

Problem Corner: Interesting Numerical Differentiation Tidbits

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Finite differences can be used to approximate values of the derivative of a differentiable function $f(x)$. Since we know that

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

we can approximate $f'(x)$ using suitably chosen values of h . Throughout this problem we will assume that $h > 0$. We naturally expect the errors in our approximations to approach 0 as $h \rightarrow 0$. Here are the perhaps surprising results we obtain for the function $f(x) = \sin(x)$ when $x = 1$ (obtained using the Maple CAS with Digits = 16).

h	Error at x = 1
1e-1	0.422e-2
1e-3	0.421e-5
1e-5	0.412e-7
1e-7	0.587e-8
1e-9	0.231e-5
1e-11	0.302e-3
1e-13	0.403e-1

1. Use your favorite calculator to do these calculations; you will obtain results exhibiting similar behavior.
2. Argue that for a given value of x the magnitude of the actual error in our approximations has the form

$$E(h) = Ah + \frac{B}{h}$$

where A and B are positive constants. The first term in $E(h)$ is the mathematical error and the second term is the roundoff error incurred due to the fact that we are not using exact arithmetic. Argue that $A \sim |(f''(x)/2)|$ and $B \sim \sqrt{10^{-m}}$ where m is the number of digits of accuracy we are using (16 in our example).

3. Find the minimum value for $E(h)$ and the corresponding value of h . Prove that we can only hope to obtain an error that is $O(\sqrt{10^{-m}})$, that is, we can obtain “half-precision” accuracy. ($y = O(x)$ means there is a constant α for which $|y(x)| \leq \alpha|x|$.)

4. For $h_1 > h_2 > \dots > h_n > 0$ suppose the corresponding errors in our approximations are $e_i, i = 1, \dots, n$. Find the values of A and B that minimize the quantity

$$\sum_{i=1}^n (E(h_i) - e_i)^2.$$

When you calculate the necessary partial derivatives, show that you obtain two linear equations that can be solved for A and B . (You have just performed a linear least squares solution to obtain the “best fit” for the errors $e_i, i = 1, \dots, n$.) Prove that your system of linear equations is nonsingular.

5. You may wish to use the attached Maple worksheet NDProb.mws to explore the various aspects of this problem.