**Problem Set 2: Interpolation, Extrapolation, and Quadrature**
**Computational Physics**
**Physics 480/680**

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**Reading**
**Numerical Recipes chapters 3 and 4, skimming the technical bits**

Exercise 2 parts (d & e) are optional for Physics 480, but (f) is expected for those in both 480 and 680.

2.1 **Methods of interpolation.** (Numerical) ③

We've implemented four different interpolation methods for the function $\sin(x)$ on the interval $(-\pi, \pi)$. On the left, we see the methods using the five points $\pm\pi$, $\pm\pi/2$, and 0; on the right we see the methods using ten points. The graphs show the interpolation, its first derivative, its second derivative, and the error. The four interpolation methods we have implemented are (1) Linear, (2) Polynomial of degree three ($M = 4$), (3) Cubic spline, and (4) Barycentric rational interpolation. *Which set of curves (A, B, C, or D) in Figure 1 corresponds with which method?*

2.2 **Numerical definite integrals.** (Numerical) ③

In this exercise we will integrate the function you graphed in the first, warmup exercise:

$$F(x) = \exp(-6\sin(x)). \tag{1}$$

As discussed in Numerical Recipes, the word *integration* is used both for the operation that is inverse to differentiation, and more generally for finding solutions to differential equations. The old-fashioned term specific to what we are doing in this exercise is *quadrature.*

(a) *Black-box. Using a professionally written black-box integration routine of your choice, integrate $F(x)$ between zero and $\pi$. Compare your answer to the analytic integral*[1] *($\approx$ 0.34542493760937693) by subtracting the analytic form from your numerical result. Read the documentation for your black box routine, and describe the combination of algorithms being used.*

(b) *Trapezoidal rule. Implement the trapezoidal rule with your own routine. Use it to calculate the same integral as in part (a). Calculate the estimated integral $Trap(h)$ for $N+1$ points spaced at $h = \pi/N$, with $N = 1, 2, 4, \ldots, 2^{10}$. Plot the estimated integral versus the spacing $h$. Does it extrapolate smoothly to the true value as $h \to 0$? With what power of $h$ does the error vanish? Replot the data as $Trap(h)$ versus $h^2$. Does the error now vanish linearly?*

[1] $\pi(\text{BesselI}[0, 6] - \text{StruveL}[0, 6])$, according to Mathematica.

