Computational Physics ps-5 Report

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1   Problem 1

The analytical formula for the derivative $f(x) = 1 + \frac{1}{2}\tanh 2x$ is

$$f'(x) = \frac{1}{\cosh^2 2x}. \tag{1}$$

The numerical derivatives computed using central difference and `jax` are shown in Figure 1 and 2 respectively.
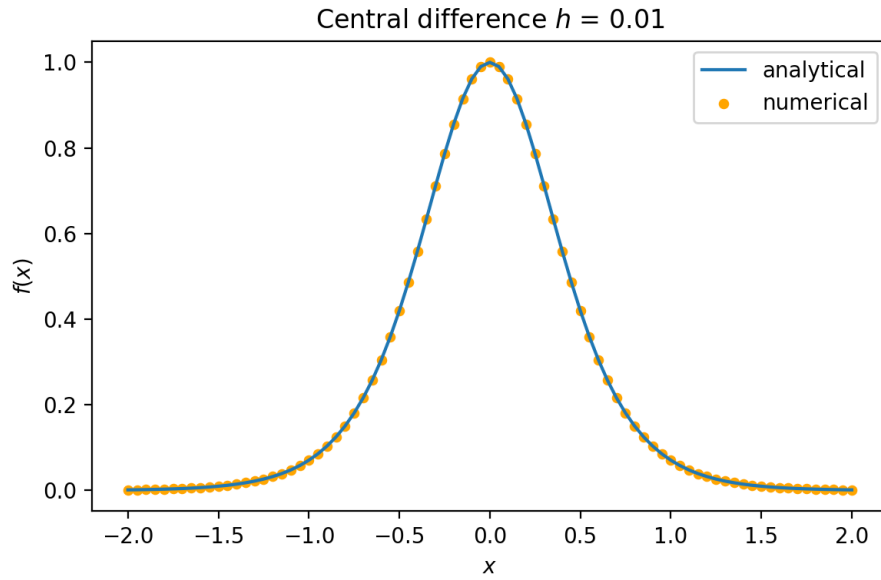

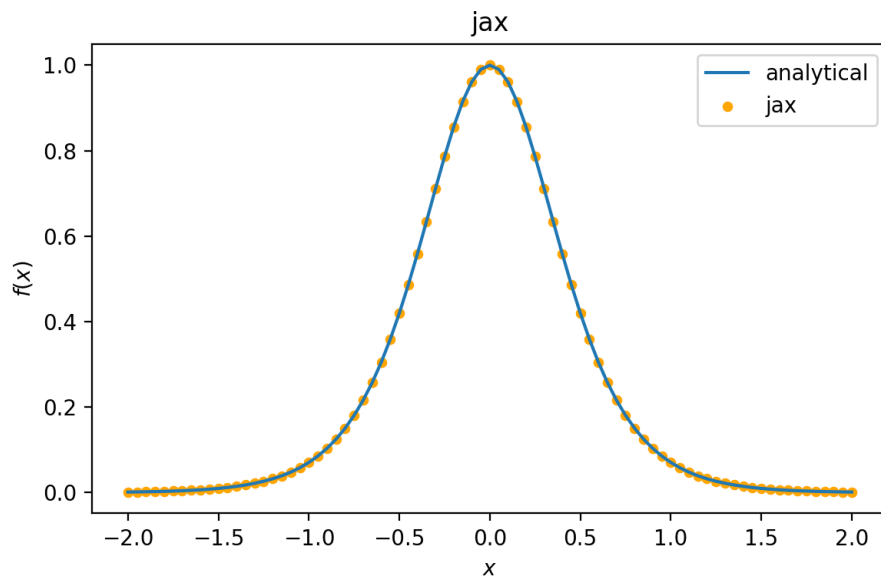Figure 1: Derivative computed using central difference.

Figure 2: Derivative computed using `jax`.

Listing 1 shows that `jax` seems to be more accurate then central difference in this particular case.

