# Computational Physics - Problem Set 5

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Github URL: https://github.com/frederikholst/phys-ga2000

## 1 Newman 5.15

We use the central difference method to compute the derivative of $1 + \frac{1}{2}\tanh(2x)$. The result is compared in Figure 1 against the analytic derivative, $\sec^2(2x)$. In Figure 2 we see the same comparison, but with the JAX method instead of the central limit derivative method.

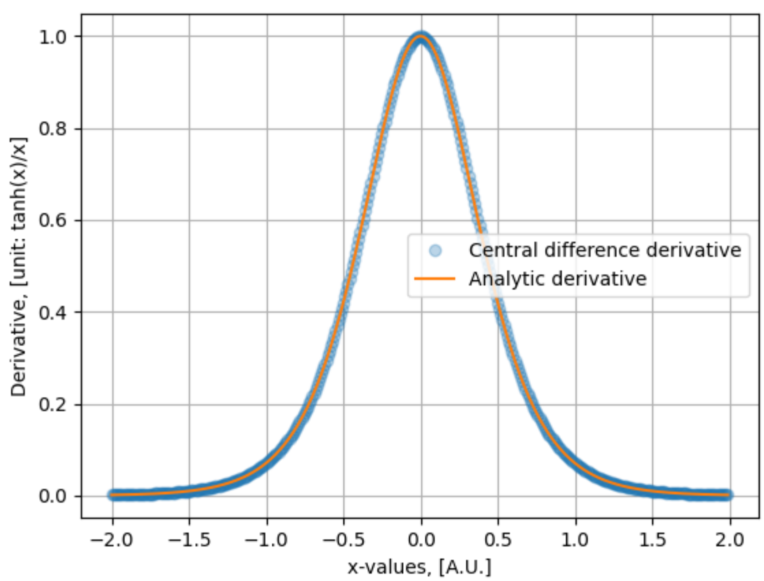


Figure 1: The analytic derivative is plotted against the numerically computed derivative using central difference method. We see very good agreement.

Finally, Figure 3 shows the residuals that are the size of machine errors.

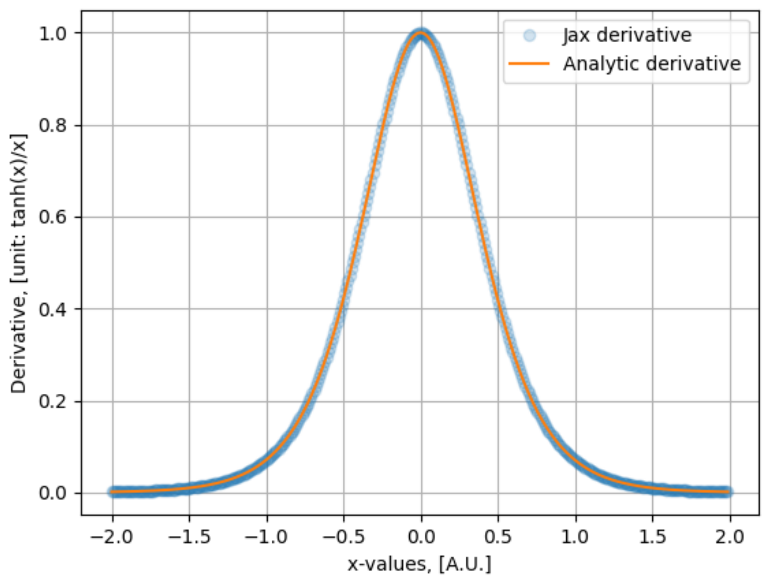


Figure 2: The analytic derivative is plotted against the derivative using JAX. Again, we see very good agreement.

## 2 Newman 5.17

Part A: In Figure 4 we see the integrand of the gamma function, $\Gamma(a) = \int_0^\infty x^{a-1}e^{-x}$ plotted for $n = 2, 3, 4$.

Part B: We now show analytically that the maximum of the integrand falls at $x = a - 1$.

$$\frac{d}{dx}x^{a-1}e^{-x} = e^{-x}((a-1)x^{a-2} - x^{a-1}) = 0$$
$$\Rightarrow ax^{a-2} - x^{a-2} - x^{a-1} = 0$$
$$\Rightarrow x^{a-2}(a-1-x) = 0$$
$$\Rightarrow x_{max} = a - 1$$

Part C: Knowing that most of the integral will fall around $x_{max} = a - 1$, we perform a change of variables using

