Numerical Analysis

Math 370 MWF 2:30-3:25
Spring 1997 201 Fowler

(03.26.97) Numerical Differentiation Continued

3-point Difference Formulae

Instead of using 2 function values x_0 and $x_1 = x_0 + h$, it is quite common to use THREE. That is, the function is evaluated at x_0, x_1 and x_2 and we use these to come up with an approximation to f'. We will use Lagrange polynomial interpolation for $f(x)$ along with the error term in order to try and approximate the derivative function $f'(x)$

Write down $L_0'(x), L_1'(x)$ and $L_2'(x)$ below:

Write down $e'(x)$ evaluated at a node (say, x_0)

If $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ the formula for $f'(x_0)$ simplifies to:

If $x_1 = x_0 + h$ and $x_2 = x_0 - h$ formula for $f'(x_0)$ simplifies to:

This second expression is called a **Centered Difference Formula**

(n+1)-point Difference Formulae

In general, if one has $n+1$ data points for $f(x)$ at $x_0, x_1, \ldots x_n$ using Lagrange interpolation we can express the function as:

$$f(x) = \sum_{k=0}^{n} f(x_k) L_{n,k}(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n)$$

Differentiating produces...

$$\begin{aligned} f'(x) &= \sum_{k=0}^{n} f(x_k) L'_{n,k}(x) + \frac{d}{dx}\left[\frac{(x-x_0)(x-x_1)\ldots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) \\ &+ \frac{(x-x_0)(x-x_1)\ldots(x-x_n)}{(n+1)!} \frac{d}{dx}[f^{(n+1)}(\xi(x))] \end{aligned}$$

But if this evaluated at x_k then write down an expression for $f'(x_k)$ below:

Taylor Expansions

Another way to compute difference formula which approximate derivatives at a point is to use Taylor Approximations. This is useful because again one gets a sense of how good the approximation is as one is making it.

For example, let's write down the third-order Taylor expansion about x_0 (with error term) for the following expressions:

$f(x_0 + h) =$

$f(x_0 - h) =$

Then subtract these two terms and solve for $f'(x_0)$

This should result in the identical form of the 2nd Order centered difference formula for $f'(x)$ obtained by using a 3-point formula.

Higher Order Derivatives
Another reason why using the Taylor Expansion method is useful is that one can use it to compute difference formulae for higher-order derivatives. All one needs to do is cancel out as many common terms of the expansion as possible.

For example, let's write down the fouth-order Taylor expansion about x_0 (with error term) for the following expressions:
$f(x_0 + h) =$

$f(x_0 - h) =$

Let's combine these in such a way that we can get a formula for $f''(x_0)$

Round-Off Error
Let's consider the first-order forward difference formula for $f'(x_0)$ again.
(Write it down below:)

Example

Consider $f(x) = \exp(x)$. I want each member of the class to come up with an approximation to $f'(1)$ using the forward difference formula with $h = 10^{-k}$ where k is an integer. We will do this in alphabetic order. The first person forms the approximation with $h = 0.1$ and so on. What do you think will happen?

h	$f(1+h)$	$f'(1)$	Error

Does it appear as if there an optimal value of h to use?

Explanation

Consider that whenever you make a function evaluation there is really some round-off error associated with it, so that $f(x) = \tilde{f}(x) + e(x)$. The $\tilde{f}$ is the machine number approximation to the exact f that you are trying to compute and e is the round-off error that the compute produces.

If we look at the forward difference formula we can obtain an expression for the error involved in approximating the derivative due to round-off error, $E(h)$

Let's assume that M is a bound for f'' and that ϵ is a bound on the round-off error. Then we can get an expression for $E(h)$ and we can find out what value of h **minimizes** it.