PHY604: homework 1

2025-09-22

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.

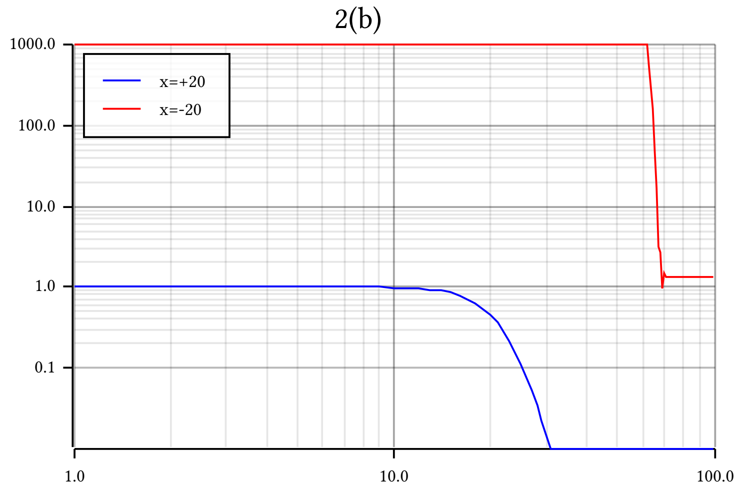
Done. See the `exponential_series` function in `hw01.rs`.

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:

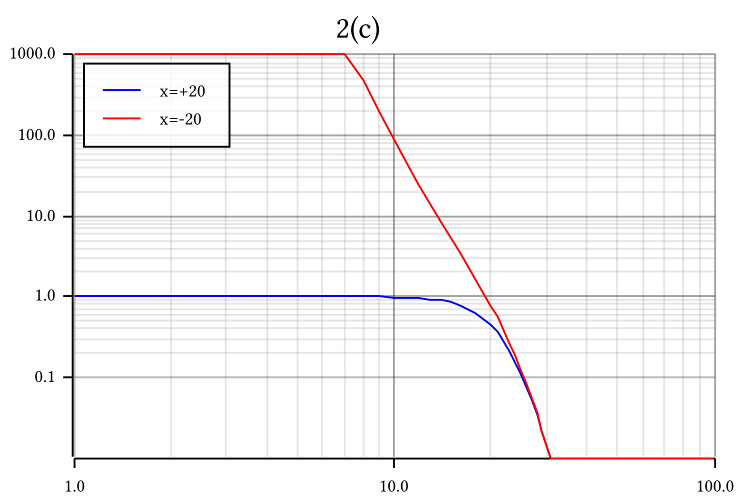


You can see that we actually never get to the correct answer for $x = -20$, because somewhere along the process of going to $n = 100$, `factorial` on a `u64` overflowed.

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

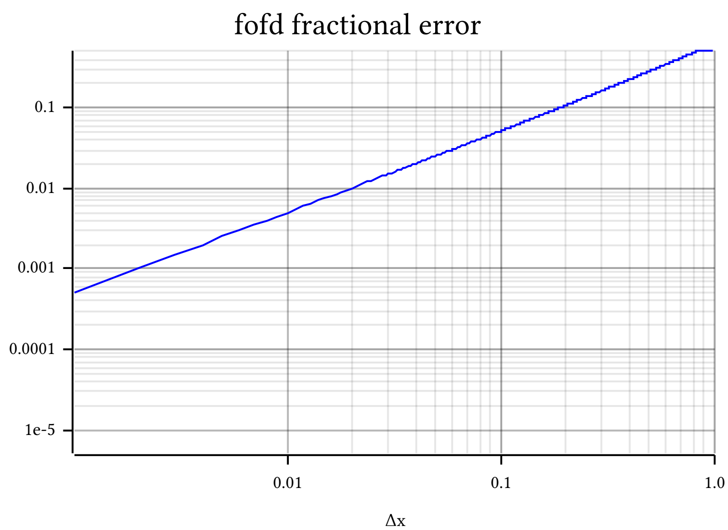
```
fn exponential_series_alt(n: u64, x: f64) -> f64 {
    return 1.0 / exponential_series(n, -x);
}
```



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:

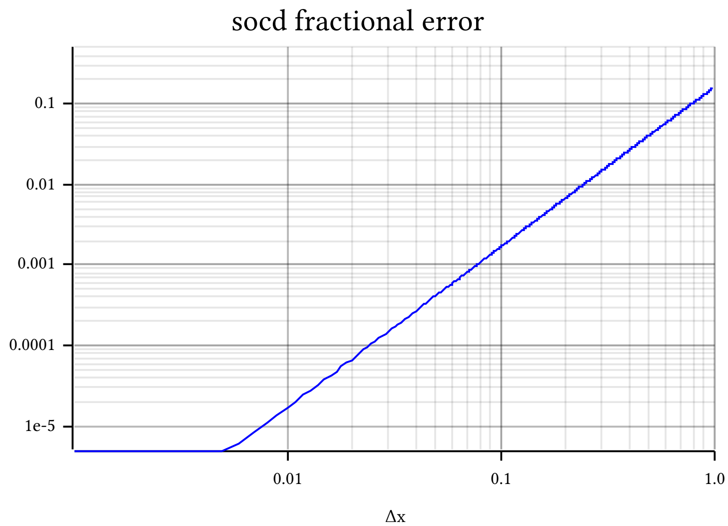


It's pretty much a straight line on a log-log plot. I think this makes sense, because the fractional error is (the magnitude of)

