第二次作业解答

1.Cholesky 消元法解方程组

第一题复用了作业一中的matrixCalc.py，得到的结果如下：

```
(base) D:\PKU\notes\Computational Physics>python homework-2/T1.py
Cholesky消元法得到的矩阵:
+0.22360680  +0.31304952  +0.26832816  +0.22360680
+0.00000000  +0.04472136  -0.08944272  -0.00000000
+0.00000000  +0.00000000  +0.14142136  +0.21213203
+0.00000000  +0.00000000  +0.00000000  +0.07071068

[0.9999999999998886, 1.0000000000000666, 1.00000000000003, 0.9999999999999819]
[1.0000000000001632, 0.999999999999899, 0.9999999999999633, 1.0000000000000222]
```

其中下方分别是通过GEM和Cholesky方法得到的方程组的解。注意到由于浮点数精度问题，得到的解并不严格等于1，而是存在很小的误差。

2.三次样条插值

设$f(x)=\cos(x^2)$，设$[x_0,x_1]$与$[x_1,x_2]$两端的三次样条函数分别为：

$$\hat{f}(x)=\begin{cases}a_1(x-x_0)^3+b_1(x-x_0)^2+c_1(x-x_0)+d_1 & x\in[x_0,x_1]\\ a_2(x-x_1)^3+b_2(x-x_1)^2+c_2(x-x_1)+d_2 & x\in[x_1,x_2]\end{cases}$$

(a) 已知端点二阶导数为零

可以列出约束方程：

$$\begin{gathered}\hat{f}''(x_0)=\hat{f}''(x_2)=0\\ \hat{f}''(x_1+0)=\hat{f}''(x_1-0)\\ \hat{f}'(x_1+0)=\hat{f}'(x_1-0)\\ \hat{f}(x_0)=f(x_0)\\ \hat{f}(x_1-0)=\hat{f}(x_1+0)=f(x_1)\\ \hat{f}(x_2)=f(x_2)\end{gathered}$$

得到：

$$\begin{gathered}b_1=0\\ 6a_2h_1+2b_2=0\end{gathered}$$

$$
\begin{gathered}
6a_1h_0 + 2b_1 = 2b_2 \\
3a_1h_0^2 + 2b_1h_0 + c_1 = c_2 \\
d_1 = f(x_0) \\
a_1h_0^3 + b_1h_0^2 + c_1h_0 + d_1 = f(x_1) \\
d_2 = f(x_1) \\
a_2h_1^3 + b_2h_1^2 + c_2h_1 + d_2 = f(x_2)
\end{gathered}
$$

其中

$$
h_i = x_{i+1} - x_i
$$

为步长，

化简得到：

$$
\begin{gathered}
b_1 = 0 \\
d_1 = f(x_0) \\
d_2 = f(x_1) \\
a_1 = \frac{b_2}{3h_0} \\
a_2 = -\frac{b_2}{3h_1} \\
\frac{b_2h_0^2}{3} + c_1h_0 = f(x_1) - f(x_0) \\
\frac{-b_2}{3}h_1^2 + b_2h_1^2 + c_2h_1 = f(x_2) - f(x_1) \\
b_2h_0 + c_1 = c_2
\end{gathered}
$$

解方程组，并将$f(x_i)$简记为

$$
y_i = f(x_i)
$$

得到：

$$
\begin{gathered}
b_2 = \frac{-3h_0y_1 + 3h_0y_2 + 3h_1y_0 - 3h_1y_1}{2h_0^2h_1 + 3h_0h_1^2 - h_1^3} \\
c_1 = \frac{h_0^3y_1 - h_0^3y_2 - 3h_0^2h_1y_0 + 3h_0^2h_1y_1 - 3h_0h_1^2y_0 + 3h_0h_1^2y_1 + h_1^3y_0 - h_1^3y_1}{2h_0^3h_1 + 3h_0^2h_1^2 - h_0h_1^3} \\
c_2 = \frac{-2h_0^3y_1 + 2h_0^3y_2 - 3h_0h_1^2y_0 + 3h_0h_1^2y_1 + h_1^3y_0 - h_1^3y_1}{2h_0^3h_1 + 3h_0^2h_1^2 - h_0h_1^3}
\end{gathered}
$$

代入数值计算得到(见T2.ipynb)：

$$
\begin{gathered}
b_2 = -1.19082 \\
c_1 = 0.13132
\end{gathered}
$$

$$
\begin{gathered}
c_2 = -0.58316 \\
b_1 = 0.00000 \\
d_1 = 1.00000 \\
d_2 = 0.93590 \\
a_1 = -0.66156 \\
a_2 = 1.32313
\end{gathered}
$$

(b) 已知端点一阶导数

与上面的方程相比，该种情形下的约束方程只需要替换前两个式子即可：

$$
\begin{gathered}
\hat{f}'(x_0) = f'(x_0) \\
\hat{f}'(x_2) = f'(x_2) \\
\hat{f}''(x_1+0) = \hat{f}''(x_1-0) \\
\hat{f}'(x_1+0) = \hat{f}'(x_1-0) \\
\hat{f}(x_0) = f(x_0) \\
\hat{f}(x_1-0) = \hat{f}(x_1+0) = f(x_1) \\
\hat{f}(x_2) = f(x_2)
\end{gathered}
$$

