April 19 Math 2335 sec 51 Spring 2016

Section 5.4: Numerical Differentiation

The mathematical models arising in diverse fields often take the form of a *differential equation*. For example, we wish to track some quantity $y = y(t)$ that depends on time, and we have information about the rate at which it changes

$$\frac{dy}{dt} = f(t, y), \quad \text{given} \quad y(0) = y_0.$$

Knowing the value that y takes when $t = 0$, and knowing how y changes, we can approximate its value a some small time in the future, say $t = 0 + \Delta t$.

To do this, we require a means of approximating a derivative $\frac{dy}{dt}$ numerically. (We won't restrict ourselves to first derivatives.)

Numerical Differentiation

Recall that if a function f is differentiable at x, then

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

From this, a reasonable rule for approximating $f'(x)$ is given by

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

for small (nonzero) h.

$D_h f(x)$ is called a **numerical derivative** of $f(x)$ with step size h.

Forward and Backward Difference

For $h > 0$ we have the names:

$$\text{Forward Difference:} \quad D_h f(x) = \frac{f(x+h) - f(x)}{h}$$

$$\text{Backward Difference:} \quad D_h f(x) = \frac{f(x) - f(x-h)}{h}$$

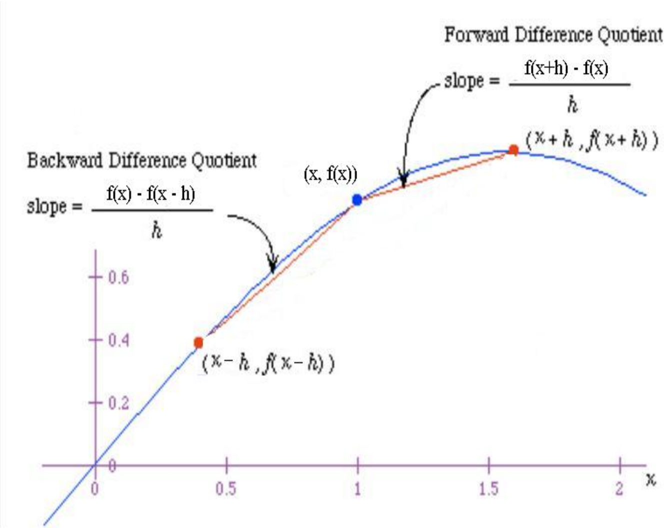

Figure: Forward and Backward Differences Illustrated

Examle

Let $f(x) = x^x$. Compute the forward difference $D_h f(x)$ at $x = 1$ for several values of h. Fill in the table on the following slide. Try to identify $f'(1)$.

Forward Difference $\quad D_h f(x) = \dfrac{f(x+h) - f(x)}{h}$

$$D_h f(1) = \frac{f(1+h) - f(1)}{h} \qquad f(1) = 1^1 = 1$$

$$= \frac{(1+h)^{1+h} - 1}{h}$$

In TI-89 put $y_1 = ((1+x)^{\wedge(1+x)} - 1)/x$ From home screen enter y1(#) hit enter.

$D_h f(1)$ for $f(x) = x^x$

h	$D_h f(1)$
0.10000	1.10534
0.01000	1.01005
0.00100	1.00100
0.00010	1.00010
0.00001	1.00001

True value

$f'(1) = 1$

Example (Euler's Method)

Suppose that an unknown function f satisfies the equation with condition

$$f'(x) = x(f(x))^2, \quad f(0) = 1$$

Use a forward difference approximation to $f'(x)$ to approximate the values of $f(0.1), f(0.2), f(0.3)$, and $f(0.4)$.

Using the forward difference

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

Replace f' w/ $D_h f$

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

Solve for $f(x+h)$

$$f(x+h) - f(x) \approx h\,x\,(f(x))^2 \quad \Rightarrow$$

$$f(x+h) \approx f(x) + h\,x\,(f(x))^2$$

Letting $x=0$ and $h=0.1$

$$f(0.1) \approx f(0) + (0.1)\cdot 0 \cdot (f(0))^2 = 1 + 0 = 1$$

Let $x=0.1$ $h=0.1$ and use $f(0.1)=1$

$$f(0.2) \approx f(0.1) + (0.1)(0.1)(f(0.1))^2 = 1.01$$

$$1 + (0.01)\cdot 1^2$$

Let $x = 0.2$, $h = 0.1$ and $f(0.2) = 1.01$

$$f(0.3) = f(0.2) + (0.1)(0.2)\left(f(0.2)\right)^2 = 1.0304$$

Let $x = 0.3$ $h = 0.1$ $f(0.3) = 1.0304$

$$f(0.4) = f(0.3) + (0.1)(0.3)\left(f(0.3)\right)^2 = 1.06225$$

Example: $\frac{d}{dx}\tan^{-1}(x)$ at $x = 1$

$$D_h f(x) = \frac{\tan^{-1}(1+h) - \tan^{-1}(1)}{h}, \quad \text{exact value:} \quad f'(1) = \frac{1}{2}$$

h	$D_h f(1)$	Err	Ratio
0.100000	0.475831	0.024168	
0.050000	0.487708	0.012291	1.966264
0.025000	0.493802	0.006197	1.983214
0.012500	0.496888	0.003111	1.991634
0.006250	0.498440	0.001559	1.995825
0.003125	0.499219	0.000780	1.997915

The quantity "Ratio" is the ratio $\dfrac{\text{Err}(h)}{\text{Err}\left(\frac{h}{2}\right)}$.