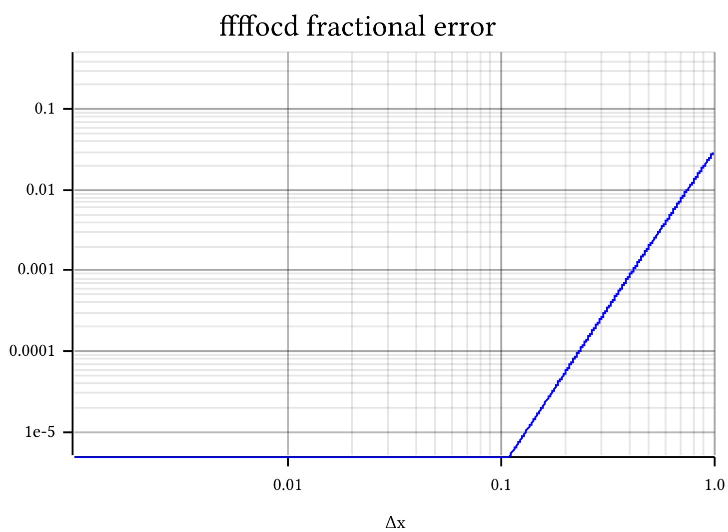
$$\frac{\frac{\sin(x+\Delta x)-\sin x}{\Delta x} - \cos x}{\cos x} = \frac{(\sin x)(\cos \Delta x - 1)}{\Delta x \cos x} - 1 \approx \frac{(\sin x)\left(-\Delta x^2\right)}{2\,\Delta x \cos x} - 1$$

which is linear.

Second order central:



Fourth order central:



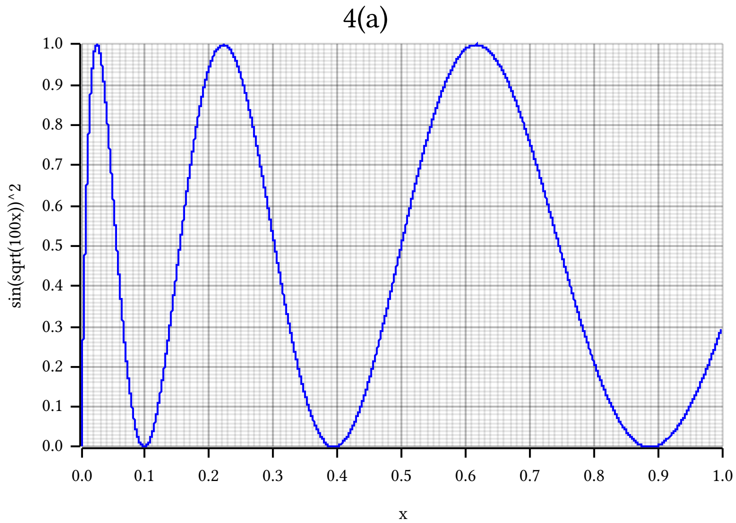
4 *comparing methods of integration*

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:



4(b) Write a program that uses the *adaptive trapezoid rule* to calculate the integral to an approximate accuracy of $\epsilon = 10^{-6}$, using the following procedure. Start with the trapezoid rule using a single subinterval. Double the number of subintervals and recalculate the integral. Continue to double the number of subintervals until the error is less than 10^{-6}. Recall that the error is given by $\epsilon_i = \frac{1}{3}(I_i - I_{i-1})$ where the number of subintervals N_i used to calculate I_i is twice that used to calculate I_{i-1}. To make your implementation more efficient, use the fact that

$$I_i = \frac{1}{2} I_{i-1} + h_i \sum_k f(a + kh_i)$$

where h_i is the width of the subinterval for the ith iteration, and k runs over *odd numbers* from 1 to $N_i - 1$.

Done in `hw01.rs` (see `trapezoid_integrate`):

```
4b: subintervals = 4096, ret = 0.455832058278271
```

4(c) Write a separate program that uses *Romberg integration* to solve the integral, also to an accuracy of 10^{-6} using the following procedure. First calculate the integral with the trapezoid rule for 1 subinterval (as you did in part (b)); we will refer to this as step $i = 1$, and the result as $I_1 = R_{1,1}$. Then calculate $I_2 = R_{2,1}$ using 2 subintervals. Using these two results, we can construct an improved estimate of the integral as: $R_{2,2} = R_{2,1} + \frac{1}{3}\left(R_{2,1} - R_{1,1}\right)$. In general

$$R_{i,m+1} = R_{i,m} + \frac{1}{4^m - 1}\left(R_{i,m} - R_{i-1,m}\right).$$

Therefore, for each iteration i (where we double the number of subintervals), we can obtain improved approximations up to $m = i - 1$ with very minor extra work. For each i and m, we can calculate the error at previous steps as

$$\epsilon_{i,m} = \frac{1}{4^m - 1}\left(R_{i,m} - R_{i-1,m}\right) .$$

Use these two equations to iterate until the error in $R_{i,i}$ is less than 10^{-6}. How significant is the improvement with respect to number of subintervals necessary compared to the approach of part (b)?