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

if $z = \frac{1}{2}$ at the maximum then $x_{max} = c$ so that

$$c = a - 1$$

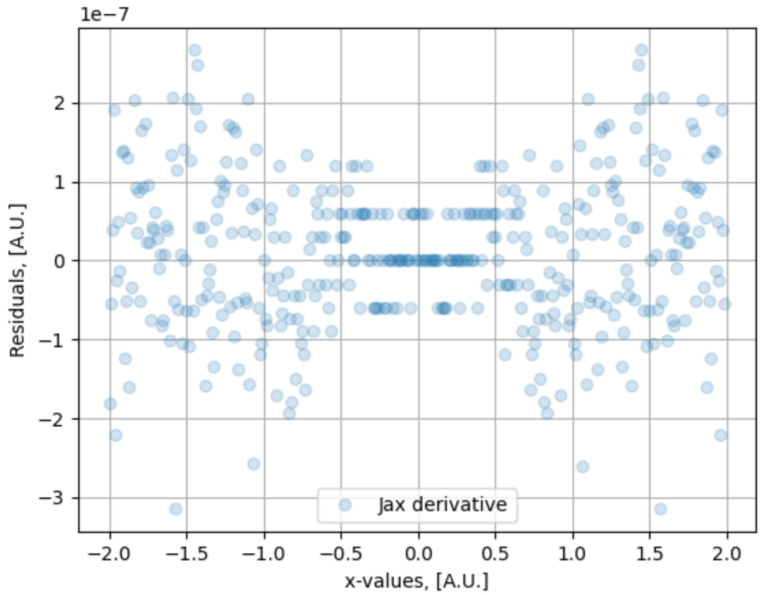


Figure 3: The residuals are very small, which confirms that the JAX derivative is a strong method for computing the derivatives.

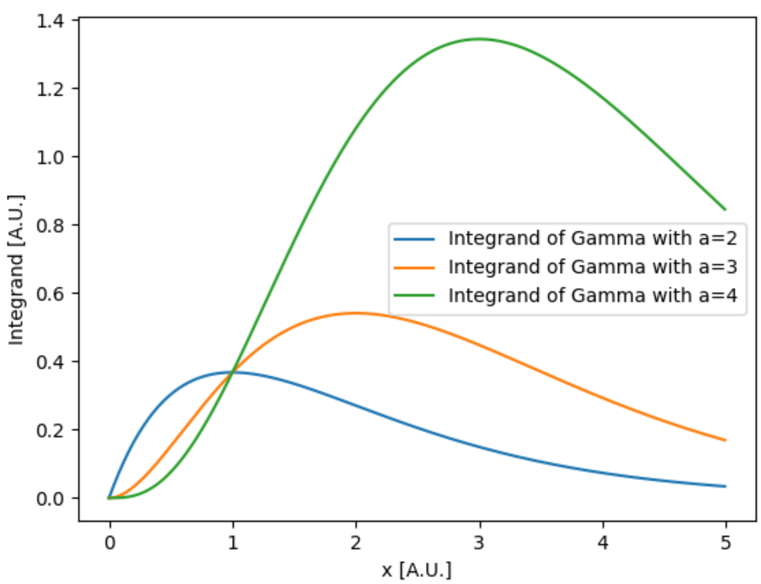


Figure 4: The integrand of the gamma function.

. And the variable change becomes:

$$z = \frac{x}{c+x}$$
$$\Rightarrow (c+x)z = x$$
$$\Rightarrow (zc = x(1-z))$$
$$\Rightarrow x = \frac{zc}{1-z}$$
$$\Rightarrow x = \frac{z(a-1)}{1-z}$$

Part D: We will now write $x^{a-1} = e^{(a-1)\ln x}$ in the integrand of the gamma function. The new expression is better that the old one, because $x^{a-1}$ can easily cause overflow, and the new form puts two exponential functions in the integrand: $e^{(a-1)\ln(x)-x}$. This avoids the issue of having a very large number multiplied with a very small one, where both could be in the danger of overflow and underflow.

Part E: We now compute the gamma function using the change of variables:

$$\frac{dx}{dz} = \frac{(a-1)}{1-z} + \frac{z(a-1)}{(1-z)^2}$$

$$\Rightarrow \frac{dx}{dz} = \frac{z(a-1)-(a-1)(z-1)}{(1-z)^2}$$
$$\Rightarrow \frac{dx}{dz} = \frac{za-z-za+a+z-1}{(1-z)^2}$$
$$\Rightarrow \frac{dx}{dz} = \frac{a-1}{(1-z)^2}$$

So that the integral becomes:

$$\Gamma(n) = \int_0^1 dz \left(\frac{(a-1)}{1-z} + \frac{z(a-1)}{(1-z)^2}\right) \exp\left[(a-1)\ln\left(\frac{z(a-1)}{1-z}\right) - \frac{z(a-1)}{1-z}\right]$$

We will use the gauss-quadrature method, and find the $\Gamma(\frac{3}{2} = 0.8862272081548225)$ at 50 sample points in the Guass-quadrature integration. If we compare to the analytic value of $\frac{1}{2}\sqrt{\pi} = 0.886$, we see very strong agreement.

