

Re: Recommendation for numerical differentiation formulas?

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- *From:* spellucci@xx (Peter Spellucci)
 - *Date:* Mon, 17 Jul 2006 13:37:54 +0000 (UTC)
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In article <1153137085.886668.152400@xx>, 1940LaSalle@xxxxxxxx writes:

Peter Spellucci wrote:

In article <1152885890.796128.65800@xx>, 1940LaSalle@xxxxxxxx writes:
>
>Peter Spellucci wrote:

no, flip in a geometric sense right to left. means

$$f'(x(n+1)) = (1/(12*h)) * (-25*f(x(n+1)) + 48*f(x(n)) - 36*f(x(n-1)) + 16*f(x(n-2)) - 3*f(x(n-3)))$$

you need these special one sided formulae only for the first data point (I named it x(0)) and the last one x(n+1) because these are not covered by the 3 point compact scheme. all other derivatives come out from the tridiagonal solve, and you are right: the right hand side is made up from the table and looking at the indices you see: f(x(0)) up to f(x(n+1)) are needed there and give you u(1) up to u(n) which correspond to f'(x(1)) up to f'(x(n))
good luck
peter

In thinking about this scheme, it seems I have a few more questions about the mechanics of it. For the sake of discussion, let's say the data involved have a total of j points. Then the right side of the equation would appear to be a matrix (that is, a vector) with one column and j-1 rows (there are no rows corresponding to x(0) and x(j)). The left side is the tridiagonal matrix we've mentioned before. I may be missing something fundamental here, so please bear with me: when one inverts the matrix on the left and does the appropriate matrix

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multiplication, one gets a solution vector (again, one column with $j-1$ rows)—at least, I believe that's the case. In that solution vector, the first row would yield the value of $u(x(1))$, the second, $u(x(2))$, etc., up to $u(x(j-1))$, correct? (What I know of matrix

yes

algebra/manipulation has been acquired purely as needed; I've never taken a formal course.)

this is a linear system of equations with a tridiagonal matrix and you never invert the matrix, you solve the system by standard Gaussian elimination with amounts in just some j arithmetic operations and hence is extremely cheap.

Also: I'd like to verify that all of the coefficients on the left side have the same sign. Unless I set up the matrices incorrectly—not out of the question—I would expect that the results would all have the same sign if the tabulated function is monotonic with no local maxima or minima within the range of the independent variable.

yes, if your function data are not subject to noise. noise will blow up by a factor $1/h$, hence this may destroy these properties if it is too large

Last but not least: what's the reference for the one-sided formulas? I'd like to see/read more.

Thanks again for your patience: this is very valuable.

the linear system is from

Quarteroni, Alfio; Sacco, Riccardo; Saleri, Fausto
Numerical mathematics. (English)
Texts in Applied Mathematics. 37. New York, NY: Springer.

the one sided formula is from
Schmeisser, Gerhard; Schirmeier, Horst

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Praktische Mathematik. (German)

de Gruyter Lehrbuch. Berlin–New York: Walter de Gruyter

but there should be other sources containing it it is obtained
simply by Taylor's formula for $f(x+k*h)$ $k=0,1,2,3$
resp. $f(x-k*h)$ and combining these values linearly such that the $f'(x)$
obtains with error term h^4

hth

peter

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