Listing 1: Some values of the derivative.

```
analytical: f'(0) = 1.0
central difference (h=0.01): f'(0) = 0.99996924
jax: f'(0) = 1.0

analytical: f'(2) = 0.0013409506
central difference (h=0.01): f'(2) = 0.001335144
jax: f'(2) = 0.0013411314
```

2   Problem 2

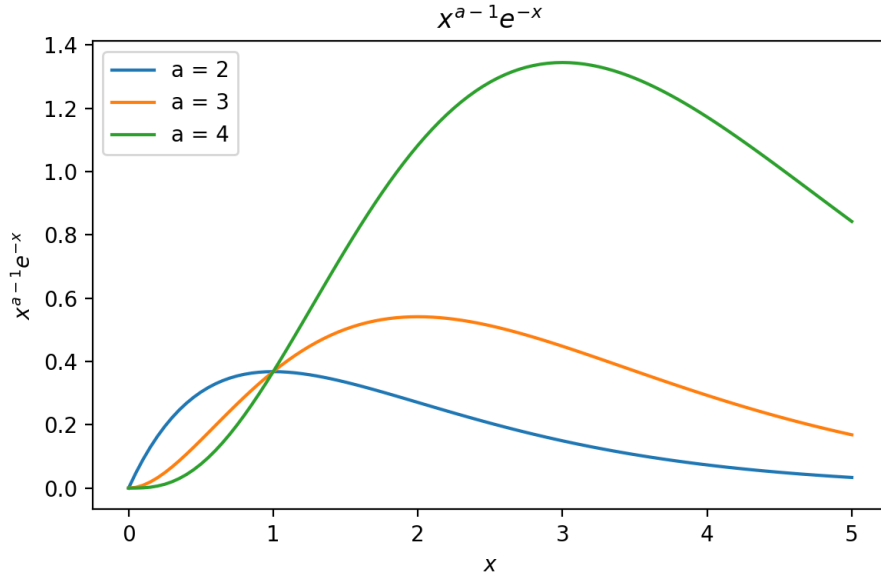## 2.1   Part (a)

Figure 3 plots the integrand of the gamma function.

2

Figure 3: Integrand of the gamma function.

2.2 Part (b)

The derivative of $f(x) = x^{a-1}e^{-x}$ is

$$f'(x) = (a - 1 - x)x^{a-2}e^{-x}. \tag{2}$$

Setting $f'(x) = 0$, we get $x = 0, (a - 1)$.

The second derivative is

$$f''(x) = -x^{a-2}e^{-x} + (a - 1 - x)(a - 2)x^{a-3}e^{-x} - (a - 1 - x)x^{a-2}e^{-x}. \tag{3}$$

Since the integral in the gamma function is from 0 to ∞, we assume that $x = a - 1 > 0$. Thus, we have

$$f''(a - 1) = -(a - 1)^{a-2}e^{a-1} > 0, \tag{4}$$

and hence $f(x)$ has a maximum at $x = a - 1$.

2.3 Part (c)

Obviously, if $x = c$, then $z = \frac{x}{c+x} = \frac{1}{2}$. Hence choosing $c = a - 1$ will put the peak of the integrand for the gamma function at $z = \frac{1}{2}$.

3

2.4 Part (d)

We can also express the integrand as

$$\begin{aligned} f(x) &= x^{a-1}e^{-x} \\ &= e^{(a-1)\ln(x)}e^{-x} \\ &= e^{(a-1)\ln(x)-x}. \end{aligned} \tag{5}$$

In the original expression, for large x, x^{a-1} may cause overflow and e^{-x} may cause underflow. The advantage of the new expression is that the $\ln(x)$ and x are less likely to cause these issues.

2.5 Part (e) and (f)

Listing 2 shows the computed values of the gamma function at some points.

Listing 2: Some values of the gamma function.

```
gamma(3/2) = 0.886226961308725
gamma(3)   = 2.000000000000008
gamma(6)   = 120.00000000000047
gamma(10)  = 362880.0000000014
```

