Math 340 • Fall 2026 • Victor Matveev

5.1. Numerical Differentiation: Finite Difference Approximation

There are many real-world functions that can be evaluated relatively accurately, but whose derivatives are not available as closed-form expressions. Consider for instance a model of average annual global temperature $T(x)$ as a function of total atmospheric CO_2 concentration x: each function value likely requires running a complicated computation taking many hours of CPU time, and its derivative $T'(x)$, which quantifies increase in global temperature with increasing CO_2 concentration, must be somehow computed separately.

Forward Finite Difference for 1st Order Derivative

Fortunately, the definition of derivative immediately provides a prescription for numerically approximating its value:

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

Even if we can't find the *exact* value of the limit, we can estimate it by choosing sufficiently small "step" size *h*:

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

As we learned in Calculus I, this is an approximation for the slope of a tangent line using the slope of a secant line.

If we don't take the limit $h \to 0$, this result is only approximate. To estimate the accuracy of this approximation, all we have to do is Taylor-expand $f(x+h)$ around argument value x, truncating the expansion at 2nd order:

$$f(x+h) = f(x) + f'(x)h + f''(c)\frac{h^2}{2}, \quad \text{where } c \in (x,\ x+h)$$

Plugging this into the approximation above yields

$$\frac{f(x+h)-f(x)}{h} = \frac{\left[\cancel{f(x)} + f'(x)h + f''(c)\frac{h^2}{2}\right] - \cancel{f(x)}}{h}$$

$$= \frac{f'(x)h + f''(c)\frac{h^2}{2}}{h} = f'(x) + \underbrace{f''(c)\frac{h}{2}}_{\text{ERROR}}$$

Thus, this approximation (known as the 2-point **forward finite difference approximation** of $f'(x)$) is only **first order accurate**, but with sufficiently small *h* values it will give sufficiently good accuracy. Note that in the absence of curvature, $f''(x) = 0$, this expression is exact, since in this case the function graph is a line of constant slope.

Summarizing our results, we found that $\underbrace{\frac{f(x+h)-f(x)}{h}}_{\text{APPROXIMATE}} = \underset{\text{EXACT}}{f'(x)} + \underbrace{f''(c)\frac{h}{2}}_{\text{ERROR = O}(h)}$, where $c \in (x,\ x+h)$

Side Note: any finite difference approximation involves subtracting values close in magnitude. Therefore, there is ***no way to avoid loss of significance*** inherent in this method. For many cases (as in your lab assignment #8), you will find that reducing *h* below about 10^{-5} to 10^{-8} will reduce the accuracy of the derivative approximation. This is the case of computation where double precision may only allow us to achieve a relatively modest accuracy.

If greater accuracy is required, one must devise an independent computational model for $f'(x)$ alongside the model of $f(x)$. In fact, for this very reason there is a whole field in computer science called *automatic differentiation* or *algorithmic differentiation*, which is beyond the scope of this course.

Backward Finite Difference for 1st Order Derivative

Backward 2-point finite difference approximation of $f'(x)$ is completely analogous to the forward one, therefore we give it without derivation:

$$\underbrace{\frac{f(x)-f(x-h)}{h}}_{\text{APPROXIMATE}} = \underbrace{f'(x)}_{\text{EXACT}} - \underbrace{f''(c)\frac{h}{2}}_{\text{ERROR = O}(h)}, \quad \text{where } c \in (x-h, x)$$

Centered Finite Difference Approximation of 1st Order Derivative

As it turns out, we can improve the accuracy of the finite difference approximation of $f'(x)$ using a more symmetric expression of the slope of the tangent line, using the slope of the secant line that is ***centered*** at x:

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

To evaluate its accuracy, we proceed as before, but this time expand both $f(x-h)$ and $f(x+h)$ around argument value x, truncating the expansion at 3rd order:

$$f(x+h) = f(x)+f'(x)h+f''(x)\frac{h^2}{2}+f'''(c_1)\frac{h^3}{3!}, \quad \text{where } c_1 \in (x,\ x+h)$$

$$f(x-h) = f(x)-f'(x)h+f''(x)\frac{h^2}{2}-f'''(c_2)\frac{h^3}{3!}, \quad \text{where } c_2 \in (x-h,\ x)$$

Plugging these expansions into the centered finite difference above, we obtain:

$$\frac{f(x+h)-f(x-h)}{2h} = \frac{\left(\cancel{f(x)}+f'(x)h+\cancel{f''(x)\frac{h^2}{2}}+f'''(c_1)\frac{h^3}{3!}\right)-\left(\cancel{f(x)}-f'(x)h+\cancel{f''(x)\frac{h^2}{2}}-f'''(c_2)\frac{h^3}{3!}\right)}{2h}$$

$$= \frac{2f'(x)h+\frac{h^3}{3!}\left[f'''(c_1)+f'''(c_2)\right]}{2h} = f'(x)+\underbrace{\frac{h^2}{12}\left[f'''(c_1)+f'''(c_2)\right]}_{\text{ERROR}}$$

By generalized intermediate value theorem, the sum of two different values of any continuous function is twice their average value achieved somewhere within the interval connecting these two values:

$$\text{Error} = \frac{h^2}{12}\left[f'''(c_1)+f'''(c_2)\right] = \frac{h^2}{12}\cdot 2f'''(c) = \boxed{\frac{f'''(c)h^2}{6}} \quad \text{where } c \in (c_1,\ c_2) \subset (x-h, x+h)$$

Thus, this symmetric, centered difference is much more accurate than the forward or backward finite differences above, achieving 2nd order accuracy.

