

Computational Physics Homework 6

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Richardson Extrapolation using the Euler-Maclaurin formula

It is of our interest to develop a method to extrapolate the value of the series:

$$\sum_{k=1}^{\infty} \frac{1}{k^s}$$

The partial sums of such series behave as:

$$\sum_{k=1}^n \frac{1}{k^s} \sim \zeta(s) - \frac{1}{(s-1)n^{s-1}} + \frac{1}{2n^s} - \sum_{i=1}^{\infty} \frac{B_{2i}}{(2i)!} \frac{(s+2i-2)!}{(s-1)!n^{s+2i-1}}$$

where the B_{2i} correspond to the Bernoulli numbers. The strategy to solve this problem is to write a system of equations for multiple partial sums:

$$\begin{aligned} A_N &= q_0 + \frac{q_1}{N^{s-1}} + \frac{q_1}{N^s} - \sum_{i=1}^{\infty} \frac{B_{2i}}{(2i)!} \frac{(s+2i-2)!}{(s-1)!N^{s+2i-1}} \\ A_{N+1} &= q_0 + \frac{q_1}{(N+1)^{s-1}} + \frac{q_1}{(N+1)^s} - \sum_{i=1}^{\infty} \frac{B_{2i}}{(2i)!} \frac{(s+2i-2)!}{(s-1)!(N+1)^{s+2i-1}} \\ &\dots \\ A_{N+p} &= q_0 + \frac{q_1}{(N+p)^{s-1}} + \frac{q_1}{(N+p)^s} - \sum_{i=1}^{\infty} \frac{B_{2i}}{(2i)!} \frac{(s+2i-2)!}{(s-1)!(N+p)^{s+2i-1}} \end{aligned}$$

Or in matrix notation:

$$\begin{pmatrix} A_N \\ A_{N+1} \\ \dots \\ A_{N+p} \end{pmatrix} = \begin{pmatrix} 1 & 1/N^{s-1} & 1/N^s & \dots \\ 1 & 1/(N+1)^{s-1} & 1/(N+1)^s & \dots \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1/(N+p)^{s-1} & 1/(N+p)^s & \dots \end{pmatrix} \begin{pmatrix} q_0 \\ q_1 \\ \vdots \\ q_p \end{pmatrix}$$

We will see in a moment how to get the dot columns in the matrix. For now, the strategy is as follows: we have a matrix equation

$$A = MQ$$

Where the only thing that is of our interest is the first entry of Q , which corresponds to the approximation of the series. Now, one way to get such vector is by calculating the inverse M^{-1} of M and apply it to both sides of the matrix equation:

$$M^{-1}A = Q$$

However, it is difficult to find an explicit formula for the inverse, specially because since the fourth column the entries take a form related to the i th dependent terms of the Euler-Maclaurin formula. So, we must calculate the partial sums A_i , $i = N, \dots, N+p$, so increasing the number of p implies increasing the size of the matrix M . We will do it numerically using `mpmath`, first up to A_{N+3} and then up to A_{N+4} .

Now we can talk about the i th dependent terms of the matrix, for the $N+3$ case:

$$M = \begin{pmatrix} 1 & 1/N^{s-1} & 1/N^s & 1/N^{s+1} \\ 1 & 1/(N+1)^{s-1} & 1/(N+1)^s & 1/(N+1)^{s+1} \\ 1 & 1/(N+2)^{s-1} & 1/(N+2)^s & 1/(N+2)^{s+1} \\ 1 & 1/(N+3)^{s-1} & 1/(N+3)^s & 1/(N+3)^{s+1} \end{pmatrix}$$

Now we can start working on the problem

```

1 import mpmath as mp
2
3 mp.dps = 100
4
5 def partial(nmax, s):
6     return mp.nsum(lambda n: mp.power(n, -s), [1, nmax])
7
8 A = mp.matrix([0,0,0,0])
9
10 k = 100 # here k corresponds to N in our previous analysis
11 s = 3/2 # the value of s
12
13 for i in range(len(A)):
14     # add the values of the partial function to the matrix A
15     nmax = i+k
16     A[i] = partial(nmax, s)
17
18 # define the matrix M
19 M = mp.matrix([[1, 1/k**(s-1), 1/k**s, 1/k**(s+1)], [1, 1/(k+1)**(s-1), 1/(k+1)**s, 1/(k+1)**(s+1)], [1, 1/(k+2)**(s-1), 1/(k+2)**s, 1/(k+2)**(s+1)], [1, 1/(k+3)**(s-1), 1/(k+3)**s, 1/(k+3)**(s+1)]])
20
21 # calculate the inverse of M
22 Minv = mp.inverse(M)
23
24 # calculate Q matrix
25 Q = Minv*A
26 print(Q)
27 >>> [ 2.61237534844416] -> The approximaton of the Riemann zeta function at s = 3/2
28     [ -1.99999999491331]
29     [ 0.49999950103022]
30     [-0.124979896719848]

```

We can see that the approximation is pretty good. For a better approximation we can increase the size of our matrix and in consequence of the vector containing the partial sums, as well as select a good choose of k:

```

1 import mpmath as mp
2
3 mp.dps = 100
4 k = 50
5 s = 3/2
6
7 def partial(nmax, s):
8     return mp.nsum(lambda n: mp.power(n, -s), [1, nmax])
9
10 B = mp.matrix([0,0,0,0,0])
11 for i in range(len(B)):
12     nmax = i+k
13     B[i] = partial(nmax, s)
14
15 T = mp.matrix([[1, 1/k**(s - 1), 1/k**(s), 1/k**(s + 1), 1/k**(s + 3)], [1, 1/(k + 1)**(s - 1), 1/(k + 1)**(s), 1/(k + 1)**(s + 1), 1/(k + 1)**(s + 3)], [1, 1/(k + 2)**(s - 1), 1/(k + 2)**(s), 1/(k + 2)**(s + 1), 1/(k + 2)**(s + 3)], [1, 1/(k + 3)**(s - 1), 1/(k + 3)**(s), 1/(k + 3)**(s + 1), 1/(k + 3)**(s + 3)], [1, 1/(k + 4)**(s - 1), 1/(k + 4)**(s), 1/(k + 4)**(s + 1), 1/(k + 4)**(s + 3)]])
16 Tinv = mp.inverse(T)
17
18 Q2 = Tinv*B
19 print(Q2)
20 >>> [ 2.61237534868775] -> The approximaton of the Riemann zeta function at s = 3/2