3 Problem 3

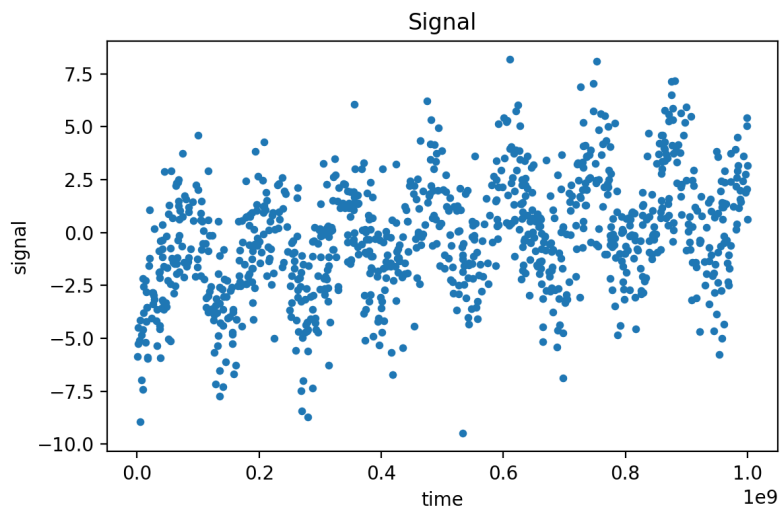## 3.1 Part (a)

Figure 4 plots the data.

Figure 4: Plot of the data.

3.2 Part (b)

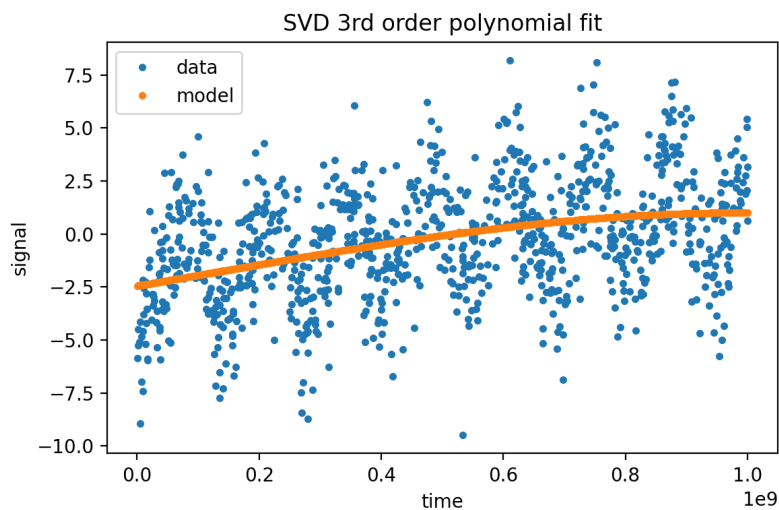Figure 5 shows the SVD 3rd-order polynomial fit.

Figure 5: SVD 3rd-order polynomial fit.

3.3 Part (c)

Listing 3 shows the condition numbers and residues of the fits performed in this problem. The 3rd-order polynomial fit is not a good explanation of the data because the residue is a bit large. Specifically, its $r/\sqrt{N}$ is greater than the uncertainty of the measurements, which is 2.0.

Listing 3: Condition numbers and residues of the SVD 3rd-order polynomial fit, 23th-order polynomial fit, 21-term Fourier series fit, and 300-term Fourier series fit.

```
condition number (3rd order): 5.919954774532443
r = 79.88708212853327
r / sqrt(N) = 2.526251351510973

condition number (23th order): 4503046701.822991
r = 64.15581991709665
r / sqrt(N) = 2.028785160936203

condition number (21 term): 1.6624737603150734
r = 71.46957923057155
r / sqrt(N) = 2.260066537824704

condition number (300 term): 8.145867733551112
r = 56.70453251408719
r / sqrt(N) = 1.7931547639958945
```

3.4   Part (d)

Figure 6 shows the SVD 23th-order polynomial fit. This is a more reasonable polynomial fit that is a better explanation of the data.

"When the condition number exceeds the dynamic range of your floating point numbers, there is no guarantee that the SVD solution will be stable. Basically, round-off error can then cause the procedure to fail."