得到：

$$
\begin{gathered}
c_1 - t_0 = 0 \\
3a_2h_1^2 + 2b_2h_1 + c_2 - t_2 = 0 \\
6a_1h_0 + 2b_1 = 2b_2 \\
3a_1h_0^2 + 2b_1h_0 + c_1 = c_2 \\
d_1 = f(x_0) \\
a_1h_0^3 + b_1h_0^2 + c_1h_0 + d_1 = f(x_1) \\
d_2 = f(x_1) \\
a_2h_1^3 + b_2h_1^2 + c_2h_1 + d_2 = f(x_2)
\end{gathered}
$$

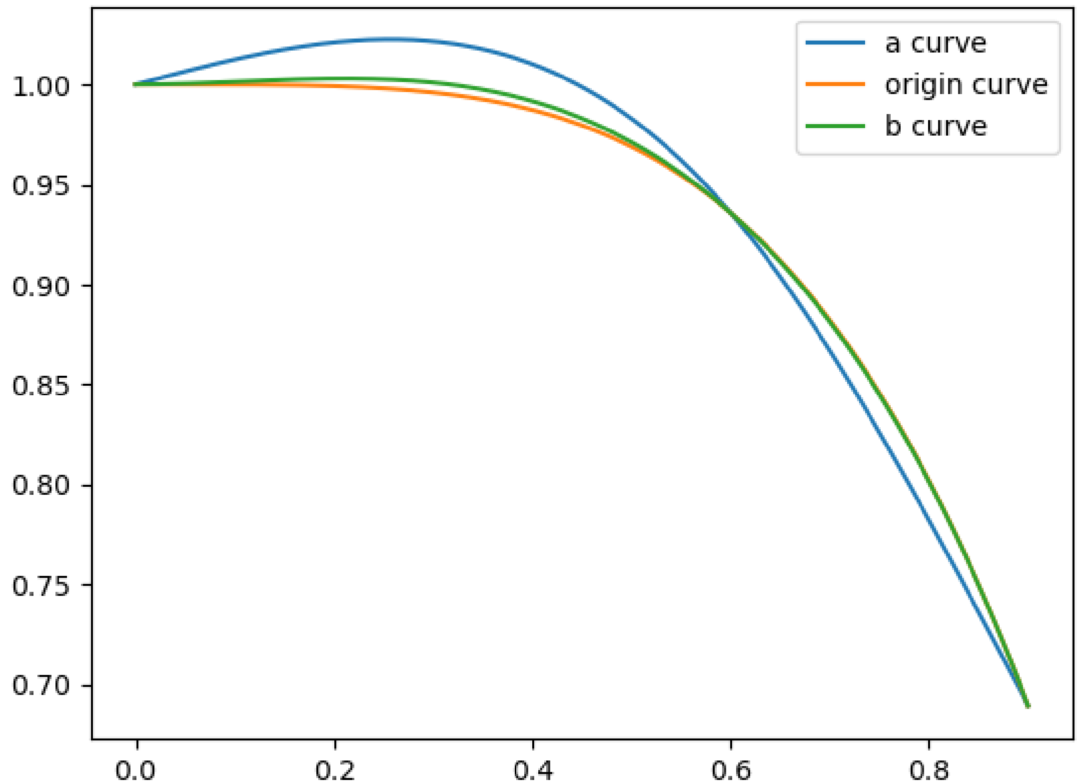
其中

$$
\begin{gathered}
t_0 = f'(0) = -2x\sin x^2|_{x=0} = 0 \\
t_2 = f'(0.9) \approx -1.30372
\end{gathered}
$$

$$
\begin{gathered}
a_1 = -0.62916 \\
a_2 = -1.12487 \\
b_1 = 0.19943 \\
b_2 = -0.93305 \\
c_1 = 0.00000 \\
c_2 = -0.44017 \\
d_1 = 1.00000
\end{gathered}
$$

$$d_2 = 0.93590$$

通过画图比较可知，第二种的拟合效果要更好。



3.Chebyshev多项式展开

展开过程：首先将$\log_2(x), x \in [1,2]$转换为$[0,1]$之间的函数：通过变量代换:$x' = 2\frac{x-1}{2-1} - 1 = 2x - 3$，得到新的函数为：

$$f(x') = f_0(x) = \log_2 \frac{x'+3}{2}$$

$f(x') = \sum_{n=0}^{\infty} c_n T_n(x')$，根据正交归一条件得到系数$c_n$为:

$$c_n = \int_{-1}^{1} \log_2 \frac{x'+3}{2} \frac{T_n(x')}{\sqrt{1-x'^2}} dx' \frac{1}{\frac{\pi}{2}(1+\delta_{n0})}$$

