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Problem Corner:
Interesting Numerical Differentiation Tidbits

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Recall from the last Problem Corner that finite differences can be used to approximate values of the derivative of a differentiable function $f(x)$. Using the forward difference approximation

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

we can approximate $f'(x)$ using suitably chosen values of h.

We saw that the magnitude of the actual error in our approximations has the form

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

where A and B are positive constants. We further saw that A and B can be estimated using linear regression.

When two point centered differences are used to approximate $f'(x)$ or three point centered differences are used to approximate $f''(x)$, we obtain similar expressions

$$E(h) = A\,h^2 + \frac{B}{h}$$

since the truncation errors for these methods are second order accurate. For either of these two methods, A and B can be estimated using linear regression. Refer to the attached Maple worksheets fdiv2.mws and fdiv3.mws for details. Proving that we are led to a nonsingular system of linear equations is more difficult for these methods.

More generally, suppose we wish to fit a set of data with a fit of the form

$$E(x) = A\,f(x) + B\,g(x).$$

This form obviously encompasses each of the three finite difference error expressions. Suppose the data in question is $(x_i, y_i)\,, i = 1, ..., n$ and we wish to approximate A and B by minimizing the sum of squares

$$r(A,B) = \sum_{i=1}^{n} \left(A\,f\left(x_i\right) + B\,g\left(x_i\right) - y_i\right)^2.$$

As before calculate the partials of $r(x)$ with respect to A and B and equate them to 0 to obtain a system of linear equations. Find a simple condition that characterizes the sets of data for which this system of equations is nonsingular and show that it holds for each of the three finite difference methods.