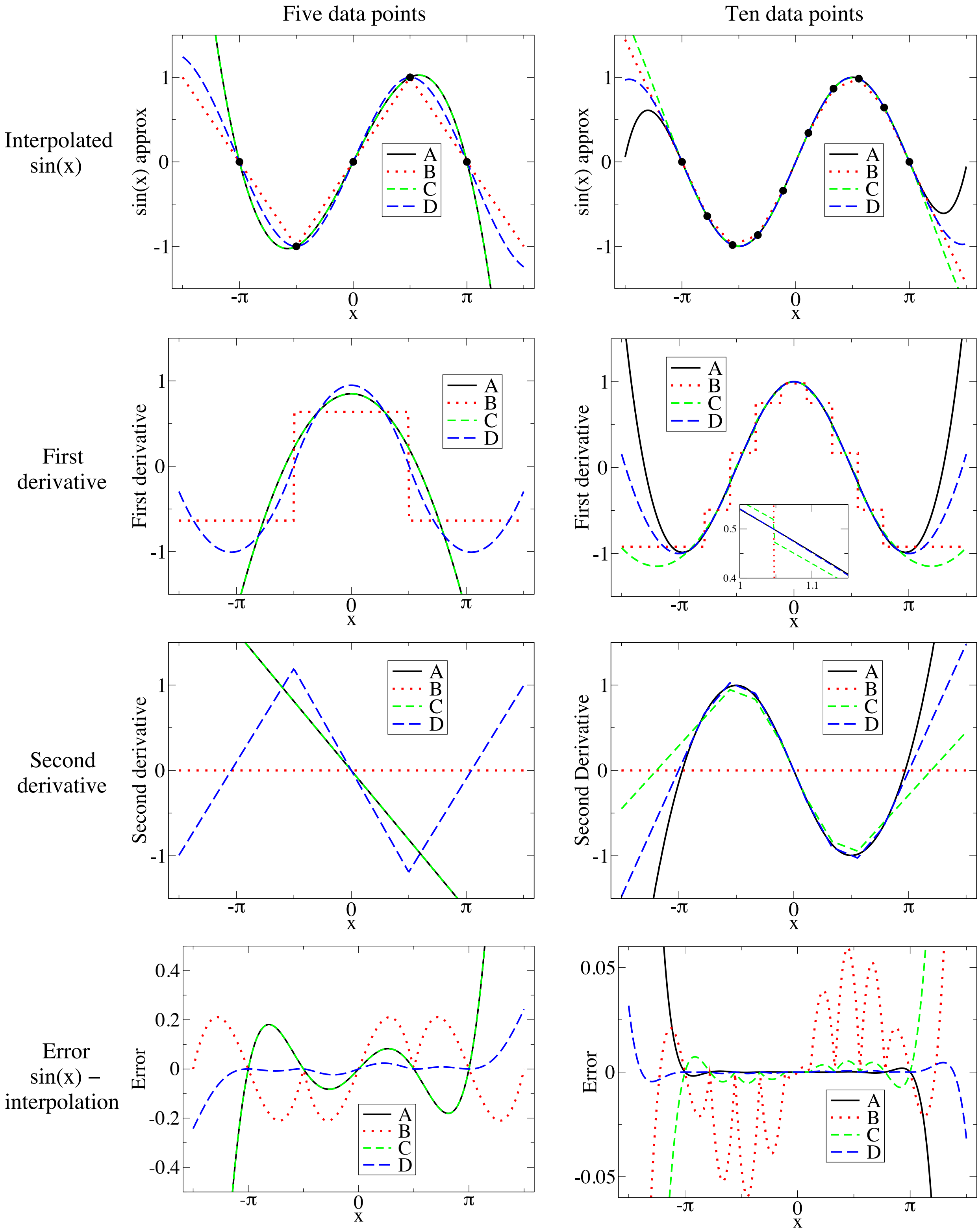


**Fig. 1 Interpolation methods**.

Numerical Recipes tells us that the error is an *even* polynomial in $h$, so we can extrapolate the results of the trapezoidal rule using polynomial interpolation in powers of $h^2$.

(c) *Simpson's rule (paper and pencil). Consider a linear fit (i.e.,* $A+Bh^2$*) to two points at* $2h_0$ *and* $h_0$ *on your* $Trap(h)$ *versus* $h^2$ *plot. Notice that the extrapolation to* $h \to 0$ *is* $A$*, and show that* $A$ *is* $4/3 \, \mathrm{Trap}(h_0) - 1/3 \, \mathrm{Trap}(2h_0)$*. What is the net weight associated with the even points and odd points? Is this Simpson's rule?*

(d) *Romberg integration. Apply* $M$*-point polynomial interpolation (here extrapolation) to the data points* $\{h^2, \mathrm{Trap}(h)\}$ *for* $h = \pi/2, \ldots, \pi/2^M$*, with values of* $M$ *between two and ten.* (Note that the independent variable is $h^2$.) *Make a log-log plot of the absolute value of the error versus* $N = 2^M$*. Does this extrapolation improve convergence?*

(e) *Gaussian Quadrature. Implement Gaussian quadrature with* $N$ *points optimally chosen on the interval* $(0, \pi)$*, with* $N = 1, 2, \ldots 5$*.* (You may find the points and the weights appropriate for integrating functions on the interval $(-1, 1)$ on the course Web site; you will need to rescale them for use on $(0, \pi)$.) *Make a log-log plot of the absolute value of your error as a function of the number of evaluation points* $N$*, along with the corresponding errors from the trapezoidal rule and Romberg integration.*

(f) *Integrals of periodic functions. Apply the trapezoidal rule to integrate* $F(x)$ *from zero to* $2\pi$*, and plot the error on a log plot (log of the absolute value of the error versus* $N$*) as a function of the number of points* $N$ *up to* $N = 20$*.* (The true value should be around 422.44623805153909946.) *Why does it converge so fast?* (Hint: Don't get distracted by the funny alternation of accuracy between even and odd points.)

The location of the Gauss points depend upon the class of functions one is integrating. In part (e), we were using Gauss-Legendre quadrature, appropriate for functions which are analytic at the endpoints of the range of integration. In part (f), we have a function with *periodic boundary conditions.* For functions with periodic boundary conditions, the end-points are no longer special. What corresponds to Gaussian quadrature for periodic functions is just the trapezoidal rule: equally-weighted points at equally spaced intervals.