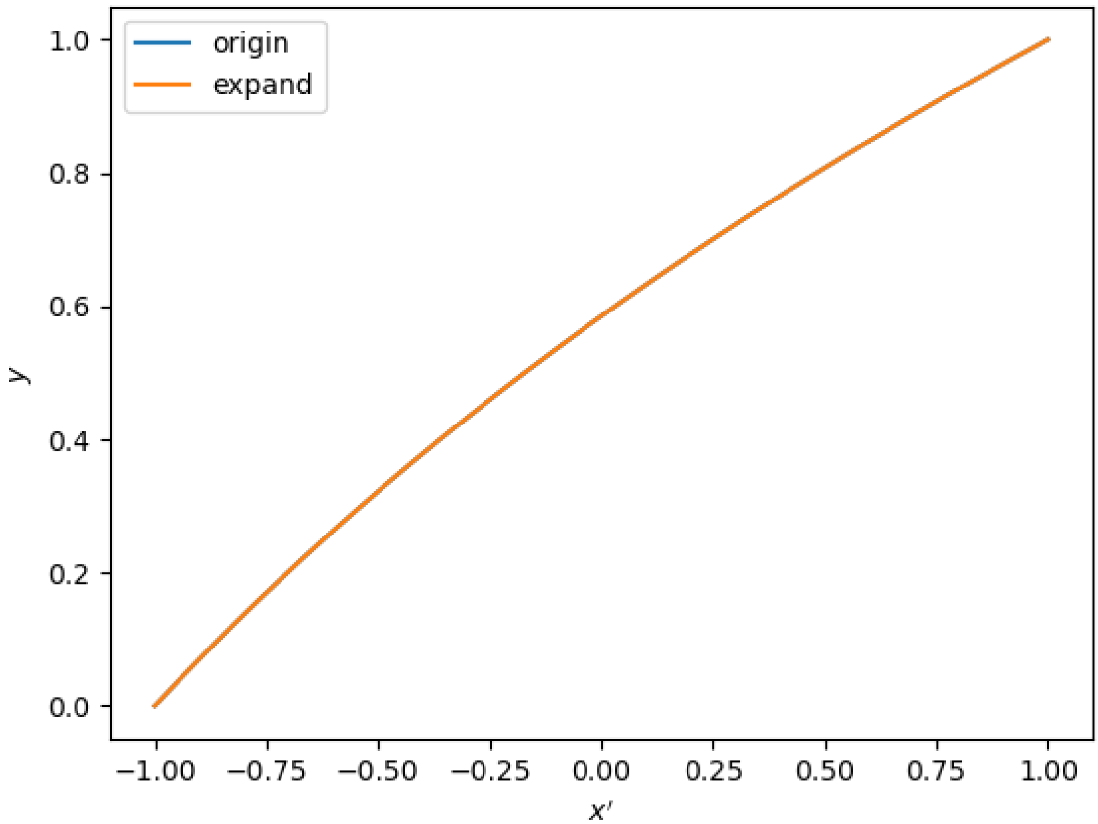
作代换：$x' = \cos\theta$，由$T_n(x) = \cos n \arccos x$,

$$c_n = \int_0^{\pi} f(\cos\theta) \cos n\theta d\theta \frac{(1-\delta_{n0})}{\pi}$$

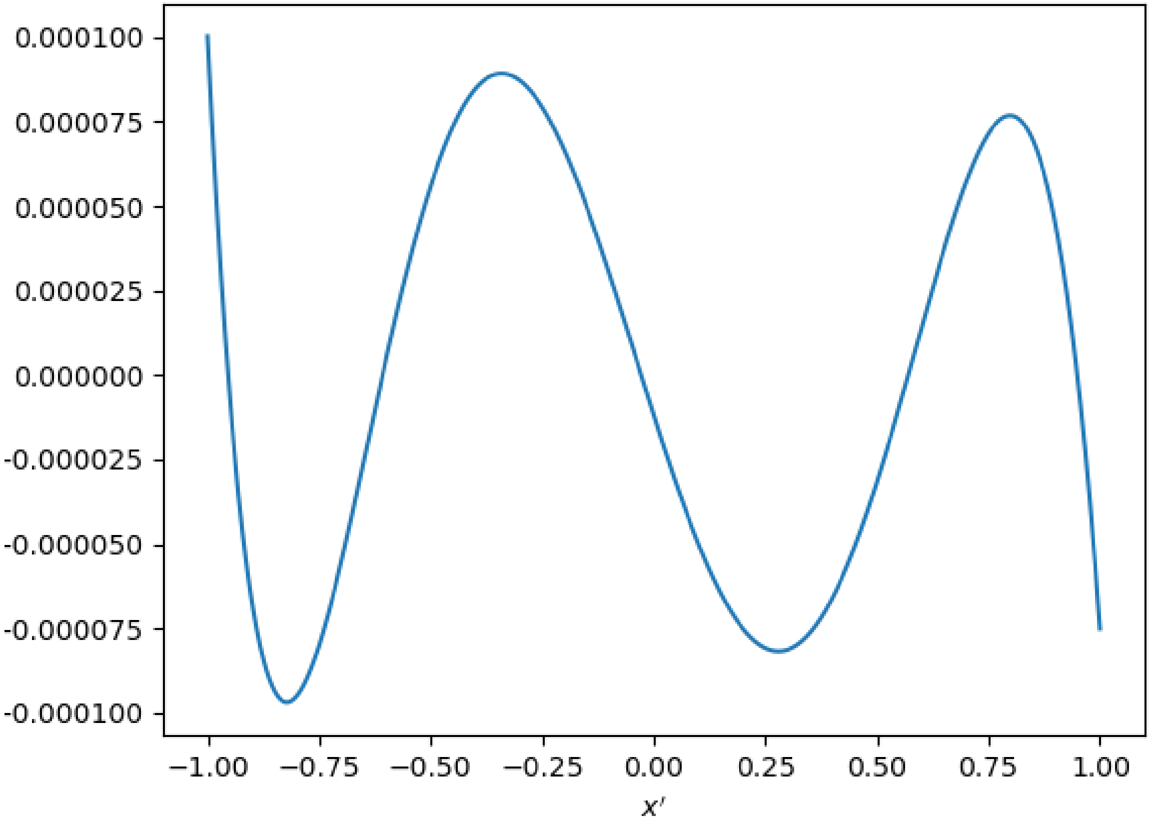
取上式的离散近似，并截断求和为N项：$\theta_k = \frac{\pi(k+1/2)}{N}$,$\Delta\theta_k = \pi/N$

$$c_n \approx c_{n,N} = \frac{2-\delta_{0m}}{N}\sum_{k=0}^{N-1} f(\cos\frac{\pi(k+1/2)}{N})\cos m\pi\frac{k+1/2}{N}$$