```

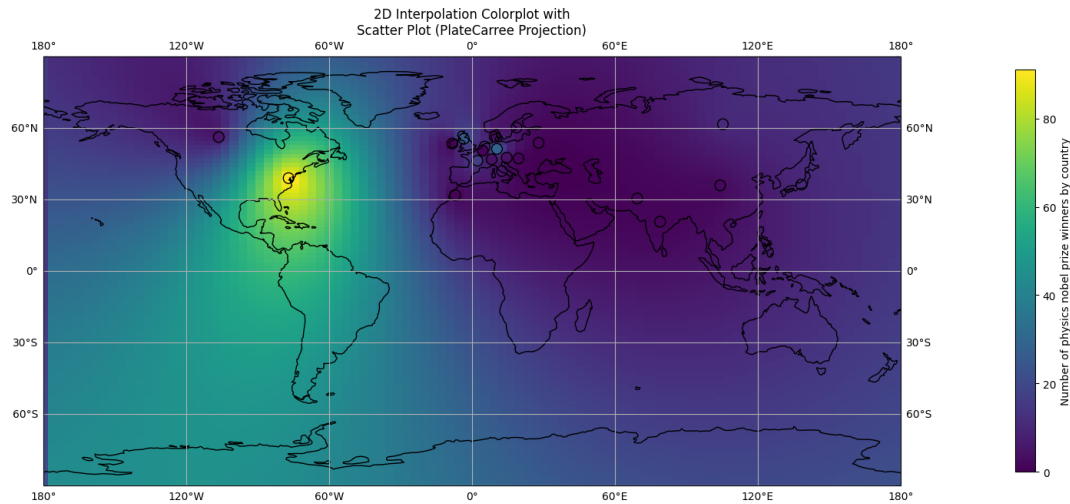
```

21 [ -2.0000000001121]
22 [ 0.5000000005620954]
23 [-0.125000118835117]
24 [0.0182315027087133]

```

So we can see that for a very slow value of p , like 4 or 5, we get a pretty good approximation of the series. Increasing the size of the matrix (i.e. increasing p) gives us a better approximation.

Radial basis functions interpolation.



```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import cartopy.crs as ccrs
4 from scipy.interpolate import Rbf
5
6 lats = [38.895,51.165691,55.378051,46.227638,61.52401,36.204824,52.132633,56.130366,
7         41.87194,60.128161,47.516231,46.818188,56.26392,35.86166,31.791702,53.41291,
8         20.593684,30.375321,50.503887,53.709807,47.162494]
9 lons = [-77.0366,10.451526,-3.435973,2.213749,105.318756,138.252924,5.291266,
10        -106.346771,12.56738,18.643501,14.550072,8.227512,9.501785,104.195397,
11        -7.09262,-8.24389,78.96288,69.345116,4.469936,27.953389,19.503304]
12 data = [96,28,25,16,11,10,9,5,5,4,4,4,3,2,1,1,1,1,1,1]
13 print(len(lats), len(lons), len(data))
14
15 # Create a meshgrid for interpolation
16 xi = np.linspace(-180, 180, 100)
17 yi = np.linspace(-90, 90, 100)
18 xi, yi = np.meshgrid(xi, yi)
19
20 # Different functions for the spherical interpolation:

```

```

21 # 'linear': Linear radial basis function
22 # 'multiquadric': Multiquadric radial basis function
23 # 'inverse': Inverse radial basis function
24 # 'gaussian': Gaussian radial basis function
25 # 'cubic': Cubic radial basis function
26 # 'quintic': Quintic radial basis function
27 # 'thin_plate': Thin-plate spline radial basis function
28
29 # Perform 2D interpolation using Rbf for spherical interpolation
30 rbf = Rbf(lons, lats, data, function='linear')
31 zi = rbf(xi, yi)
32
33 # Create a Cartopy PlateCarree projection centered at lon = 0
34 ax = plt.axes(projection=ccrs.PlateCarree(central_longitude=0))
35
36 # Add coastlines and gridlines
37 ax.coastlines()
38 ax.gridlines(draw_labels=True)
39
40 # Set extent of the plot
41 ax.set_extent([-180, 180, -90, 90], crs=ccrs.PlateCarree())
42
43 # Create color plot
44 plt.pcolormesh(xi, yi, zi, shading='auto', cmap='viridis')
45
46 # Create scatter plot with data as color
47 scatter = ax.scatter(lons, lats, c=data, cmap='viridis', s=100,\
48                     edgecolors='black', linewidths=1,\
49                     transform=ccrs.PlateCarree())
50
51 # Add colorbar
52 cbar = plt.colorbar(scatter, label='Number of physics nobel prize winners by country↵',
53                    ax=ax, shrink=0.7, pad = .1)
54 cbar.mappable.set_clim(0, 91)
55
56 # Add title
57 plt.title('2D Interpolation Colorplot with\nScatter Plot (PlateCarree Projection)')
58 plt.show()

```