EXAMPLE. To understand these expressions better, it is useful to see how they work by applying them to simple functions. For instance, let's apply the centered difference expression above to the function $f(x) = x^3$:

$$\frac{f(x+h)-f(x-h)}{2h} = \frac{(x+h)^3-(x-h)^3}{2h} = \frac{\left(\cancel{x^3}+3x^2h+\cancel{3xh^2}+h^3\right)-\left(\cancel{x^3}-3x^2h+\cancel{3xh^2}-h^3\right)}{2h} = \frac{6x^2h+2h^3}{2h} = \underbrace{3x^2}_{f'(x)}+\underbrace{h^2}_{\text{ERROR}}$$

Let's check that this agrees with the error in the general expression: $f''' = (x^3)''' = 6$, therefore $\frac{f'''(c)h^2}{6} = \frac{6h^2}{6} = h^2$ ☺

Centered Finite Difference Approximation of 2nd Order Derivative

We can find similar expressions for any higher-order derivatives using the same method. For instance, the following is a widely used 3-point finite difference approximation of 2nd derivative:

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

To see that it indeed approximates $f''(x)$, and to determine its error, we can use the same expansions that we used for the centered difference approximation of $f'(x)$ on the previous page, but increasing the expansion order:

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f'''(x)\frac{h^3}{3!} + f^{(4)}(c_1)\frac{h^4}{4!}, \quad \text{where } c_1 \in (x,\ x+h)$$

$$f(x-h) = f(x) - f'(x)h + f''(x)\frac{h^2}{2} - f'''(x)\frac{h^3}{3!} + f^{(4)}(c_2)\frac{h^4}{4!}, \quad \text{where } c_2 \in (x-h,\ x)$$

Plugging these expansions into the centered finite difference above, we obtain:

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

$$= \frac{\left(\cancel{f(x)} + \cancel{f'(x)h} + f''(x)\frac{h^2}{2} + \cancel{f'''(x)\frac{h^3}{3!}} + f^{(4)}(c_1)\frac{h^4}{4!}\right) - \cancel{2f(x)} + \left(\cancel{f(x)} - \cancel{f'(x)h} + f''(x)\frac{h^2}{2} - \cancel{f'''(x)\frac{h^3}{3!}} + f^{(4)}(c_2)\frac{h^4}{4!}\right)}{h^2}$$

$$= \frac{\cancel{2}f''(x)\frac{h^2}{\cancel{2}} + \left[f^{(4)}(c_1) + f^{(4)}(c_2)\right]\frac{h^4}{4!}}{h^2}$$

$$= f''(x) + \underbrace{\frac{h^2}{4!}\left[f^{(4)}(c_1) + f^{(4)}(c_2)\right]}_{\text{ERROR}} = f''(x) + \underbrace{\frac{h^2}{4!}2f^{(4)}(c)}_{\text{ERROR}} = \boxed{f''(x) + \underbrace{\frac{h^2}{12}f^{(4)}(c)}_{\text{ERROR}}} \quad \text{where } c \in (x-h,\ x+h)$$

Centered Finite Difference Approximation of 2nd Order Derivative: Alternative Derivation

It is useful to obtain this approximation of 2nd derivative considered above as a repeated application of centered difference of 1st derivative.

Consider the interval $(x - h, x)$. We learned that $f'(x)$ in the middle of this interval is given by:

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

Equivalently, considering the middle of the interval $(x, x + h)$, we obtain:

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

Now we can approximate 2nd derivative as the centered difference between these two lower-order centered differences for the 1st derivative, noting that the distance between the two mid-points that we consider equals *h*:

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

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

The error of this expression we already computed in the previous subsection.

Obtaining finite difference derivative approximations using arbitrary set of points

Problem: Find the finite difference approximation of $\boldsymbol{f''(x)}$ using values $\boldsymbol{f(x-2h)}$, $\boldsymbol{f(x)}$, and $\boldsymbol{f(x+h)}$.