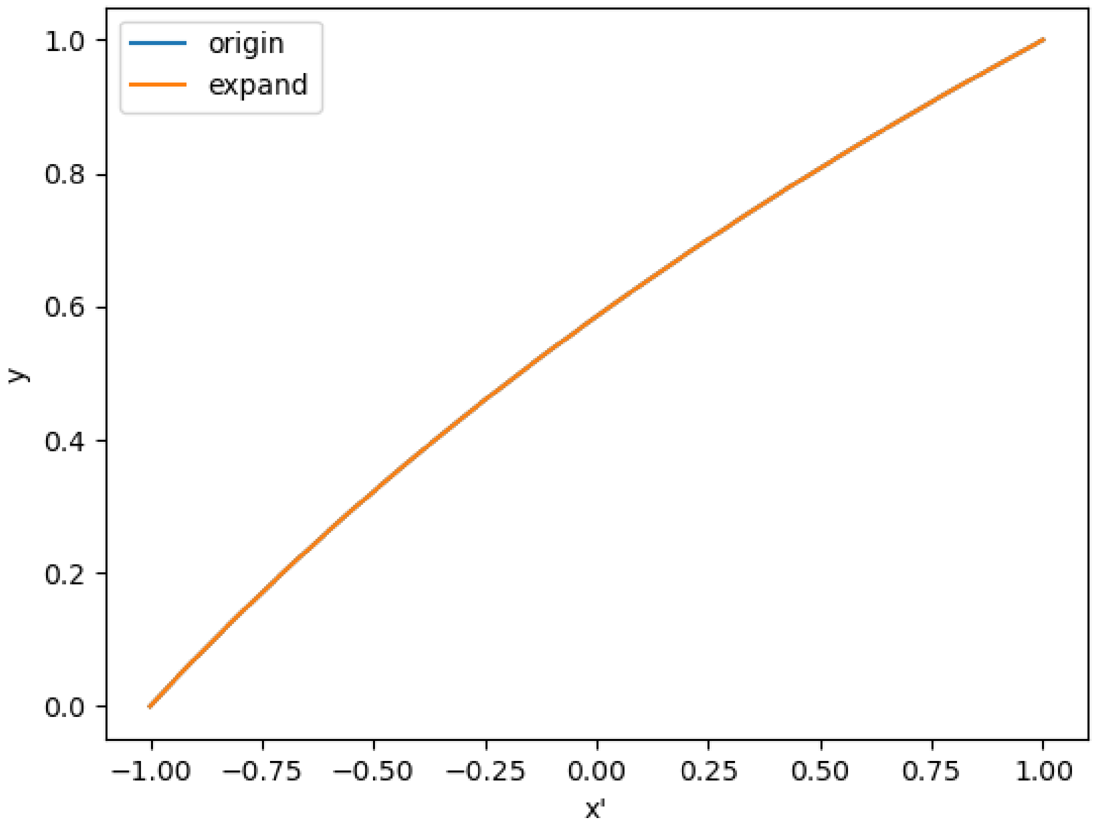
取0-4阶进行比较作图，可以看到二者的曲线十分接近：

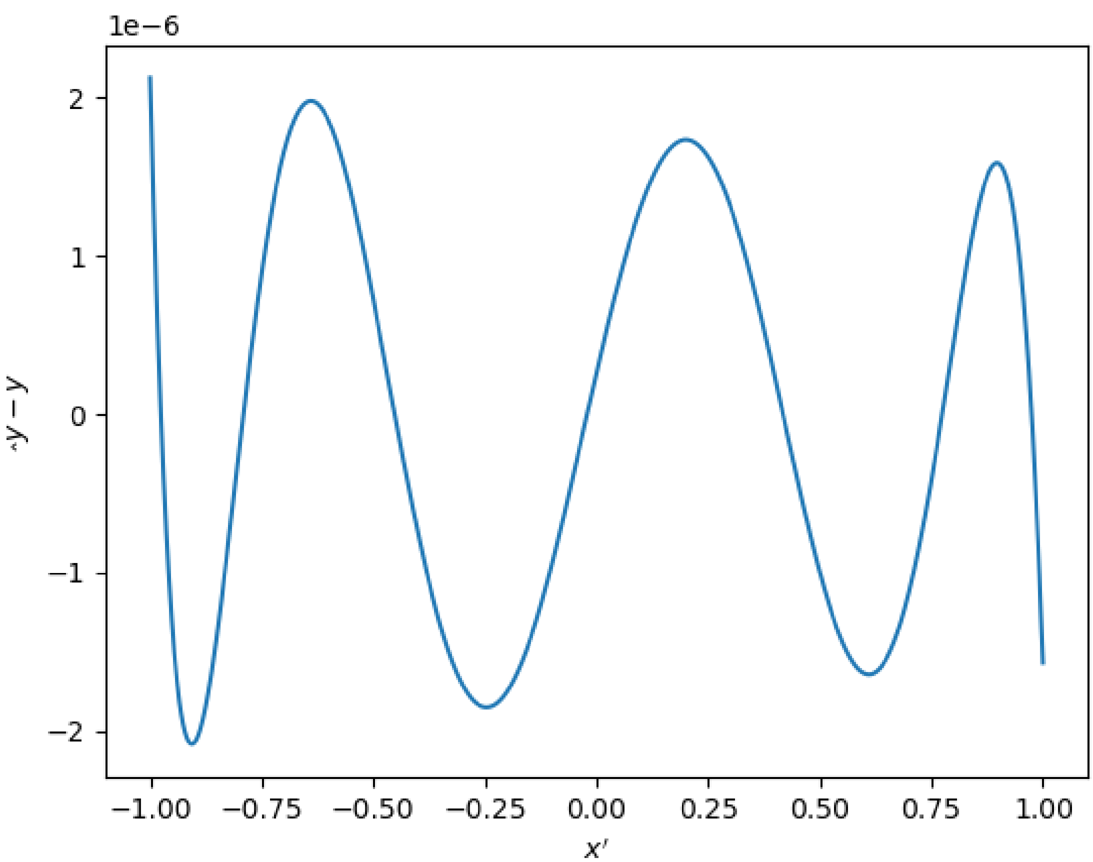


作差分析误差，可以看到误差在$\sim 10^{-5}$量级，而且在0两侧接近对称分布：



对0-6阶进行同样的分析，得到的误差将变得更小：

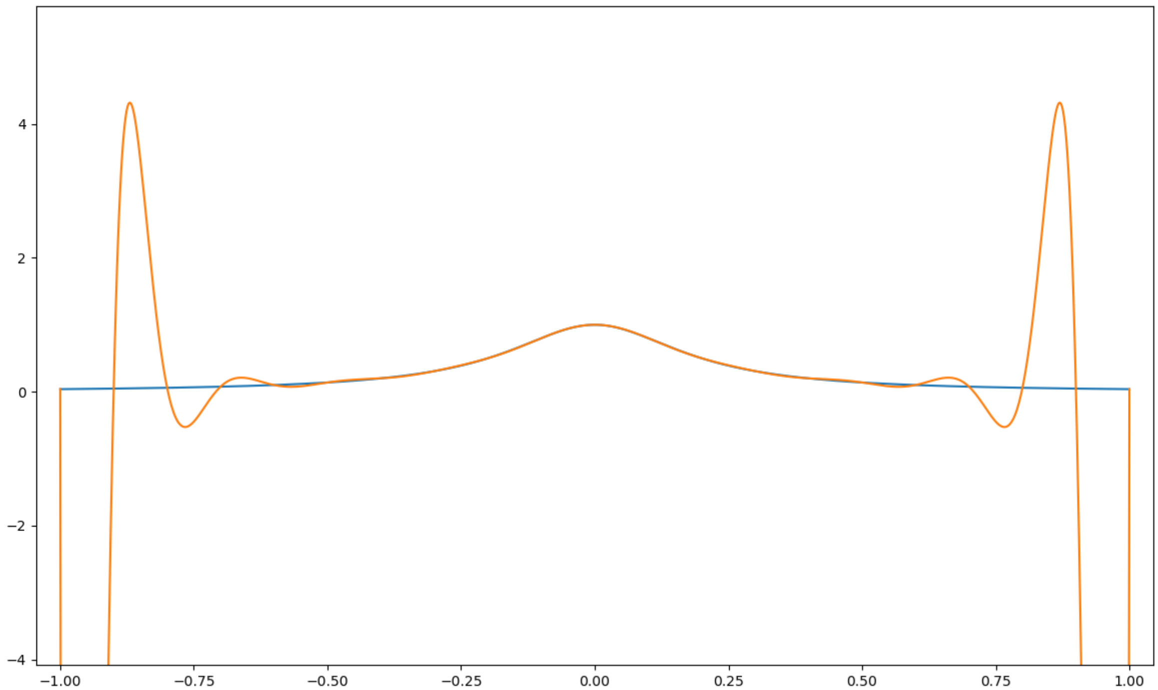

origin
expand
1.0
0.8
0.6
0.4
0.2
0.0
y
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x'


1e−6
2
1
0
−1
−2
$\hat{y} - y$
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
x'

