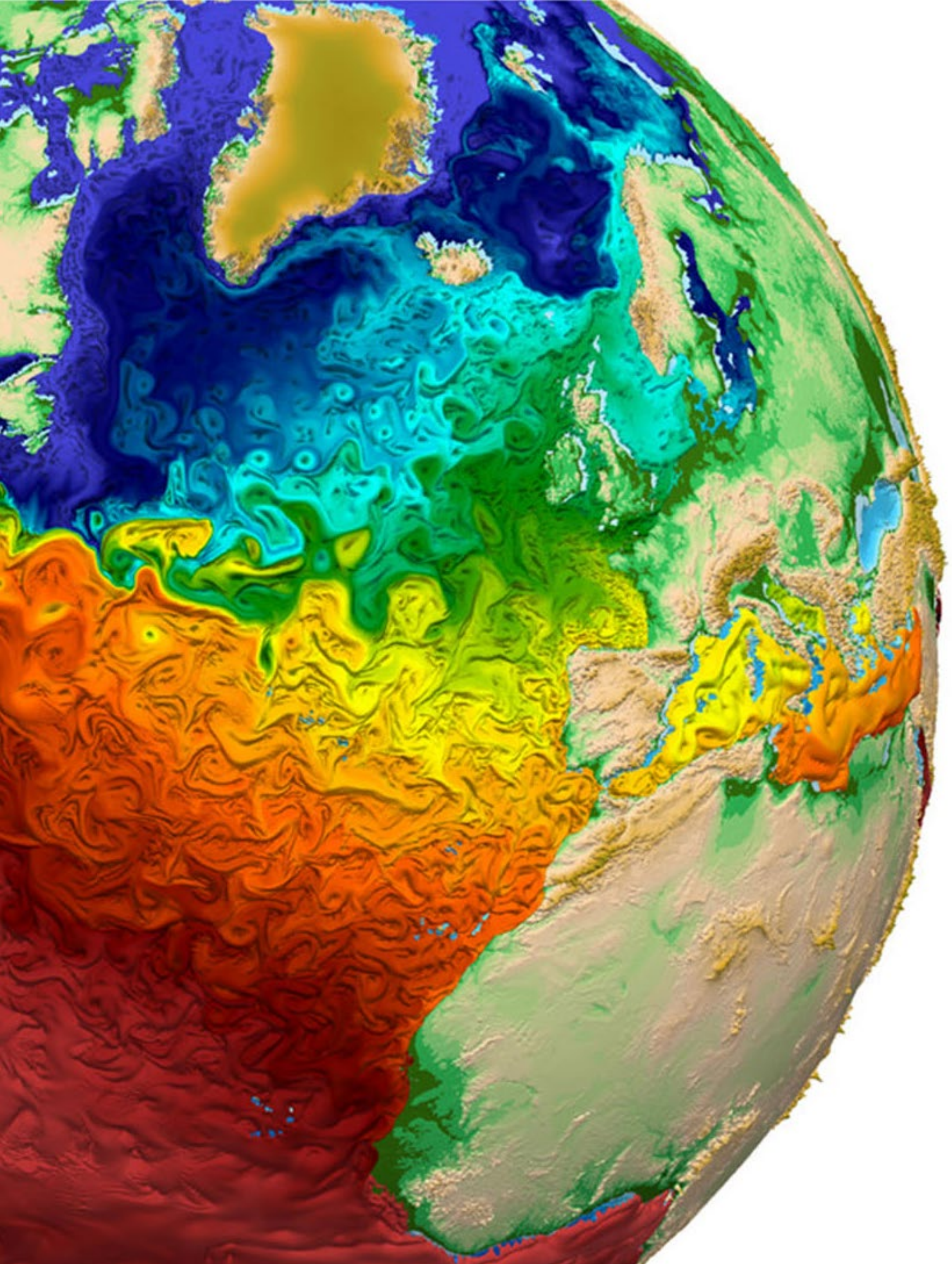

Numerical Differentiation

Finite Difference Methods

Scientific Visualization

Professor Eric Shaffer

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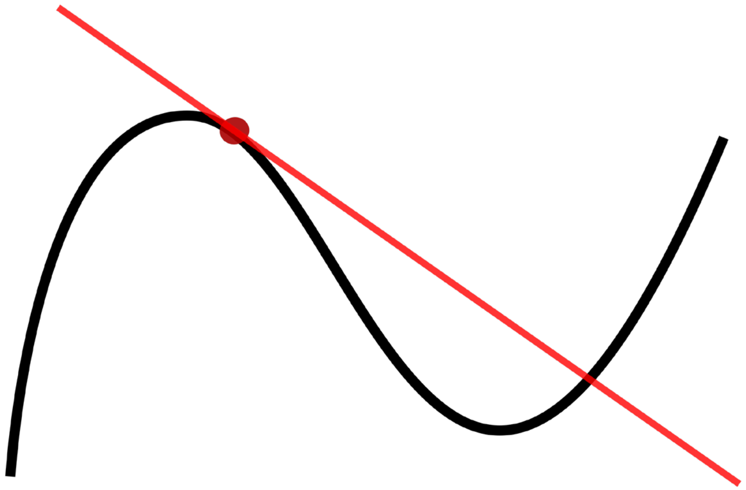
Differentiation

Differentiation is the process of finding the derivative of a function

The derivative expresses the rate of change of an output with respect to a change in the input

“the ratio of the instantaneous change in the dependent variable to that of the independent variable”



Really it’s a fundamental element of data science…helps analyze change…

Numerical Differetiatiom

Analytical differentiation finds a derivative through symbolic manipulation

This is often ideal…no error and sometimes fast evaluation of the derivative

"Evaluate" means to compute the value of a function (or derivative…which is also a function) for a specific input.

This is not always possible

- We may only have sampled data
- Derivative can be difficult or impossible to compute analytically
- Derivative may be prohibitively expensive to evaluate

Numerical methods are an alternative…approximate the analytical solution

Centered Difference Formula

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

h is called the step-size

