PHY604: homework 1

2025-09-17

1 *understanding round-off error (no program required)*

Consider a quadratic equation of the form $ax^2 + bx + c = 0$. The two solutions of this are:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}\,.$$

1(a) Explain how this expression may be problematic with respect to roundoff errors if b is much larger than a and c. Recall that such errors often occur when subtracting close large numbers.

If $b^2 \gg 4ac$, then $\sqrt{b^2 - 4ac} \approx b$, in which case the $+$ solution with end up with something asymptotic to $-b + b$ in the numerator, which is prone to roundoff error. □

1(b) Provide an alternative expression that will have smaller errors in the situation you describe in (a).

The $-$ solution is not a risk, so we ignore it for now. For the $+$ solution, we multiply by one:

$$x = \frac{-b + \sqrt{b^2 - 4ac}}{2a}\left(\frac{b + \sqrt{b^2 - 4ac}}{b + \sqrt{b^2 - 4ac}}\right) = \frac{4ac}{2a\left(b + \sqrt{b^2 - 4ac}\right)}\,.$$

2 *round-off error and accurate calculation of the exponential series*

Consider the series expansion for an exponential function:

$$e^x \approx S_n(x) := 1 + \frac{x}{1!} + \frac{x^2}{2!} + \ldots + \frac{x^n}{n!}\,.$$

2(a) Write a program that computes the exponential function using this series expansion for a given number of terms n.

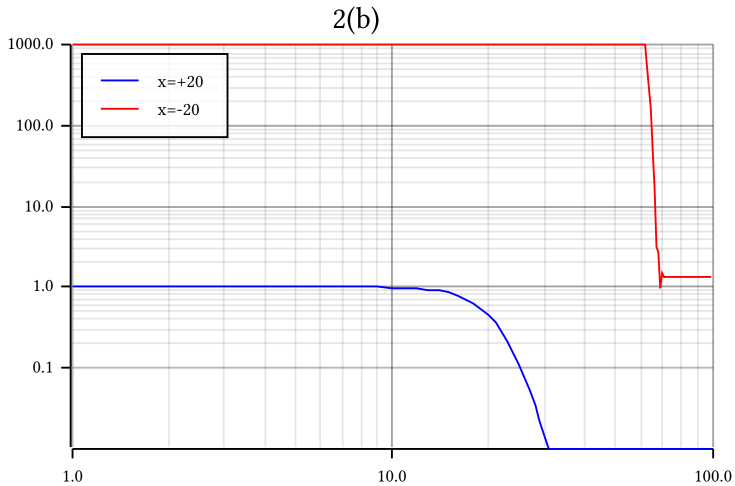
Done. See the `exponential_series` function in `hw01.rs`.

2(b) For n ranging between 0 and 100, compare the result with the exponent calculated with a built-in function or function from a numerical library (e.g. `numpy.exp`) in the following way. Plot the error defined by

$$\epsilon_n := \frac{|e^x - S_n(x)|}{e^x}$$

on a log-log plot for a large positive and large negative exponent (e.g., $x = 20$ and $x = -20$). Describe what you see.

The plot:

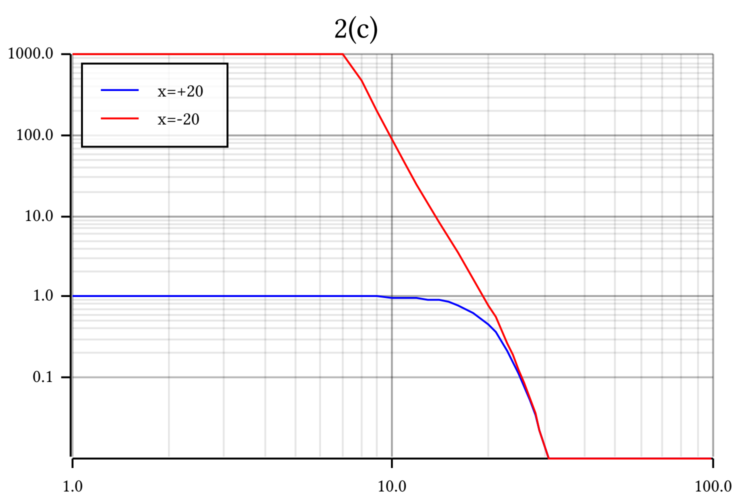


You can see that we actually never get to the correct answer for $x = -20$, because somewhere along the process of going to $n = 100$, `factorial` on a `u64` overflowed.