4.Runge效应

a. Lagrange插值

通过拉格朗日插值法得到$P_{20}(x)$，作图得到：



拉格朗日插值法在插值区域中心处近似比较好，但在两端会出现剧烈震荡。

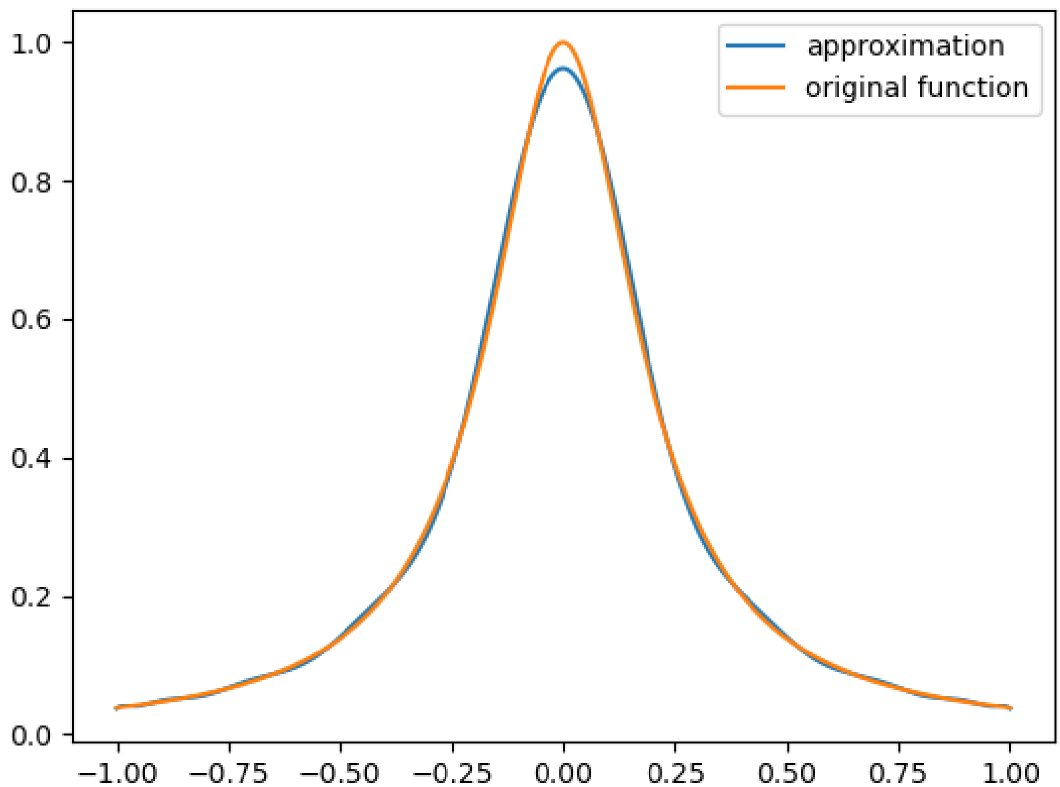
做表格如下所示：

```
x        origin  Lagrange        abs
----------------------------------------
-1.0000 +0.0385 +0.0385 +0.0000
-0.9500 +0.0424 -39.9524         +39.9949
-0.9000 +0.0471 +0.0471 +0.0000
-0.8500 +0.0525 +3.4550 +3.4025
-0.8000 +0.0588 +0.0588 +0.0000
-0.7500 +0.0664 -0.4471 +0.5134
-0.7000 +0.0755 +0.0755 +0.0000
-0.6500 +0.0865 +0.2024 +0.1159
-0.6000 +0.1000 +0.1000 +0.0000
-0.5500 +0.1168 +0.0807 +0.0361
-0.5000 +0.1379 +0.1379 +0.0000
-0.4500 +0.1649 +0.1798 +0.0148
-0.4000 +0.2000 +0.2000 +0.0000
-0.3500 +0.2462 +0.2384 +0.0077
-0.3000 +0.3077 +0.3077 +0.0000
-0.2500 +0.3902 +0.3951 +0.0048
-0.2000 +0.5000 +0.5000 +0.0000
-0.1500 +0.6400 +0.6368 +0.0032
-0.1000 +0.8000 +0.8000 +0.0000
-0.0500 +0.9412 +0.9425 +0.0013
0.0000  +1.0000 +1.0000 +0.0000
0.0500  +0.9412 +0.9425 +0.0013
0.1000  +0.8000 +0.8000 +0.0000
0.1500  +0.6400 +0.6368 +0.0032
0.2000  +0.5000 +0.5000 +0.0000
0.2500  +0.3902 +0.3951 +0.0048
0.3000  +0.3077 +0.3077 +0.0000
0.3500  +0.2462 +0.2384 +0.0077
0.4000  +0.2000 +0.2000 +0.0000
0.4500  +0.1649 +0.1798 +0.0148
0.5000  +0.1379 +0.1379 +0.0000
0.5500  +0.1168 +0.0807 +0.0361
0.6000  +0.1000 +0.1000 +0.0000
0.6500  +0.0865 +0.2024 +0.1159
0.7000  +0.0755 +0.0755 +0.0000
0.7500  +0.0664 -0.4471 +0.5134
0.8000  +0.0588 +0.0588 +0.0000
0.8500  +0.0525 +3.4550 +3.4025
0.9000  +0.0471 +0.0471 +0.0000
0.9500  +0.0424 -39.9524         +39.9949
```

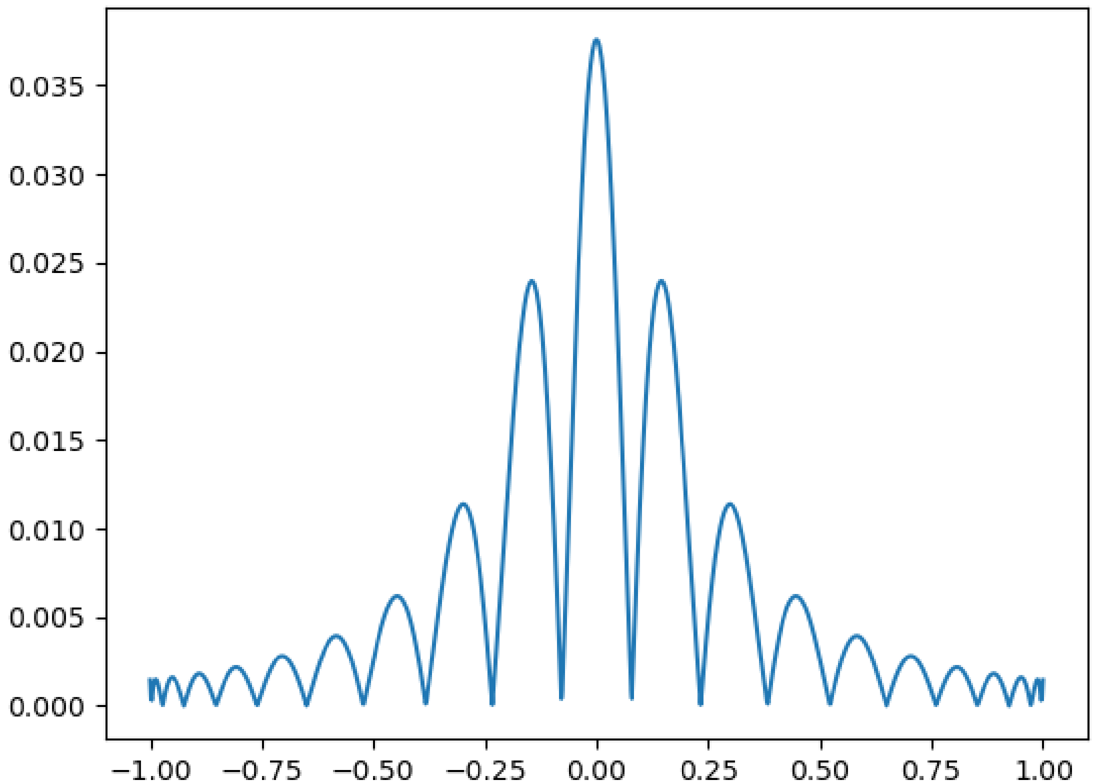
```
0.9500  +0.0424 -39.9524        +39.9949
1.0000  +0.0385 +0.0385 +0.0000
```