Error for These Rules

The ratios in this example illustrate that cutting the step size in half seems to cut the error in half. That is

$$\mathrm{Err} \propto h.$$

Defintion: If the error for a particular rule satisfies

$$\mathrm{Err} = Ch^p, \quad \text{for some constants } C \text{ and } p,$$

we will say that the rule is of **order** p.

We expect that the forward and backward difference are order 1.

Error for Forward & Backward Difference

Use

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(c) \quad \text{(for some } c \text{ between } x \text{ and } x+h\text{)}$$

to show that Err $\propto h$.

Note $$f(x+h) - f(x) = h f'(x) + \frac{1}{2} h^2 f''(c)$$

$$\frac{f(x+h) - f(x)}{h} = \frac{h f'(x) + \frac{1}{2} h^2 f''(c)}{h}$$

$$\frac{f(x+h) - f(x)}{h} = f'(x) + \frac{1}{2} h f''(c)$$

$$D_h f(x) = f'(x) + \frac{1}{2} h f''(c)$$

$$f'(x) - D_h f(x) = -\frac{1}{2} h f''(c)$$

$$\mathrm{Err}\left(D_h f(x)\right) = Ch \qquad \text{where } C = \frac{-1}{2} f''(c)$$

The same approach for backward difference starts w/

$$f(x-h) = f(x) - h f'(x) + \frac{1}{2} h^2 f''(c)$$ for some c between x and $x-h$

Central Difference Formula

An alternative to estimating $f'(x)$ is to consider both points

$$(x+h, f(x+h)), \quad \text{and} \quad (x-h, f(x-h)).$$

This gives the **central difference formula**

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

Central Difference Formula for $f'(x)$

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

Find the average of the forward and backward differences.

Forward $\quad D_h f(x) = \dfrac{f(x+h) - f(x)}{h}$

Backward $\quad D_h f(x) = \dfrac{f(x) - f(x-h)}{h}$

avg. $\quad \dfrac{\dfrac{f(x+h)-f(x)}{h} + \dfrac{f(x)-f(x-h)}{h}}{2} = \dfrac{f(x+h) - f(x) + f(x) - f(x-h)}{2h}$

= Central Difference.

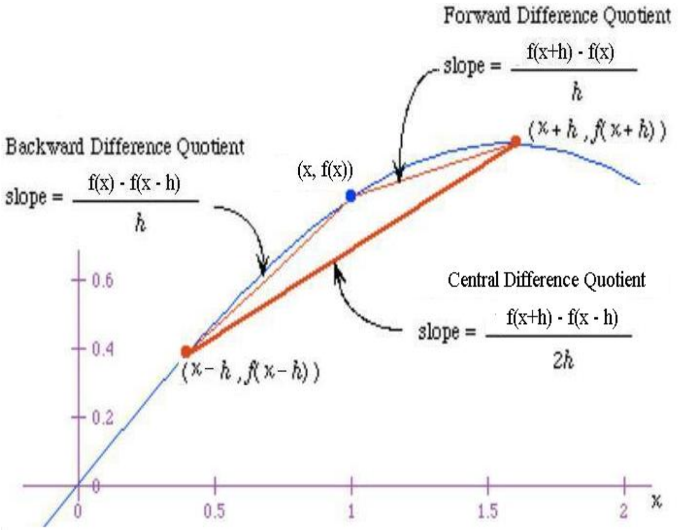

Figure: Forwards, Backward, and Central Difference Quotients

Example: $\frac{d}{dx}\tan^{-1}(x)$ at $x = 1$

$$D_h f(x) = \frac{\tan^{-1}(1+h) - \tan^{-1}(1-h)}{2h}, \quad \text{exact value:} \quad f'(1) = \frac{1}{2}$$

h	$D_h f(1)$	Err	Ratio
0.100000	0.500830	−0.000830	
0.050000	0.500208	−0.000208	3.990953
0.025000	0.500052	−0.000052	3.997747
0.012500	0.500013	−0.000013	3.999437
0.006250	0.500003	−0.000003	3.999859
0.003125	0.500000	−0.000000	3.999964

We notice that cutting the step size by a factor of 2 reduces the error by about a factor of 4.

