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A Wacky Graph of a Simple Looking Function: The Explanation and a Solution

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Abstract: Graphing of a seemingly simple function can sometimes give unexpected wacky results that are due to the finiteness of the underlying floating-point system.

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Last Revision Date: January 19, 2005

We now want to understand the reasons why the graph of the function

$$f(x) = \frac{1 - \cos(x)}{x^2}, \tag{1}$$

has problems when x is small. We need to analyze the behavior of the function in that region. We know that for small x,

$$\cos(x) \approx 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots. \tag{2}$$

and so the numerator appearing in $f(x)$ behaves like

$$1 - \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots\right) = \frac{x^2}{2!} - \frac{x^4}{4!} + \dots.$$

Dividing this by x^2 we see that

$$f(x) \approx \frac{1}{2} - \frac{x^2}{24} + \dots,$$

when x is small. Again we see that the function should be given by $1/2$ near the origin.

The problem has two major sources because in computing $f(x)$ the way implied by Eq. (1) we first compute the cosine term and then we obtain the numerator by subtracting it from 1. First there is rounding error associated with the computation of $\cos(x)$. Then since $\cos(x)$ is almost equal to 1 when x is small, there is catastrophic cancellation when it is being subtracted from 1 in the formula.

A very convincing indication that the interpretation given above is indeed correct can be obtained by computing $f(x)$ where we replace $\cos(x)$ by $1 - \frac{x^2}{2}$. The result is found to be almost indistinguishable from that obtained using the original function for x in the range of interest here.

Next we want to understand why we get such a peculiar result when we compute

$$f_1(x) = \frac{1 - \left(1 - \frac{x^2}{2}\right)}{x^2}, \tag{3}$$

which, after all, is mathematically exactly equal to a half. We start by explaining why Eq. (3) gives a zero when x is less than about 0.1×10^{-7}. Notice that in order to evaluate the function the way it

is expressed in Eq. (1) or (3), the cosine is first computed. It is then subtract off from 1 and the result is then divided by x^2. Although we do not know how MATLAB computes $\cos(x)$, but when x is small, the result for $\cos(x)$ must be the same as if it was computed using Eq. (2) without the quartic term. We see that when $x^2/2 \leq \epsilon_{\text{mach}}/2$ the $\cos(x)$ term is always evaluated to give 1. This value is then subtracted from 1 and so the numerator is always equal to 0. Since x^2 is not 0, the value we get for $f(x)$ is therefore given by 0. This occurs whenever x is less than or equal to $\sqrt{\epsilon_{\text{mach}}} \approx 1.05 \times 10^{-8}$. This agrees with the result from the graph.

Now if x is infinitesimally larger than $\sqrt{\epsilon_{\text{mach}}}$, the $\cos(x)$ term evaluates to $1 - \epsilon_{\text{mach}}$. The numerator gives $1 - (1 - \epsilon_{\text{mach}}) = \epsilon_{\text{mach}}$. The denominator x^2 is also given by ϵ_{mach}, and therefore $f(x)$ evaluates to 1. This agrees exactly with what we see from the graph.

For x increasing from $\sqrt{\epsilon_{\text{mach}}}$ to $\sqrt{3\,\epsilon_{\text{mach}}} \approx 1.8 \times 10^{-8}$, the numerator remains at ϵ_{mach} while the denominator increases from ϵ_{mach} to $3\,\epsilon_{\text{mach}}$. Therefore $f(x)$ decreases from 1 to 1/3. For x slightly larger than $\sqrt{3\,\epsilon_{\text{mach}}}$, the $\cos(x)$ term jumps to the value

$1 - 2\,\epsilon_{\rm mach}$, and so the numerator evaluates to $2\,\epsilon_{\rm mach}$. Therefore $f(x)$ jumps from $1/3$ to $2/3$.