Done in `hw01.rs` (see `romberg_integrate`):

```
4c: subintervals = 64, ret = 0.45583249446137863
```

You can see that the number of subintervals reduced from 4096 to 64.

4(d) Use the Gauss–Legendre approach to calculate the integral. What order (i.e., how many points) do you need to obtain an accuracy below 10^{-6}? You can find tabulated weights and points online.

Done in `hw01.rs`, `quadgl.rs`, and `quadgl/quadgl_data.rs`. We see:

```
4d: n = 2, ret = 0.6273262731105194
4d: n = 3, ret = 0.23603692720508807
4d: n = 4, ret = 0.4267093047956246
4d: n = 5, ret = 0.5631145323435273
4d: n = 6, ret = 0.470222775561266
4d: n = 7, ret = 0.45644586447958324
4d: n = 8, ret = 0.45584440641945256
4d: n = 9, ret = 0.455832655443542
4d: n = 10, ret = 0.455832533065431
4d: n = 11, ret = 0.4558325323120352
4d: n = 12, ret = 0.4558325323090928
```

Doing analytic integration in SageMath, we can see that the actual answer is 0.455832532309085:

```
sage: N(integrate(sin(sqrt(100*x))^2, x, 0, 1))
0.455832532309085
```

and we are within 10^{-6} of that with just $n = 9$.

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:

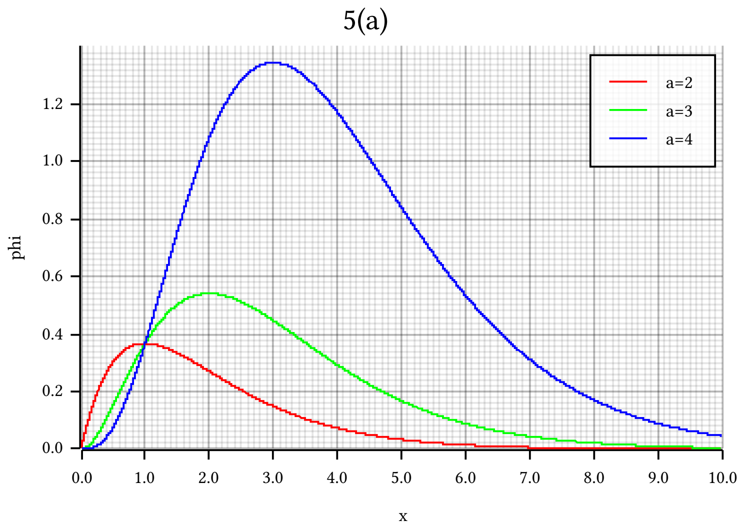
$$z = \frac{x}{x + c} .$$

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?

Setting the derivative equal to zero:

$$0 = \frac{\mathrm{d}}{\mathrm{d}x}\phi(x) = e^{-x}(a-1)x^{a-2} - x^{a-1}e^{-x} \quad \Rightarrow \quad (a-1)x^{a-2} = x^{a-1} \quad \Rightarrow \quad x = (a-1)\,.$$

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 $0 \le z \le 1$, making our numerical integration more accurate.

Simply:

$$\frac{1}{2} = \frac{a-1}{a-1+c} \quad \Rightarrow \quad c = a-1\,.$$

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 ($N \le 50$).

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.

We have

$$z(x+c) = x \quad \Rightarrow \quad x = \frac{cz}{1-z} \quad \Rightarrow \quad \mathrm{d}x = \left(\frac{c}{1-z} + \frac{cz}{(1-z)^2}\right)\mathrm{d}z = \frac{c}{(1-z)^2}\,\mathrm{d}z$$

Our new integral is

$$\Gamma(a) = \int_0^1 \left(\frac{cz}{1-z}\right)^c \exp\left(-\frac{cz}{1-z}\right)\frac{c}{(1-z)^2}\,\mathrm{d}z = \int_0^1 c\frac{(cz)^c}{(1-z)^{2+c}} \exp\left(-\frac{cz}{1-z}\right)\mathrm{d}z$$

and with quadgl integration in `hw01.rs` we see

```
5d: a = 1+1, ret = 1.0000000000058678
5d: a = 2+1, ret = 2.0000000000000653
5d: a = 3+1, ret = 5.999999999999983
```

which is pretty close to the analytical values of 1, 2, and 6.