As shown in Listing 3, the conditional number for the 23th-order polynomial fit is not too large comparing to the dynamic range. And its residue is smaller.
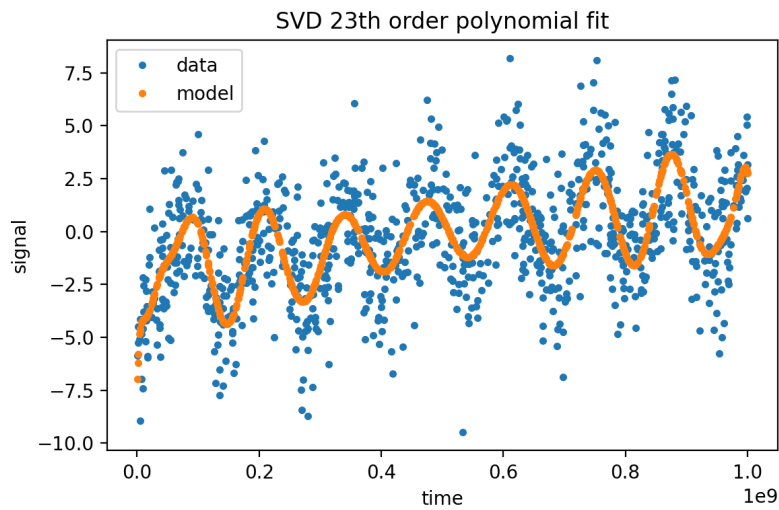

Figure 6: SVD 23th-order polynomial fit.

3.5   Part (e)

Figure 7 and 8 show the SVD 21-term and 300-term Fourier series fits respectively.

The models do a good job explaining the data. As shown in Listing 3, both fits have condition numbers that are small enough to be reasonable. And the 300-term Fourier series fits has smaller residue.

From figure 4, we can notice a typical periodicity about $T \approx 1.35 \times 10^8$ unit time.
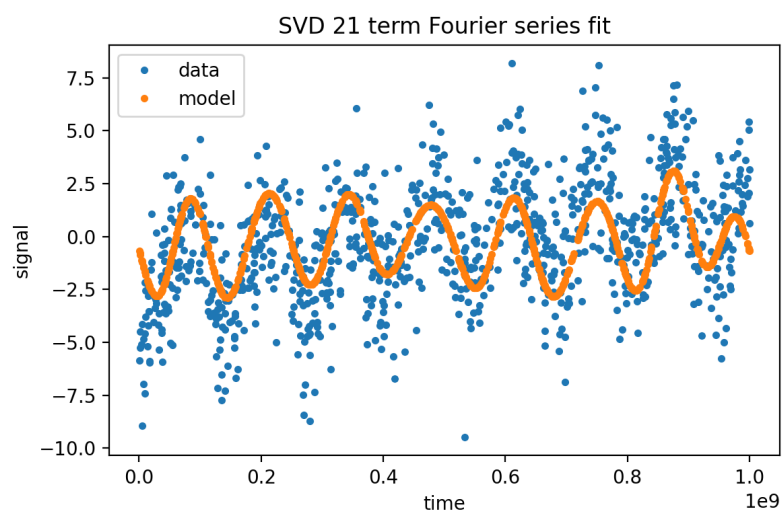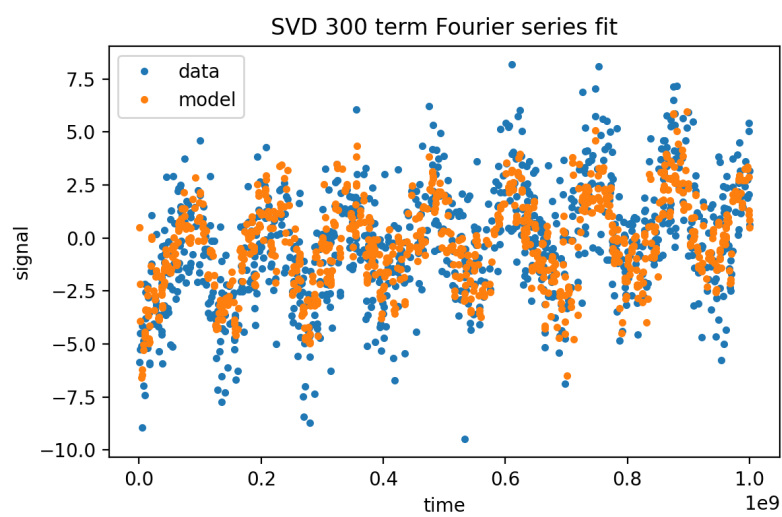
Figure 7: SVD 21-term Fourier series fit.

Figure 8: SVD 300-term Fourier series fit.