Mathematics 373 Workshop 5 Solutions

Extrapolation

Fall 2003

Problem 1

We give a rigorous derivation of a numerical differentiation formula with error term.

1a Statement

Expand the **divided difference** $f[x, x, y, z]$ to get its value in terms of x, y, z, $f(x)$, $f(y)$, $f(z)$, and $f'(x)$.

1a Solution

$$
\begin{aligned}
f[x,x,y,z] &= \frac{f[x,y,z] - f[x,x,y]}{z-x} \\
&= \frac{f[x,z,y] - f[x,x,y]}{z-x} \\
&= \frac{\big(f[z,y] - f[x,z]\big) - \big(f[x,y] - f[x,x]\big)}{(z-x)(y-x)} \\
&= \frac{f[z,y] - f[x,z] - f[x,y] + f[x,x]}{(z-x)(y-x)} \\
&= \frac{\frac{f(z)-f(y)}{z-y} - \frac{f(z)-f(x)}{z-x} - \frac{f(y)-f(x)}{y-x} + f'(x)}{(z-x)(y-x)} \\
&= \frac{(y+z-2x)\,f(x)}{(z-x)^2(y-x)^2} + \frac{f(y)}{(y-z)(y-x)^2} + \frac{f(z)}{(z-y)(z-x)^2} + \frac{f'(x)}{(z-x)(y-x)}
\end{aligned}
$$

It should also be noted that

$$
\begin{aligned}
f[x,x,y,z] &= \frac{\partial}{\partial x} f[x,y,z] \\
&= \frac{\partial}{\partial x} \frac{f[x,y] - f[y,z]}{x-z} \\
&= \frac{(x-z)\,f[x,x,y] - \big(f[x,y] - f[y,z]\big)}{(x-z)^2} \\
&= \frac{(x-z)\,\frac{f[x,y]-f[x,x]}{y-x} - \big(f[x,y] - f[y,z]\big)}{(x-z)^2} \\
&= f[x,y]\frac{(x-z)-(y-x)}{(x-z)^2(y-x)} + \frac{f[y,z]}{(x-z)^2} - \frac{f[x,x]}{(y-x)(x-z)}
\end{aligned}
$$

This will simplify to the same expression when fully expanded. The second calculation is a rigorous version of the suggestion in the textbook that one could differentiate an interpolation formula including its error term. This looks suspect if the error term is expressed in terms of $\xi(x)$ which is not guaranteed to be smooth, but **is** possible if the error term is expressed as a divided difference. Also note that identifying $f[x, x, y, z]$

with the partial derivative with respect to x requires that y and z be independent of x. Although the desired formula uses points in that keep a fixed distance from x, the proof requires that x move relative to fixed locations of y and z in the description of $f'(x)$.

1b Statement

Solve the equation in (a) for $f'(x)$.

1b Solution

Rearranging the terms from the end of the first calculation in (1a):

$$\frac{f'(x)}{(z-x)(y-x)} = \frac{(2x-y-z)f(x)}{(z-x)^2(y-x)^2} - \frac{f(y)}{(y-z)(y-x)^2} - \frac{f(z)}{(z-y)(z-x)^2} - f[x,x,y,z]$$

$$f'(x) = f(x)\frac{(2x-y-z)}{(z-x)(y-x)} - f(y)\frac{z-x}{(y-z)(y-x)} - f(z)\frac{y-x}{(z-y)(z-x)} - f[x,x,y,z](z-x)(y-x)$$

Note that this result is **symmetric** in y and z, i.e., it is unchanged if these two variables are interchanged.

1c Statement

The **mean value theorem** (in the form of a **generalized Rolle's theorem**) implies that $f[x,x,y,z] = f'''(\xi)/6$ for some ξ in an interval x, y and z. Use this to get a general **three point formula** for $f'(x)$ that includes all special cases described in the text.

1c Solution

Making the indicated substitution in the result of (1b) gives

$$f'(x) = f(x)\frac{(2x-y-z)}{(z-x)(y-x)} - f(y)\frac{z-x}{(y-z)(y-x)} - f(z)\frac{y-x}{(z-y)(z-x)} - (z-x)(y-x)\frac{f'''(\xi)}{6}$$

Note that the sum of the coefficients of the $f(x)$, $f(y)$ and $f(z)$ is zero because these arose from expanding first order divided differences.