2(c) Consider the following (trivial) equality: $e^{-x} = \left(e^{-1}\right)^x$. Write a program that utilizes this equality to get a more accurate series expansion for large negative exponents. Plot ϵ_n on a log-log plot to demonstrate that you have achieved this.

This one's easy; we just rerun with

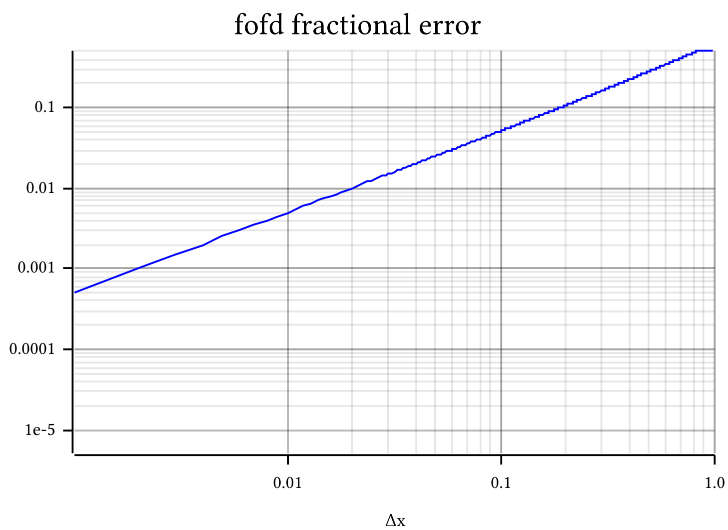
```
fn exponential_series_alt(n: u64, x: f64) -> f64 {
    return 1.0 / exponential_series(n, -x);
}
```



3 *errors in numerical differentiation*

Calculate the derivative of the function $f(x) = \sin x$ at the point $x = \pi/4$ using the first-order forward difference. Plot on a log-log plot the error with respect to the analytical derivative for a wide range of Δx. Describe the behavior you see (especially for very small Δx) and the reason for the trends. How does it change if you use a second-order central difference? How about a fourth-order central difference?

First order forward:

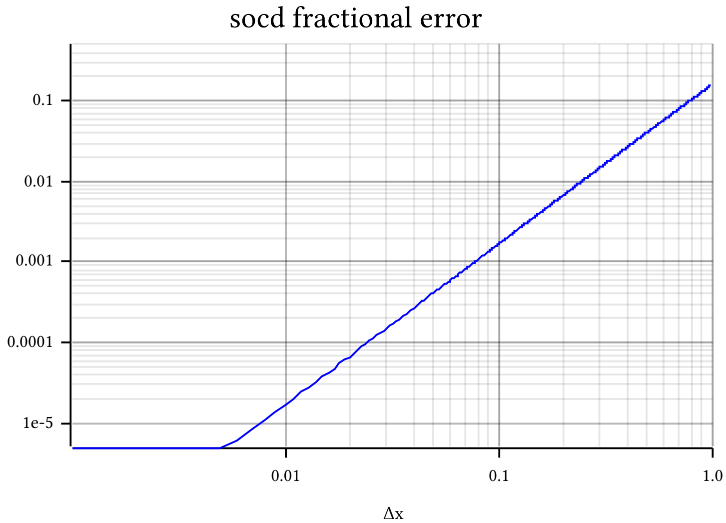


It's pretty much a straight line on a log-log plot. I think this makes sense, because the fractional error is (the magnitude of)

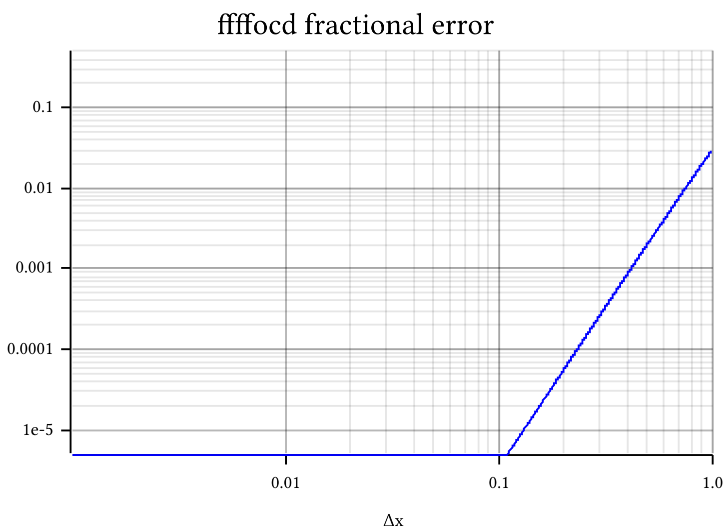
$$\frac{\frac{\sin(x+\Delta x)-\sin x}{\Delta x} - \cos x}{\cos x} = \frac{(\sin x)(\cos\Delta x - 1)}{\Delta x \cos x} - 1 \approx \frac{(\sin x)\left(-\Delta x^2\right)}{2\,\Delta x \cos x} - 1$$

which is linear.