This is essentially a linear algebra problem: we have to find constants (a, b, c) so that

$$f''(x) \approx a f(x-2h) + b f(x) + c f(x+h)$$

Taylor expanding around *x* gives

$$f''(x) \approx a\left[f(x) - f'(x)(2h) + f''(x)\frac{(2h)^2}{2} - f'''(x)\frac{(2h)^3}{3!} + \ldots \right] + bf(x) + c\left[f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f'''(x)\frac{h^3}{3!} + \ldots \right]$$

Now, terms proportional to $f(x)$ and $f'(x)$ should vanish; factors multiplying $f''(x)$ should add to one, and the remaining terms form the error. Let's take this into account, collecting factors of $f(x)$ and its derivatives:

$$\begin{cases} f(x): & a+b+c=0 \\ f'(x): & (-2a+c)h=0 \\ f''(x): & (4a+c)\dfrac{h^2}{2}=1 \\ Error \approx f'''(x)(-8a+c)\dfrac{h^3}{3!} \end{cases}$$

The first 3 equations form a simple 3x3 linear system: $\begin{cases} a+b+c=0 \\ -2a+c=0 \\ 4a+c=\dfrac{2}{h^2} \end{cases}$

We could use linear algebra, but this system is too simple: from the last 2 equations we obtain $\boldsymbol{6a = \frac{2}{h^2}}$, so $\boldsymbol{a = \frac{1}{3h^2}}$. Therefore, $\boldsymbol{c = 2a = \frac{2}{3h^2}}$, and $\boldsymbol{b = -a - c = -\frac{3}{3h^2}}$. Thus, our finite difference is

$$f''(x) \approx \frac{f(x-2h) - 3f(x) + 2f(x+h)}{3h^2}$$

And the error is

$$Error \approx f'''(x)(-8a+c)\frac{h^3}{3!} = f'''(x)\left(-\frac{8}{3h^2} + \frac{2}{3h^2}\right)\frac{h^3}{3!} = \boxed{-f'''(x)\frac{h}{3}}$$

Thus, this non-centered difference is only 1st order accurate.

Note: using the same 3 values, you can find a **2nd order accurate** approximation of **1st derivative**, by solving instead the following system (in fact, we did this in class):

$$\begin{cases} f(x): & a+b+c=0 \\ f'(x): & (-2a+c)h=1 \\ f''(x): & (4a+c)\dfrac{h^2}{2}=0 \\ Error \approx f'''(x)(-8a+c)\dfrac{h^3}{3!} \end{cases}$$

Richardson Extrapolation

Richardson extrapolation is a clever way of combining a numerical approximation of certain accuracy with a less accurate approximation to obtain a result that is more accurate than either of the two approximations! This elegant method can be applied to any numerical computation that has a definite order of accuracy, for example root-finding. Here we will apply it to our finite difference approximation of function derivatives.

Let's consider for instance the centered finite difference for the first derivative considered above:

$$\frac{f(x+h)-f(x-h)}{2h} = f'(x) + \underbrace{\frac{f'''(x)}{6}h^2 + O(h^4)}_{\text{ERROR}}$$

Denoting the finite difference approximation as $F(h)$ and the corresponding exact value of the derivative as $\boldsymbol{Q}$, with the error coefficient denoted $\boldsymbol{K} = \frac{\boldsymbol{f'''(x)}}{\boldsymbol{6}}$, we can write the above as

$$F(h) = Q + Kh^2 + O(h^4)$$

We can then consider the error arising from using a less accurate approximation using twice the step $2h$ instead of h:

$$F(2h) = Q + K(2h)^2 + O(h^4) = Q + 4Kh^2 + O(h^4)$$

Thus, we obtain a simple linear system with 2 unknowns:

$$\begin{cases} F(h) \approx Q + Kh^2 \\ F(2h) \approx Q + 4Kh^2 \end{cases}$$

Considering the linear system above, we can easily eliminate the error using linear combination $4F(h) - F(2h) = 3Q$:

$$\boldsymbol{Q \approx \frac{4F(h) - F(2h)}{3}}$$

Let's now plug in our finite differences into this expression:

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

$$F(2h) = \frac{f(x+2h) - f(x-2h)}{4h}$$

we then obtain:

$$f'(x) \equiv Q \approx \frac{4}{3}F(h) - \frac{1}{3}F(2h) = \frac{1}{3}\left[\frac{4f(x+h) - 4f(x-h)}{2h}\right] - \frac{1}{3}\left[\frac{f(x+2h) - f(x-2h)}{4h}\right]$$

$$= \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}$$

NOTE: we did not, in fact, completely cancel the error, since we neglected terms of order h^4 and higher. We did however rigorously cancel error terms of order h^2, leaving only error terms of order h^4 (the error of a centered difference is a sum of even powers due to its symmetry)

Using Taylor expansion, we find that the error of the above approximation is:

$$Error[Q] = -\frac{[-2^5 + 8 + 8 - 2^5]}{12h} \cdot \frac{f^{(5)}(x)h^5 + O(h^7)}{5!} = -\frac{f^{(5)}(x)}{30}h^4 + O(h^6)$$

This error is two orders of magnitude smaller than the error of the original centered difference approximation that we started with, and is **exact for polynomials up to 4th degree**!