Part F: Computing $\Gamma(a)$ with interger values of $a$ replicates that of the theoretical analytic values $a-1!$ with strong precision:

$$\Gamma(3) = 2.000000000000057, (3-1)! = 2$$

$$\Gamma(6) = 119.99999999999946, (6-1)! = 120$$
$$\Gamma(10) = 362879.99999999825, (10-1)! = 362880$$

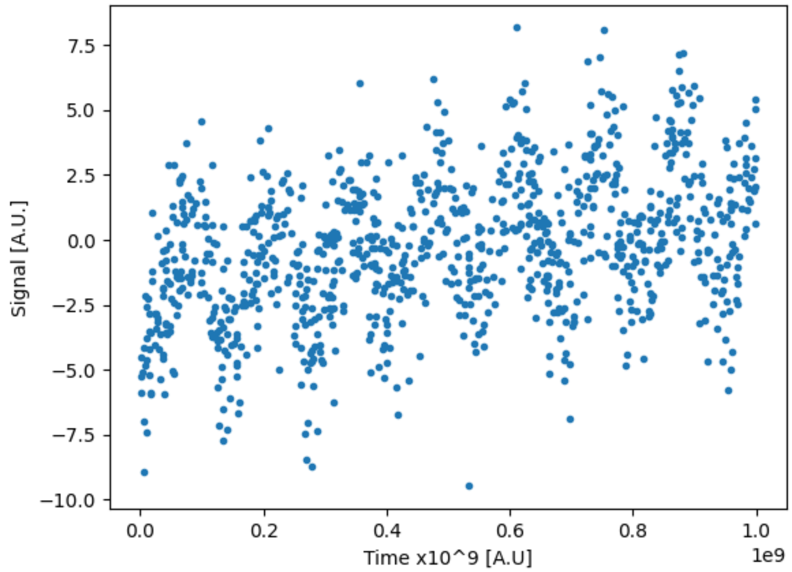


Figure 5: The noisy signal is shown with normalized time. This will make approximation erros less likely later on.

# 3 Problem 3

Part A: We import plot the data as seen in Figure 5.

Part B: Choosing a model that is a third order polynomial, we use the SVP method to perform the fit of the signal. See Figure 6:

Part C: The residuals of the model against the data are shown in Figure 7

Part D: We now try with a polynomial of order $n = 20$ to see if that makes a better fit for our noisy data. The condition number is now: $9.1 \times 10^{14}$, which is a lot higher, meaning we are in the danger of overfitting. See Figure 8.

Part E: We now try a Fourier series of order $n = 18$, where the fit nicely follows that of the oscillations burried in the noise, as seen in Figure 9. The condition number is now $1.8 \times 10^{14}$.

From this fit we find the period in the scaled units to be around 0.15, which corresponds to around 5 years if the original time unit were in seconds. This could, likely, be the period of an exoplanet orbiting a distant star.

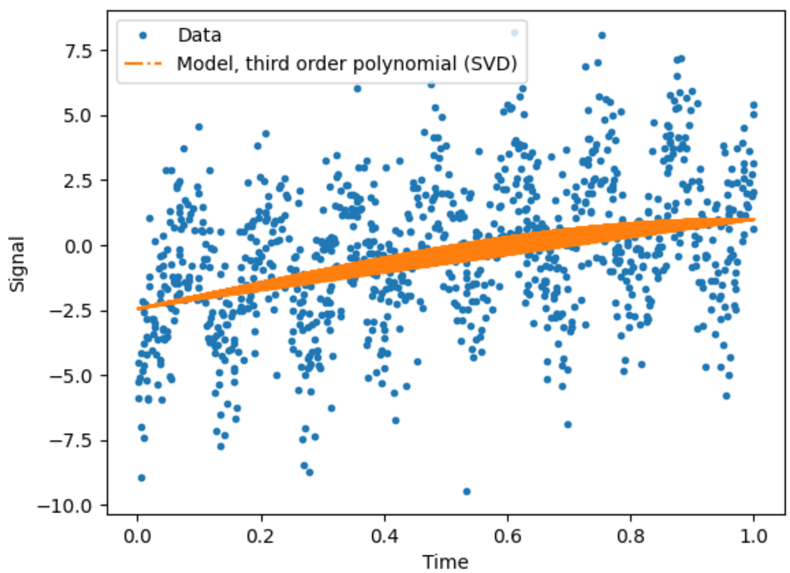


Figure 6: The thrid order polynomial is clearly not suited to fit the signal. This gives us no prediction power, and we have to improve the design matrix, A to include higher order terms in our model