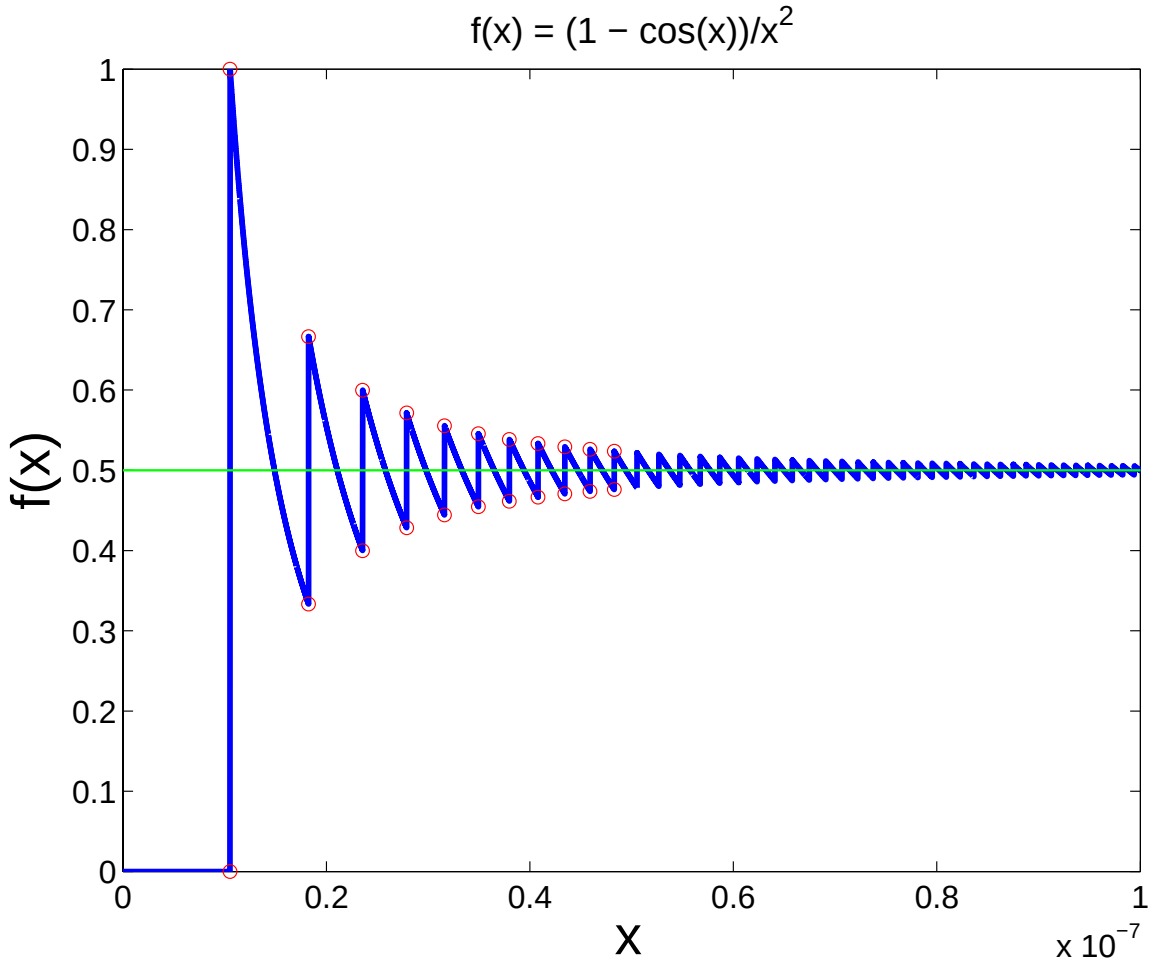
In general, for a real number r very close to and less than 1, discontinuities in $fl(r)$ occur at $r = 1 - (2n+1) * \epsilon_{\rm mach}/2$, where $n = 0, 1, \ldots$. Putting $r = \cos(x) \approx 1 - x^2/2$, we see that $fl(\cos(x))$ has discontinuities at $x_n = \sqrt{(2n+1)\,\epsilon_{\rm mach}}$, and

$$fl(\cos(x_n \mp \delta)) = \begin{cases} 1 - n\,\epsilon_{\rm mach} \\ 1 - (n+1)\,\epsilon_{\rm mach} \end{cases}$$

where δ is an infinitesimal positive quantity. Therefore we have

$$\frac{1-\cos(x_n \mp \delta)}{x_n^2} = \begin{cases} \dfrac{1-(1-n\,\epsilon_{\rm mach})}{(2n+1)\,\epsilon_{\rm mach}} \\ \dfrac{1-[1-(n+1)\,\epsilon_{\rm mach}]}{(2n+1)\,\epsilon_{\rm mach}} \end{cases} = \begin{cases} \dfrac{n}{2n+1} \\ \dfrac{n+1}{2n+1} \end{cases}$$

Therefore when $f(x)$ is computed according to Eq. (1), we find $f(0) = 0$, and as x is increased from 0, $f(x)$ jumps from $n/(2n+1)$ to $(n+1)/(2n+1)$ at each $x = x_n$. We plot these jump-off points as red circles in the following graph. One can see that they coincide


f(x) = (1 − cos(x))/x^2
f(x)
x
x 10^−7
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1

with the discontinuities of the original graph.