b. Chebyshev多项式插值

进行Chebyshev多项式插值，得到的结果如下图所示：



计算二者差的绝对值，作图得到：


0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

或用数据表表示：

x	origin	Chebyshev	abs
-1.0000	+0.0385	+0.0370	+0.0014
-0.9500	+0.0424	+0.0408	+0.0016
-0.9000	+0.0471	+0.0487	+0.0016
-0.8500	+0.0525	+0.0523	+0.0002
-0.8000	+0.0588	+0.0567	+0.0021
-0.7500	+0.0664	+0.0672	+0.0008
-0.7000	+0.0755	+0.0783	+0.0028
-0.6500	+0.0865	+0.0865	+0.0000
-0.6000	+0.1000	+0.0964	+0.0036
-0.5500	+0.1168	+0.1141	+0.0027
-0.5000	+0.1379	+0.1405	+0.0026
-0.4500	+0.1649	+0.1711	+0.0062
-0.4000	+0.2000	+0.2028	+0.0028
-0.3500	+0.2462	+0.2402	+0.0060
-0.3000	+0.3077	+0.2963	+0.0114
-0.2500	+0.3902	+0.3853	+0.0049
-0.2000	+0.5000	+0.5119	+0.0119
-0.1500	+0.6400	+0.6639	+0.0239
-0.1000	+0.8000	+0.8126	+0.0126
-0.0500	+0.9412	+0.9221	+0.0191
0.0000	+1.0000	+0.9624	+0.0376
0.0500	+0.9412	+0.9221	+0.0191
0.1000	+0.8000	+0.8126	+0.0126
0.1500	+0.6400	+0.6639	+0.0239
0.2000	+0.5000	+0.5119	+0.0119
0.2500	+0.3902	+0.3853	+0.0049
0.3000	+0.3077	+0.2963	+0.0114
0.3500	+0.2462	+0.2402	+0.0060
0.4000	+0.2000	+0.2028	+0.0028
0.4500	+0.1649	+0.1711	+0.0062
0.5000	+0.1379	+0.1405	+0.0026
0.5500	+0.1168	+0.1141	+0.0027
0.6000	+0.1000	+0.0964	+0.0036
0.6500	+0.0865	+0.0865	+0.0000
0.7000	+0.0755	+0.0783	+0.0028
0.7500	+0.0664	+0.0672	+0.0008
0.8000	+0.0588	+0.0567	+0.0021
0.8500	+0.0525	+0.0523	+0.0002
0.9000	+0.0471	+0.0487	+0.0016
0.9500	+0.0424	+0.0408	+0.0016

```
1.0000  +0.0385 +0.0370 +0.0014
```