Second order central:



Fourth order central:



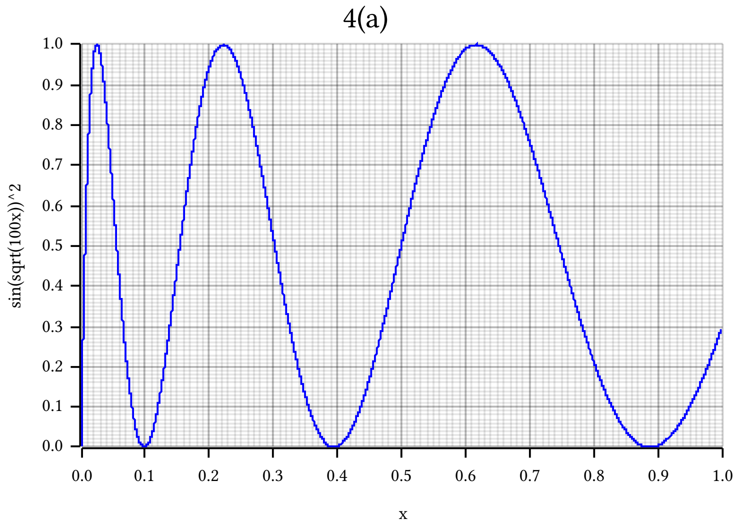
4 *comparing methods of integration*

Consider the variable

$$I = \int_0^1 \left(\sin\sqrt{100x}\right)^2 \, \mathrm{d}x$$

4(a) Plot the integrand over the range of the integral.

As instructed:



5 *integration to ∞*

Consider the gamma function,

$$\Gamma(a) = \int_0^\infty x^{a-1} e^{-x}\, \mathrm{d}x \, .$$

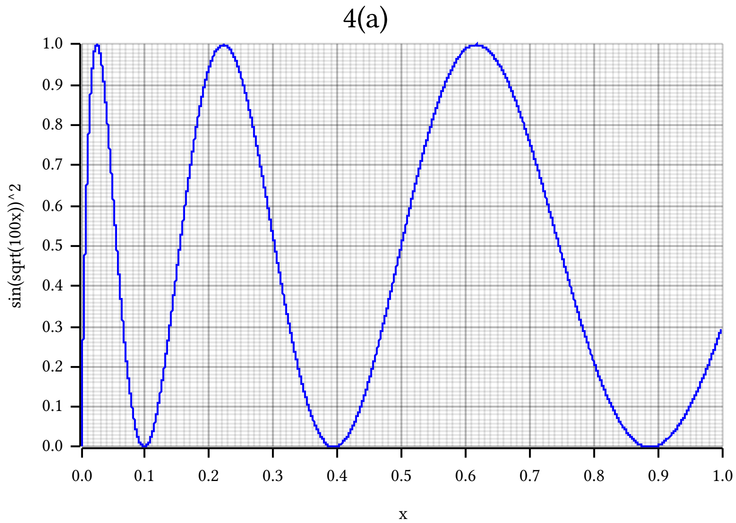
We want to evaluate this numerically, and we will focus on $a > 1$. Consider a variable transformation of the form:

$$z = \frac{x}{x+c} \, .$$

This will map $0 \le x < \infty$ to $0 \le z \le 1$, allowing us to do this integral numerically in terms of z. For convenience, we express the integrand as $\phi(x) = x^{a-1} e^{-x}$.

5(a) Plot $\phi(x)$ for $a \in \{2, 3, 4\}$.

As instructed:



5(b) For what value of x is the integrand $\phi(x)$ maximum?

5(c) Choose the value c in our transformation such that the peak of the integrand occurs at $z = 1/2$. What value is c?

This choice spreads the interesting regions of integrand over the domain $0 \leq z \leq 1$, making our numerical integration more accurate.

5(d) Find $\Gamma(a)$ for a few different values of $a > 1$ using any numerical integration method you wish, integrating from $z = 0$ to $z = 1$. Keep the number of points in your quadrature to a reasonable amount ($N \leq 50$).

Don't forget to include the factors you pick up when changing $\mathrm{d}x$ to $\mathrm{d}z$.

Note that roundoff error may come into play in the integrand. Recognizing that you can write $x^{a-1} = e^{(a-1)\ln x}$ can help minimize this.