Now that we understand the reasons for the numerical problems, we want to see if these problems can be avoided. The most important problem is due to the cancellation of 1 and the $\cos(x)$ term. We want to be able to do that without cancellation.

We recall from trigonometry that

$$\cos 2\theta = \cos^2\theta - \sin^2\theta = (1 - \sin^2\theta) - \sin^2\theta = 1 - 2\sin^2\theta.$$

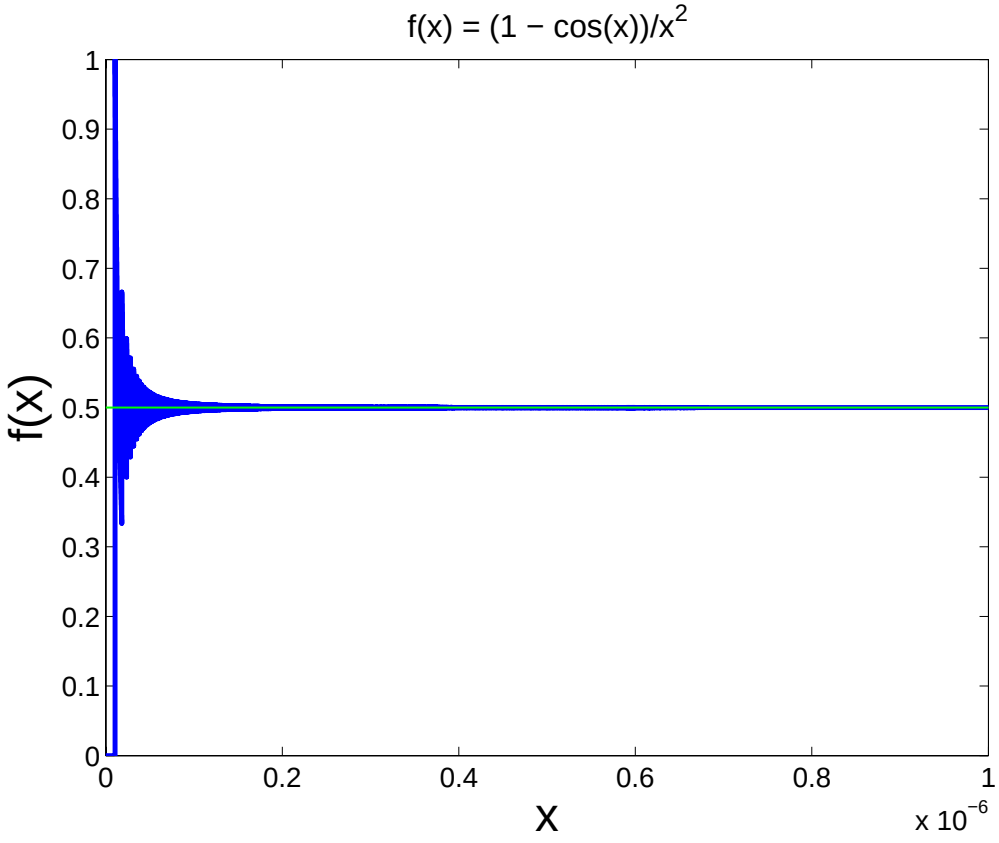
Therefore

$$1 - \cos 2\theta = 2\sin^2\theta.$$

Letting $\theta = x/2$, we see that $f(x)$ can be rewritten as

$$f(x) = 2\frac{\sin^2\frac{x}{2}}{x^2} = \frac{1}{2}\frac{\sin^2\frac{x}{2}}{\left(\frac{x}{2}\right)^2}.$$

This form for $f(x)$ is free from cancellation error. The result of using it to compute $f(x)$ is shown by the green curve in the following graph. Of course in this range the function is essentially given by a half.


f(x) = (1 − cos(x))/x^2
f(x)
x
x 10^−6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0.2
0.4
0.6
0.8