- smaller step-size will result in less error
- error is on the order of $O(h^2)$

x is the location in the domain at which we evaluate the derivative

this is a *finite difference method*

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Understanding Error

- Differentiation is an inherently sensitive operation
  - Derivative of some functions changes rapidly..small input error can have great impact

- The centered difference formula can be derived from Taylor Series

$$
\begin{aligned}
f'(x) &= \frac{f(x+h)-f(x-h)}{2h} - \frac{f'''(x)}{6}h^2 + \cdots \\
&\approx \frac{f(x+h)-f(x-h)}{2h},
\end{aligned}
$$

Reducing step-size by $\frac{1}{2}$ reduces errors by $\frac{1}{4}$

- Can see that truncation error is $O(h^2)$

Derivatives of Sampled Data

People frequently use the centered difference formula…it's fast and easy

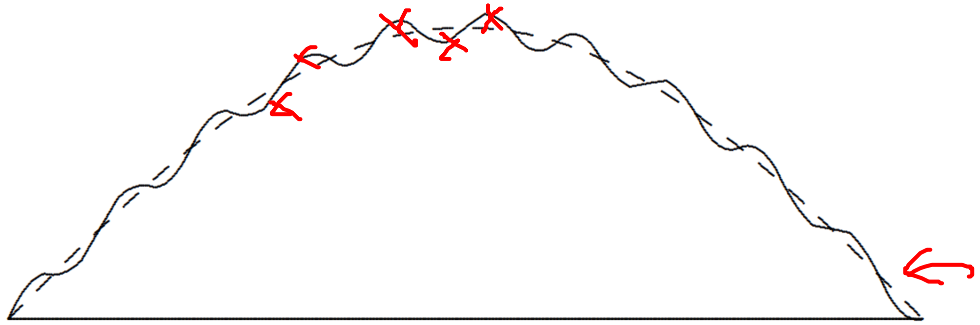
- Appropriate when function is known and we want fast approximation
- Not really appropriate for sampled or noisy data

Better approach for sampled data

- Fit an approximate function to data
- Take the derivative of the approximate function

Example:

- Least-squares best fit of quadratic function
- Then differentiate quadratic



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