Day 10: Numeric Differentiation and Integration

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1 Differentiation

To compute the derivative $f'(x)$, we can appeal to the definition

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

This gives us our first rule, 5.4

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

A better approximation is 5.7,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12} f'''(c)$$

A good estimate of the second derivative is

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} + \frac{h^2}{12} f^{(iv)}(c)$$

The accuracy increases as we decrease h, but there is a point of diminishing returns.

2 Method of Undetermined Coefficients

We will derive the approximation (5.7) above using the method of Undetermined Coefficients. We decide to measure $f(x)$ at three points: x, $x+h$ and $x-h$. This is called a **Central Difference** equation, as we are evaluating at x in the center of the trio of points.

We wish to have a formula of the form

$$f'(x_0) \approx Af(x_0 - h) + Bf(x_0) + Cf(x_0 + h)$$

and we wish to find A, B, and C. We would like the formula to be accurate on constant functions, on lines, and on quadratic functions. While we could use a general form of each equation, it is usually enough to try it on representatives. Here we will use $f_1(x) = 1$, $f_2(x) = (x - x_0)$ and $f_3(x) = (x - x_0)^2$

Plug these three functions into the equation above, evaluate at x_0, and compute the derivative for the left hand side. The three function give the following three equations:

$$0 = A + B + C$$

$$1 = A \times (-h) + B \times 0 + C \times h = h(C - A)$$

$$0 = A \times h^2 + B \times 0 + C \times h^2 = h^2(A + C)$$

The last equation tells us that $A = -C$.

When we insert $A = -C$ into the first equation, we see that $B = 0$.

The last two equations tell us that $C = \frac{1}{2h}$. We can put this all together to get

$$f'(x) \approx -\frac{1}{2h}f(x - h) + 0 \times f(x) + \frac{1}{2h}f(x + h) = \frac{f(x + h) - f(x - h)}{2h}$$

We will apply this technique to find Integration formulas as well.

3 Integration

Each of the equations below includes a formula with an error term. The greater the degree of the error term, the better for $h < 1$.

The Trapezoid Rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12}f''(c)$$

Simpson's Rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{3}(f(x_0) + 4f(\frac{x_1 - x_0}{2}) + f(x_1)) - \frac{h^5}{90}f^{(iv)}(c)$$

Midpoint Rule

$$\int_{x_0}^{x_1} f(x)dx = 2hf(\frac{x_1 - x_0}{2}) - \frac{h^3}{3}f''(c)$$

Romberg Integration, based on Richardson Extrapolation.

```
% Program 5.1 Romberg integration
% Computes approximation to definite integral
% Inputs: Matlab inline function specifying integrand f,
%    a,b integration interval, n=number of rows
% Output: Romberg tableau r
% Timothy Sauer
function r=romberg(f,a,b,n)
h=(b-a)./(2.^(0:n-1));
r(1,1)=(b-a)*(f(a)+f(b))/2;
for j=2:n
    subtotal = 0;
    for i=1:2^(j-2)
        subtotal = subtotal + f(a+(2*i-1)*h(j));
    end
    r(j,1) = r(j-1,1)/2+h(j)*subtotal;
    for k=2:j
        r(j,k) = (4^(k-1)*r(j,k-1)-r(j-1,k-1))/(4^(k-1)-1);
    end
end
```

```
   2.000000000000000
   2.732050807568877   2.976067743425169
   2.995709068102441   3.083595154946962   3.090763649048415
   3.089819144357174   3.121189169775418   3.123695437430648   3.124218164230366
```