Computational Physics: Homework 1

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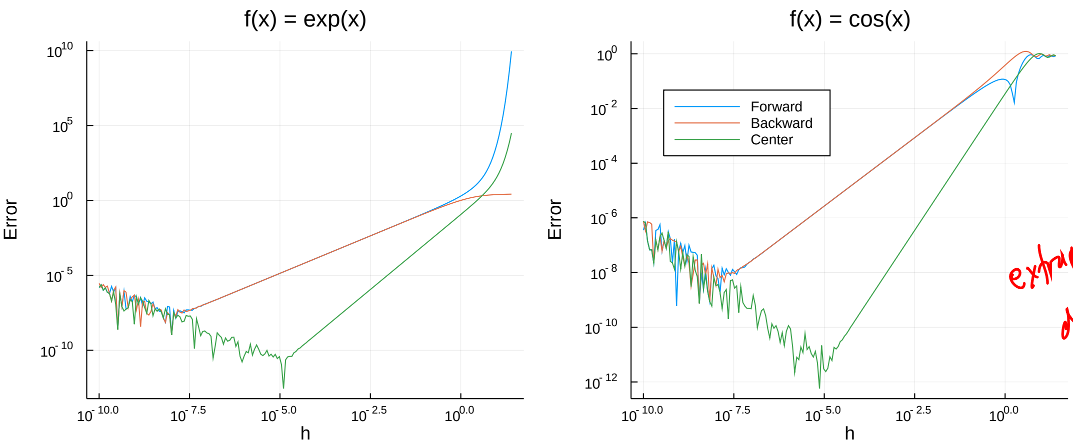
This homework was done using the Julia programming language.

Problem 1

After implementing simple functions (differentiation.jl) for forward, backward and central differences, we used them on exp & cos. The results can be found in Fig. 1.



extrapolated difference method?

Figure 1: Error scaling for forward, backward and central difference approximation to derivatives. "Error" on the y-axis stands for $|D - D_h|$ where D is the true derivative value at $x_0 = 1$ and D_h is the finite difference h approximation.

In Fig. 1 we can clearly identify three regimes on both panels:

- The noisy regime on the left is a consequence of the rounding error for small numbers discussed in Newman. When we subtract $f(x_0 + h)$ and $f(x_0)$ for a continuous function, we are subtracting two very similar floating point numbers. Additional division by a very small h is then just multiplying an unreliable result with a large number.

well, for truncation

- The middle regime represents the true error scaling. We can clearly observe that the central difference method is an order of magnitude better, as expected. In addition it can achieve lower error values before the rounding error regime takes over.

- The noisy regime on the right is a consequence of h-values which are too large to reliably estimate a derivative. At that point, we are essentially calculating the slope of a secant instead of a tangent line.

Problem 2

Integration algorithms were implemented in integration.jl and were used to calculate the value of

$$I = \int_0^1 e^{-x} \mathrm{d}x = 1 - {}^{1}\!/_{e} \, . \tag{1}$$

Error scaling can be found in Fig. 2.