The special cases mentioned in the text are:
(1) $y = x+h$, $z = x-h$, where $2x-y-z=0$, so

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} + h^2\frac{f'''(\xi)}{6}$$

and
(2) $y = x+h$, $z = x+2h$ which gives

$$\begin{aligned} f'(x) &= -f(x)\frac{3}{2h} + f(x+h)\frac{2}{h} - f(x+2h)\frac{1}{2h} - h^2\frac{f'''(\xi)}{3} \\ &= \frac{4f(x+h)-3f(x)-f(x+2h)}{2h} - h^2\frac{f'''(\xi)}{3} \end{aligned}$$

The three point formula containing x, $x-h$ and $x-2h$ can be obtained from this by replacing h by $-h$.

These are typical of the use of the formula. All differences between two of x, y, and z will be small, and these values will be comparable. A ratio of a linear expression to a quadratic expression will introduce a numerical coefficient depending on the configuration of the three points divided by a **measure of size** denoted by h. When the points are close, the **truncation error**, which is proportional to h^2, is small, but dividing by h amplifies **roundoff error**. The combination of function values that will be divided by h has coefficients that sum to zero. This eliminates any contribution of the size of the function at the base point but numbers are entered at that scale, so the cancellation that leaves a result whose size is comparable to h causes a loss of accuracy. The best choice of size is one for which the two errors are roughly equal.

Problem 2

Specializing the formula of Problem 1 to the case where $y = x + h$ and $z = x + 2h$ gives

$$f'(x) = \frac{2}{h} f(x+h) - \frac{1}{2h} f(x+2h) - \frac{3}{2h} f(x) + 2h^2 f[x, x, x+h, x+2h], \tag{A}$$

which leads to the formula in the textbook by identifying the **third order** divided difference with $1/6$ of the value of the third derivative *somewhere*.

2a Statement

Replace h by $h/2$ in (A) to get an expression for $f'(x)$ in terms of $f(x)$, $f(x+h/2)$, and $f(x+h)$,

2a Solution

$$f'(x) = \frac{4}{h} f(x + \frac{h}{2}) - \frac{1}{h} f(x+h) - \frac{3}{h} f(x) + \frac{h^2}{2} f[x, x, x + \frac{h}{2}, x+h].$$

2b Statement

Scale the two formulas you have so that the divided difference error terms have the same coefficient and subtract.

2b Solution

This can be accomplished by copying (A) unchanged and multiplying the answer to (2a) by 4. Since both have $f'(x)$ on the left side, subtracting (A) from the modified answer to (2a) yields

$$\begin{aligned} 3 f'(x) = & \frac{16}{h} f(x + \frac{h}{2}) - \frac{6}{h} f(x+h) + \frac{1}{2h} f(x+2h) - \frac{21}{2h} f(x) + \\ & + 2h^2 \big(f[x, x, x + \frac{h}{2}, x+h] - f[x, x, x+h, x+2h] \big) \end{aligned}$$

2c Statement

The difference of divided differences in the result of (b) can be written as a multiple of a divided difference of higher order. Do this. Then write this divided difference as a value of a derivative *somewhere*.

2c Solution

The difference of divided differences is $-3/2\, f[x, x, x + \frac{h}{2}, x+h, x+2h]h$. Dividing by 3 then gives

$$f'(x) = \frac{32 f(x + \frac{h}{2}) - 12 f(x+h) + f(x+2h) - 21 f(x)}{6h} - h^3 f[x, x, x + \frac{h}{2}, x+h, x+2h]$$

A simple way to check this formula is to apply it to the special cases $f(x) = x^k$ for $k = 0, 1, 2, 3, 4$.

The error term can be written as $-h^3 f^{(4)}(\xi)/24$ by applying the mean value theorem. A benefit of extrapolation is that the error term is a single divided difference, so that the application of the mean value theorem expresses it in terms of a higher order derivative at a single unknown point ξ.

End of workshop 5