Problem Corner:
Interesting Numerical Differentiation Tidbits

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Solutions and Comments

When we calculate the partials of $r(A,B)$ and equate them to 0, we obtain the linear system

$$\sum_{i=1}^{n}\left(Af_i+Bg_i-y_i\right)f_i=0 \tag{1}$$

$$\sum_{i=1}^{n}\left(Af_i+Bg_i-y_i\right)g_i=0 \tag{2}$$

where $f_i=f\left(x_i\right)$ and $g_i=g\left(x_i\right)$. We rewrite this system as

$$A\sum_{i=1}^{n}f_i^2+B\sum_{i=1}^{n}f_ig_i=\sum_{i=1}^{n}f_iy_i \tag{3}$$

$$A\sum_{i=1}^{n}f_ig_i+B\sum_{i=1}^{n}g_i^2=\sum_{i=1}^{n}g_iy_i. \tag{4}$$

Denote by F and G respectively the vectors with components f_i and g_i and by θ the angle between F and G. The determinant of this system is then $||F||^2\,||G||^2 - (F\cdot G)^2$ which in turn is equal to $||F||^2\,||G||^2 - ||F||^2\,||G||^2\cos^2(\theta)$ or $||F||^2\,||G||^2\sin^2(\theta)$. Assuming neither F nor G is the zero vector we see that the determinant is 0 if and only if F and G are parallel so that they differ by a common scalar multiple.

For the forward difference approximations $F_i=h_i$ and $G_i=\dfrac{1}{h_i}$. Thus, $F_i=h_i^2\,G_i$. Since the h_i are distinct, this shows that G is not a scalar multiple of F so the two vectors are not parallel. For both centered difference approximations, $F_i=h_i^2>$ and $G_i=\dfrac{1}{h_i}$ and we see again that F and G are not parallel. Hence, the corresponding systems of linear equations are nonsingular so that A and B are determined uniquely for each of the three derivative approximations.

For a simple example of singularity, suppose we wish to fit two points (x_1,y_1) and (x_2,y_2) with a function of the form Ax^2+Bx where $x_1\neq x_2$. The determinant of the linear system is $x_1^2x_2^2(x_1-x_2)^2$. The system is singular if, say, $x_1=0$. In this case there are an infinite number of parabolas passing through the two points. Note that $F=<0,x_2^2>$ and $G=<0,x_2>$ are parallel since $F=x_2\,G$. If both x_1 and x_2 are nonzero the system is nonsingular. This is due to the fact that our fit must also pass through the point $(0,0)$ and there is a unique parabola passing through the three points.