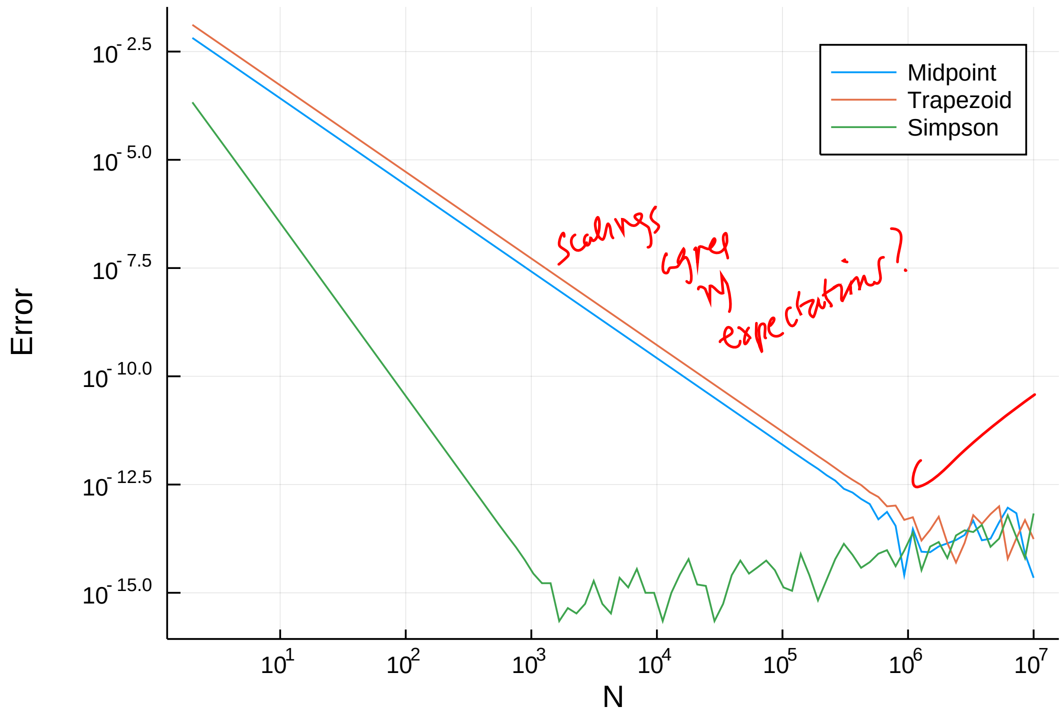


Figure 2: Error scaling for the midpoint, trapezoidal and Simpson's rules. "Error" on the y-axis stands for $|I - I_N|$ where I is the true integral value defined in Eq. 1 and I_N is the numerical integration result using N bins.

Similar to the the previous problem, we can identify two regimes: real error scaling and machine precision saturation. The noisy behavior on the right is a consequence of our accuracy reaching machine precision and rounding errors taking over. We can see that Simpson's rule produces a order of magnitude better results than either midpoint or trapezoid rules, as expected.

Problem 3

We loaded the power spectrum data and plotted it in Fig. 3.

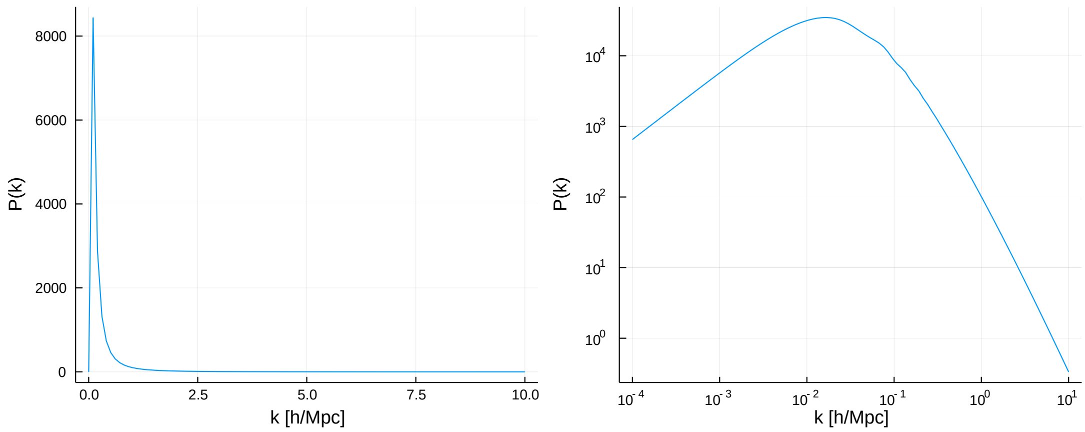
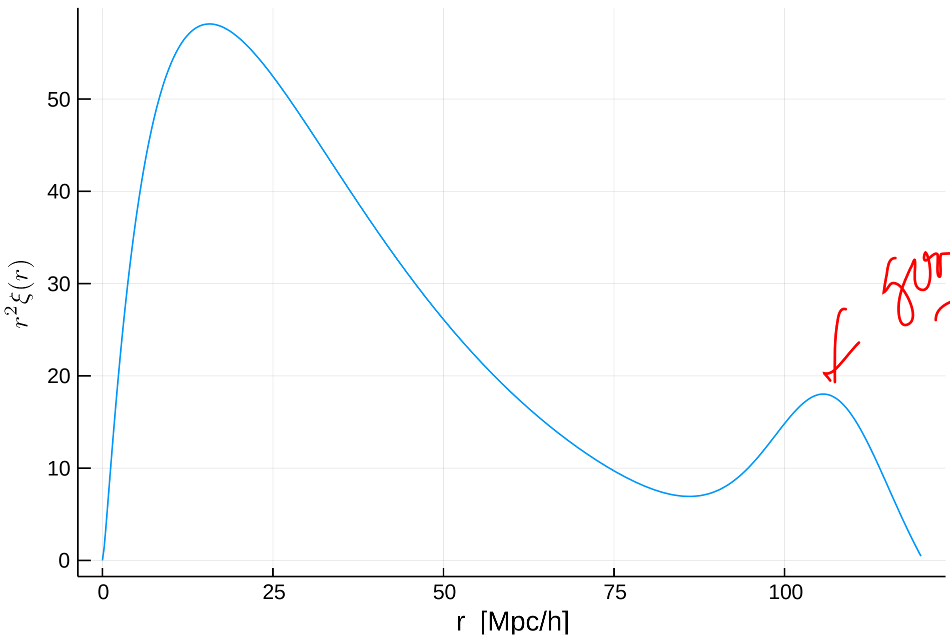


Figure 3: Overdensity power spectrum linear (left panel) and log-log plot (right panel).

