Numerical Methods

Math 3338 – Spring 2022

Worksheet 9

Differentiation

Reading

CP	5.10
NMEP	5.1, 5.2

Table 1: Sections Covered

1 Derivatives

As we saw in Worksheet 4, the standard definition the derivative

$$f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h} \tag{1}$$

Add more explanation

is inadequate as there can be numeric error in the division. There actually isn't anything we can do about this.

Motivate This.

Let's do some Taylor series. Recall,

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \cdots \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \cdots. \end{aligned}$$

Add Graphs?

Subtract these and solve for $f'(x)$ to see,

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} + \mathcal{O}(h^2). \tag{2}$$

This is called a *central difference* and it's order h^2 which is better than order h, like (**??**)[1]. Central differences are more accurate using larger values of h.

There are also *forward differences*, this is (**??**), and *backward differences*. You should be able to guess what a backward difference is, but just in case,

$$\frac{f(x)-f(x-h)}{h}$$

You'll primarily use forward and backward differences when dealing with sequential data. If your data looks like $x_0, x_1, x_2, \ldots$, you can't use central differences to evaluate the derivative at x_0, you must use a forward difference.

2 Second Derivatives and Higher Order

When posed with a problem, the only logical solution is Taylor series. The idea with be to expand $f(x+ih)$ for numbers i (preferably integers) and solve for $f^{(n)}(x)$ canceling lower order derivatives.

[1] Why is (**??**) order h?

For example, using the following expansions,

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \cdots \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \cdots \\
f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x) + \frac{8h^3}{6}f'''(x) + \cdots \\
f(x-2h) &= f(x) - 2hf'(x) + \frac{4h^2}{2}f''(x) - \frac{8h^3}{6}f'''(x) + \cdots .
\end{aligned}
$$

We can find that,

$$
\begin{aligned}
f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2) \\
f^{(3)}(x) &= \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3} + \mathcal{O}(h^2) \\
f^{(4)}(x) &= \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4} + \mathcal{O}(h^2).
\end{aligned}
$$

These are all central differences, similar formulas exists for noncentral differences.

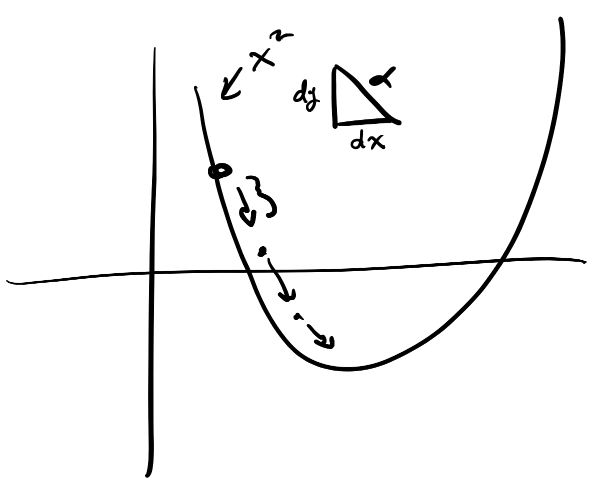
3 The Problem with Derivatives

We'll always be dividing by small numbers. This is especially true for $f^{(n)}(x)$. Combine this with,

1. Most problems being able to be phrased in terms of an integral
2. We can easily evaluate all explicit derivatives

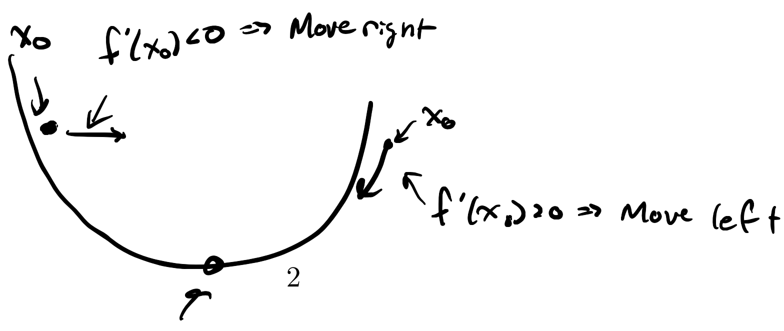
and we tend to not use differentiation that frequently. There are situations where differentiation is essential. But that's a future problem.

4. Numeric Optimization.



$$x_i = x_{i-1} - \alpha \underbrace{f'(x_{i-1})}_{\text{Near min, this is close to 0. So we go slower.}}$$

Idea:



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Homework 9 (Due: Tuesday, February 15)

Problem 1 (1 pt) Write two functions, `diff` and `diff_2` for the first and second derivatives using central differences. The input of these should be `f,x,h=.01` where f is a function.

Problem 2 (1 pt) Given $f(x) = 3x^4 + 3x^3 - 2x + 1$ find $f'(x)$ and $f''(x)$ by hand. Use your programs to compare the exact answers with approximation for $x \in \{-5, -4, \dots, 4, 5\}$. Make a table and put in a PDF.

Problem 3 (1 pt) Given $f(x) = \frac{1}{1+e^{-x}}$ find $f'(x)$ and $f''(x)$ by hand. Use your programs to compare the exact answers with approximation for $x \in \{-5, -4, \dots, 4, 5\}$. Make a table and put in a PDF.

Problem 4 (1 pt) Let $f(x, y)$ be a function. The partial derivative, $\frac{\partial f}{\partial x}$ at the point (a, b) is defined as,

$$\lim_{h \to 0} \frac{f(a+h, b) - f(a, b)}{h}.$$

This is the non-central difference, you can write a similar expression for the central difference.

1. $f(x, y) = \sin(x^2)e^{y-x}$, compute $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$ at the point $(1, 2)$.
2. $g(x, y, z) = x - \sqrt{y^2 + z^2}$, compute $\frac{\partial g}{\partial x}$, $\frac{\partial g}{\partial y}$, and $\frac{\partial g}{\partial z}$ at the point $(0, 0, 0)$
3. $h(x, y) = \ln(x + y)$, compute $\frac{\partial h}{\partial x}$ and $\frac{\partial h}{\partial x}$ at the point $(0, 0)$.

You should be able to use `diff` along with a lambda function to compute most of these. Some may give an error in which case you will have to think about what to do. You can always check you answers using MATH.