Error in Central Difference

Use the Taylor expansions to obtain an expression for the error $f'(x) - D_h f(x)$ for the central difference formula:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(c_1)$$

Subtract second line from first

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(c_2)$$

$$f(x+h) - f(x-h) = 2h\, f'(x) + \frac{h^3}{6}\left(f'''(c_1) + f'''(c_2) \right)$$

The numbers c_1 and c_2 are some numbers between $x - h$ and $x + h$.

$$\frac{f(x+h)-f(x-h)}{2h} = \frac{2h\,f'(x) + \frac{h^3}{6}\left(f'''(c_1)+f'''(c_2)\right)}{2h}$$

$$D_h f(x) = f'(x) + \frac{h^2}{12}\left(f'''(c_1)+f'''(c_2)\right)$$

$$f'(x) - D_h f(x) = \frac{-h^2}{12}\left(f'''(c_1)+f'''(c_2)\right)$$

$$\mathrm{Err}\left(D_h f(x)\right) = C h^2$$

where $C = \frac{-1}{12}\left(f'''(c_1)+f'''(c_2)\right)$

The central difference formula is order 2.

Higher Order Derivatives and Notation

If we have a scheme to approximate the first derivative $f'(x)$, we're using the notation

$$f'(x) \approx D_h f(x), \quad \text{for step size } h.$$

If we want to approximate $f''(x)$, we'll use a superscript with parentheses

$$f''(x) \approx D_h^{(2)} f(x) \quad \text{for step size } h.$$

For an n^{th} derivative, we write

$$f^{(n)}(x) \approx D_h^{(n)} f(x) \quad \text{for step size } h.$$

The Method Undetermined Coefficients

The use of Taylor series expansions can help us to define new numerical differentiation rules as well as analyze the error for a rule.

The Method of Undetermined Coefficients involves setting up a **form** the rule is to take, and then finding out what coefficients are needed.

The Method Undetermined Coefficients an Example

Suppose we wish to approximate a second derivative

$$f''(x) \approx D_h^{(2)} f(x).$$

We begin by deciding how many points to use, such as x, $x+h$, and $x-h$ (or $x+2h$ etc.), then write out a general form.

$$D_h^{(2)} f(x) = Af(x+h) + Bf(x) + Cf(x-h)$$

Then, we determine the values of the unknown coefficients A, B, and C using Taylor series.

Taylor Series

It is helpful to remember that if a function f is at least $n+1$ continuously differentiable on an interval, then for x and $x+\Delta x$ in this interval

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{(\Delta x)^2}{2!} f''(x) + \cdots +$$

$$+ \frac{(\Delta x)^{n-1}}{(n-1)!} f^{(n-1)}(x) + \frac{(\Delta x)^n}{n!} f^{(n)}(c)$$

for some c between x and $x+\Delta x$.

The Method Undetermined Coefficients an Example

$$D_h^{(2)} f(x) = Af(x+h) + Bf(x) + Cf(x-h)$$

Use Taylor series to obtain three equations in the three unknowns, and solve for A, B, and C.

$$Af(x+h) = Af(x) + Ahf'(x) + A\frac{h^2}{2}f''(x) + A\frac{h^3}{3!}f'''(x) + A\frac{h^4}{4!}f^{(4)}(x) + \ldots$$

$$Bf(x) = Bf(x)$$

$$Cf(x-h) = Cf(x) - Chf'(x) + C\frac{h^2}{2}f''(x) - C\frac{h^3}{3!}f'''(x) + C\frac{h^4}{4!}f^{(4)}(x) + \ldots$$

add the three lines

$$Af(x+h) + Bf(x) + Cf(x-h) =$$

$$(A+B+C)f(x) + (Ah - Ch)f'(x) + \left(A\frac{h^2}{2} + C\frac{h^2}{2}\right)f''(x) + \left(A\frac{h^3}{6} - C\frac{h^3}{6}\right)f'''(x)$$

$$+ \cdots$$

We want this to equal $f''(x)$ with some hopefully small error.

We'll set the coefficients of $f(x)$ and $f'(x)$ to zero and that of $f''(x)$ to 1.

$$A + B + C = 0$$

$$Ah \qquad - Ch = 0$$

$$A\frac{h^2}{2} + C\frac{h^2}{2} = 1$$

From $Ah - Ch = 0$ $\quad (A - C)h = 0 \Rightarrow A = C$

From $\frac{h^2}{2}A + \frac{h^2}{2}C = 1$ and $A = C$

$$\frac{h^2}{2}A + \frac{h^2}{2}A = 1 \Rightarrow h^2 A = 1 \Rightarrow A = \frac{1}{h^2}$$

So $\quad C = \frac{1}{h^2}$

$$B = -C - A = \frac{-1}{h^2} - \frac{1}{h^2} = \frac{-2}{h^2}$$

Our formula $Af(x+h) + Bf(x) + Cf(x-h)$ is

$$D_h^{(2)} f(x) = \frac{1}{h^2} f(x+h) - \frac{2}{h^2} f(x) + \frac{1}{h^2} f(x-h)$$

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