After performing the angular integrals in **k**-space, we can recover the real-space correlation function through:

$$\xi(r) = \frac{1}{2\pi^2} \int_0^\infty \mathrm{d}k\, k^2\, P(k) \frac{\sin(kr)}{kr} \tag{2}$$

We perform the integral in Eq. 2 for each value of r separately. However, before integrating, we interpolated between the exponentially separated data points of $P(k)$ using a cubic spline, through the Dierckx package. After that, we sampled an equidistant set of points to use with Simpson's rule.



good.

Figure 4: Real-space correlation function obtained from the tabulated power spectrum data points.

$N = 10\,000$ equidistant points were chosen to use with Simpson's rule and $k_{\max} =$

100 h/Mpc was chosen to replace infinity in the upper limit of the integral in Eq. 2.[1] We report the value of the BAO peak at $r_{\mathrm{BAO}} \approx 106$ Mpc.

Finally, to provide an argument towards the robustness of $k_{\max}$, we study the Mean Square Error (MSE) as our measure of deviation from $\xi^{(0)}$ shown in Fig. 4. It is defined as:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}\left[r_i^2\xi^{(k_{\max})}(r_i) - r_i^2\xi^{(0)}(r_i)\right]^2 \tag{3}$$

– ok, but could be dominated by r's outside region of interest. what is your $\{r_i\}$?!

for an equidistant set of points $\{r_i\}$. The implicit dependence of ξ on $k_{\max}$ is denoted through an extra superscript. A MSE vs. $k_{\max}$ plot can be found in Fig. 5.

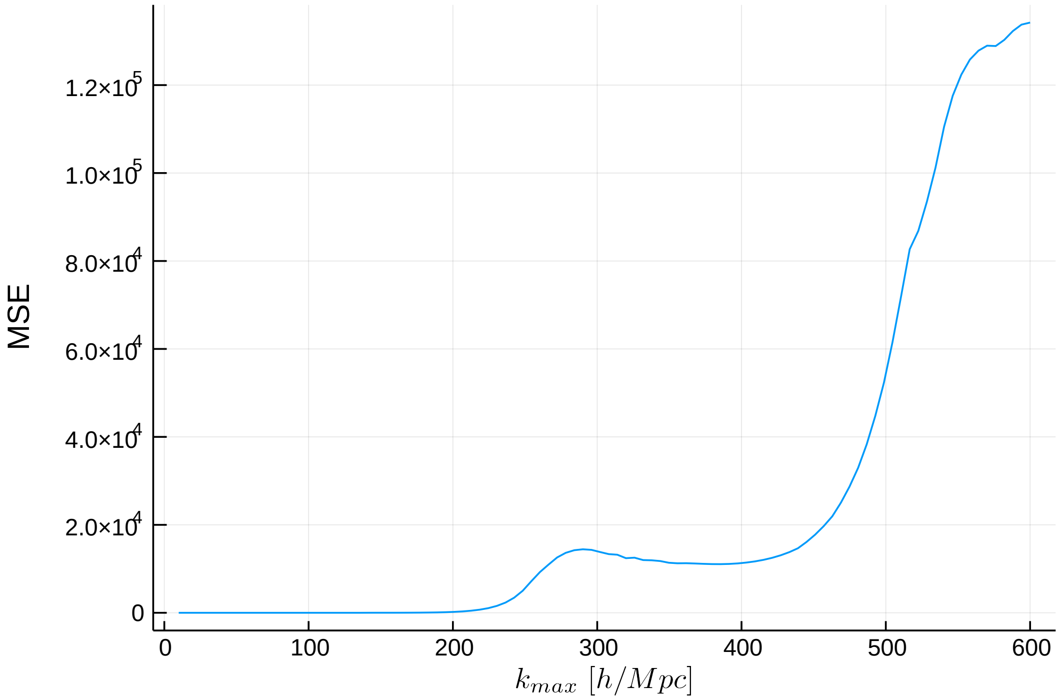


Figure 5: Mean square error dependence on wave number cutoff $k_{\max}$.

We notice that, as soon as we increase $k_{\max}$ the fixed number of points used for Simpson's rule becomes too thin to adequately sample the sharp peak at low k-values, shown on the left panel of Fig. 3. If we wanted to reduce error further, that would have to happen alongside with a significant increase in the bin count used for Simpson's rule. However, the dominant contribution to the integral comes from $k \lesssim 2.5$ h/Mpc so we would not gain much accuracy if we do increase $k_{\max}$. Therefore, the fact that the MSE plateaus towards zero for $k_{\max} \lesssim 200$ Mpc indicates that our result is robust in the sense that it has picked up the dominant contribution of the integral.

[1]That value seems like at least an order of magnitude larger than what should be necessary (based on the left panel of Fig. 3) but choosing a lower cutoff resulted in "ringing" effects on top of the expected curve shape.