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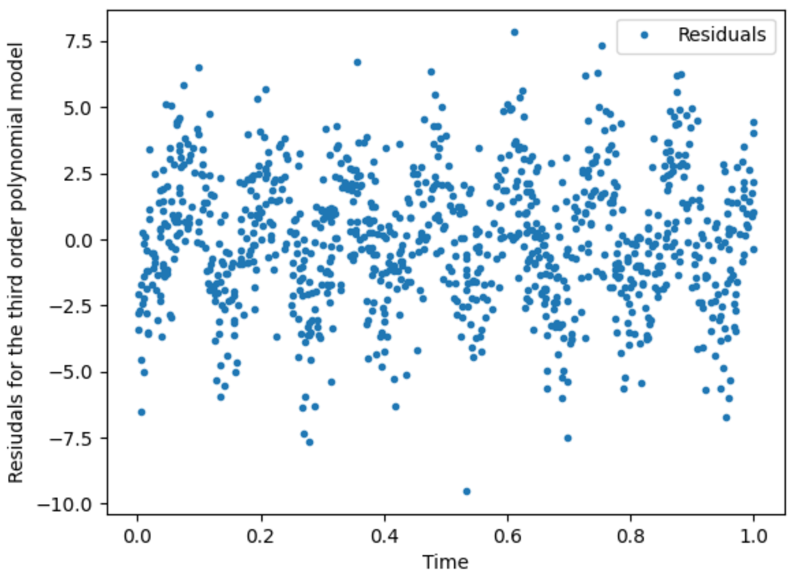


Figure 7: The residuals are found to be significantly larger than that of the uncertainty of 2.0 in signal units. Unfortunately, we cannot learn much of the fit from the residuals.

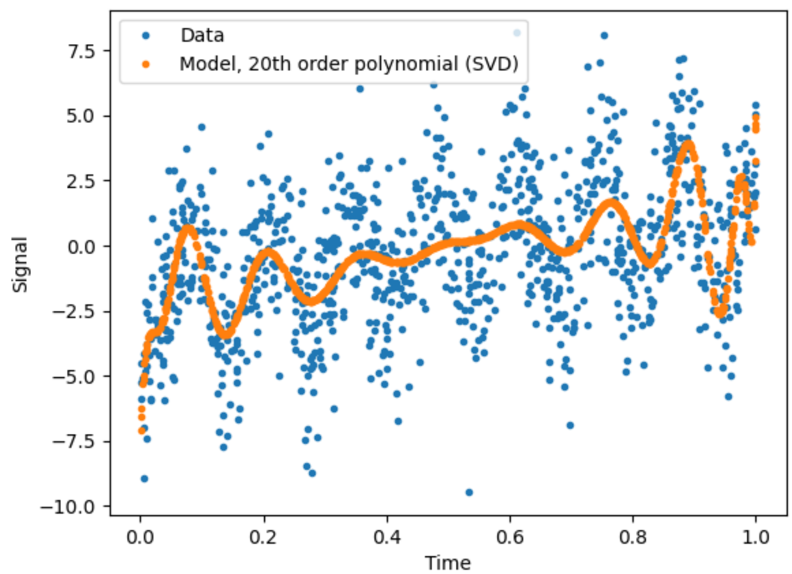


Figure 8: The fit is much better, since it captures the oscillatory behavior, but still not quite good enough at the beginning and end of the fit

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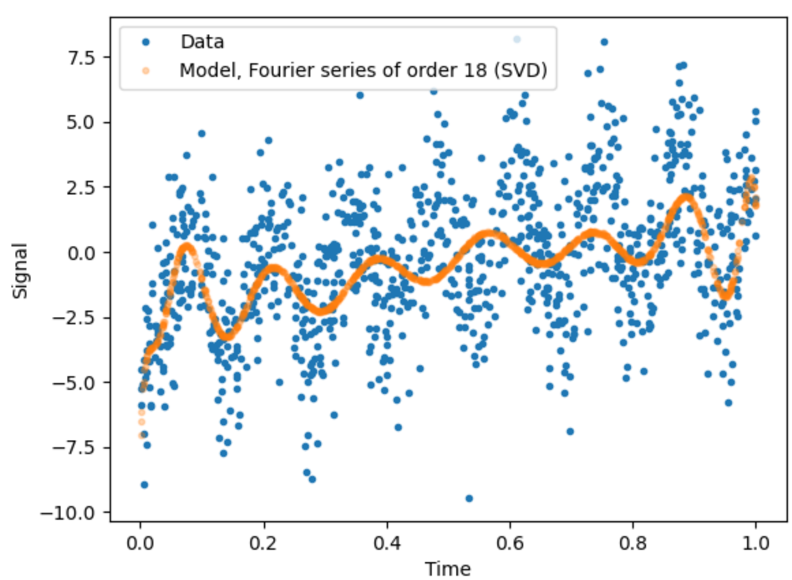


Figure 9: The Fourier series fits the data at order $n = 18$.