Numerical Analysis: Numerical Differentiation

Natasha S. Sharma, PhD

Mathematical Question we are interested in answering numerically

- How to we evaluate

$$f'(x) \equiv \frac{df}{dx}?$$

- Calculus tells us that

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

- Goal is to approximate $f'(x)$ by a numerical derivative denoted by $D_h(f)$.

Why do we need to approximate derivatives?

1. Even if there exists an underlying function that we need to differentiate, we might know its values only at a sampled data set without knowing the function itself.
   For example,

x	f(x)
1	2.71
2	7.38
4	54.6

2. There are times in which exact formulas are available but they are very complicated to the point that an exact computation of the derivative requires a lot of function evaluations. It might be significantly simpler to approximate the derivative instead of computing its exact value.

Why do we need to approximate derivatives?

3. When approximating solutions to ordinary differential equations of the form:

$$\frac{dy}{dx} = f(x)$$

we typically represent the solution as a discrete approximation that is defined on a grid.
Since we then have to evaluate derivatives at the grid points, we need to be able to come up with methods for approximating the derivatives at these points.
Idea here is replace $\frac{dy}{dx}$ by $D_h(y)$ and numerically be able to solve the ordinary differential equation.

Numerical Differentiation: A General Framework

Definition (Forward Difference Numerical Derivative Formula)

For a given function $f(x)$, the numerical derivative is given by

$$D_h^+ f(x) = \frac{f(x+h) - f(x)}{h}.$$

with stepsize h.

Example

Example

Recall, the discrete set of data

x	f(x)
1	2.71
2	7.38
4	54.6

For $h = 1$, $D_h^+ f(1) = \frac{f(2)-f(1)}{2-1} = 4.67$.

For $h = 2$, $D_h^+ f(2) = \frac{f(4)-f(2)}{4-2} = 23.61$.

Numerical Differentiation: A General Framework

Definition (Backward Difference Numerical Derivative Formula)

For a given function $f(x)$, the numerical derivative is given by

$$D_h^- f(x) = \frac{f(x) - f(x-h)}{h}.$$

with stepsize h.

Example

Example

Recall, the discrete set of data

x	f(x)
1	2.71
2	7.38
4	54.6

For $h = 1$, $D_h^- f(2) = \frac{f(2)-f(1)}{2-1} = 4.67.$

For $h = 2$, $D_h^- f(4) = \frac{f(4)-f(2)}{4-2} = 23.61.$

Differentiation using Interpolation

The idea of using forward and backward difference formula for approximating derivatives was inspired by the very definition of $f'(x)$.

Taking inspiration from the approach followed for numerical integration,

$$f(x) \approx p_2(x) \implies f'(x) \approx p_2'(x).$$

This simplifies to the following formula (verfiy!)

Definition (Central Difference Numerical Derivative Formula)

For a given function $f(x)$, the numerical derivative is given by

$$D_h f(x) = \frac{f(x+h) - f(x-h)}{2h}.$$

with stepsize h.

Example

Example

Consider the discrete set of data

x	f(x)
1	2.71
2	7.38
3	20.1

$$h = 1, \; D_h f(2) = \frac{f(3) - f(1)}{2h} = 17.39/2 \approx 8.7.$$