可以看到，切比雪夫近似在$x = 0$附近的误差最大，相对误差远小于拉格朗日插值近似

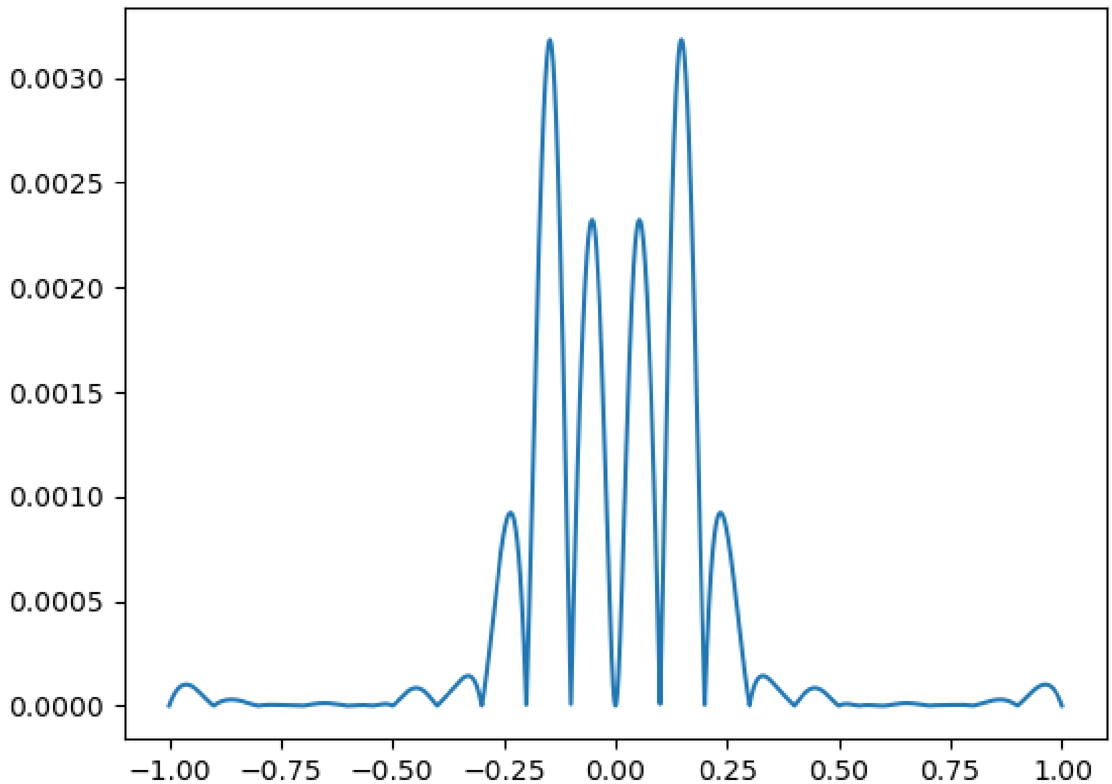
c. 三次样条函数插值

编写三次样条插值程序spline_interpolation.py和自动测试程序autotest.py，得到三次样条函数插值曲线（由于该种插值方法与原函数贴合紧密，无法看出区别，故只作出二者绝对值随x变化）：

数据表：

```
(base) D:\PKU\notes\Computational Physics\homework-2>python T4_cubic_spline.py
----------------------------------------
-1.0000 +0.0385 +0.0385 +0.0000
-0.9500 +0.0424 +0.0425 +0.0001
-0.9000 +0.0471 +0.0471 +0.0000
-0.8500 +0.0525 +0.0524 +0.0000
-0.8000 +0.0588 +0.0588 +0.0000
-0.7500 +0.0664 +0.0664 +0.0000
-0.7000 +0.0755 +0.0755 +0.0000
-0.6500 +0.0865 +0.0865 +0.0000
-0.6000 +0.1000 +0.1000 +0.0000
-0.5500 +0.1168 +0.1168 +0.0000
-0.5000 +0.1379 +0.1379 +0.0000
-0.4500 +0.1649 +0.1649 +0.0001
-0.4000 +0.2000 +0.2000 +0.0000
-0.3500 +0.2462 +0.2463 +0.0001
-0.3000 +0.3077 +0.3077 +0.0000
-0.2500 +0.3902 +0.3894 +0.0008
-0.2000 +0.5000 +0.5000 +0.0000
-0.1500 +0.6400 +0.6432 +0.0032
-0.1000 +0.8000 +0.8000 +0.0000
-0.0500 +0.9412 +0.9389 +0.0023
0.0000  +1.0000 +1.0000 +0.0000
0.0500  +0.9412 +0.9389 +0.0023
0.1000  +0.8000 +0.8000 +0.0000
0.1500  +0.6400 +0.6432 +0.0032
0.2000  +0.5000 +0.5000 +0.0000
0.2500  +0.3902 +0.3894 +0.0008
0.3000  +0.3077 +0.3077 +0.0000
0.3500  +0.2462 +0.2463 +0.0001
0.4000  +0.2000 +0.2000 +0.0000
0.4500  +0.1649 +0.1649 +0.0001
0.5000  +0.1379 +0.1379 +0.0000
0.5500  +0.1168 +0.1168 +0.0000
0.6000  +0.1000 +0.1000 +0.0000
0.6500  +0.0865 +0.0865 +0.0000
0.7000  +0.0755 +0.0755 +0.0000
0.7500  +0.0664 +0.0664 +0.0000
0.8000  +0.0588 +0.0588 +0.0000
0.8500  +0.0525 +0.0524 +0.0000
0.9000  +0.0471 +0.0471 +0.0000
0.9500  +0.0424 +0.0425 +0.0001
1.0000  +0.0385 +0.0385 +0.0000
```

图像：



可以看到，二者最大误差在0.003左右，是切比雪夫多项式的拟合最大误差的$1/10$。

5. 样条函数在计算机绘图中的应用

(a)

选取$t=0,1,2,\cdots,8$, 给出$x_t=r(\phi)\cos\phi$和$y_t=r(\phi)\sin\phi$的数值。将数值作为精确的数值列到一个表中。

t	x_t	y_t
0	0	0
1	$\frac{\sqrt{2}\left(1-\frac{\sqrt{2}}{2}\right)}{2}$	$\frac{\sqrt{2}\left(1-\frac{\sqrt{2}}{2}\right)}{2}$
2	0	1
3	$-\frac{\sqrt{2}\left(\frac{\sqrt{2}}{2}+1\right)}{2}$	$\frac{\sqrt{2}\left(\frac{\sqrt{2}}{2}+1\right)}{2}$
4	-2	0

t	x_t	y_t
5	$-\frac{\sqrt{2}\left(\frac{\sqrt{2}}{2}+1\right)}{2}$	$\frac{\sqrt{2}\left(\frac{\sqrt{2}}{2}+1\right)}{2}$
6	0	-1
7	$\frac{\sqrt{2}\left(1-\frac{\sqrt{2}}{2}\right)}{2}$	$-\frac{\sqrt{2}\left(1-\frac{\sqrt{2}}{2}\right)}{2}$

b)给出三次样条函数$S_\Delta(X;t)$和$S_\Delta(Y;t)$

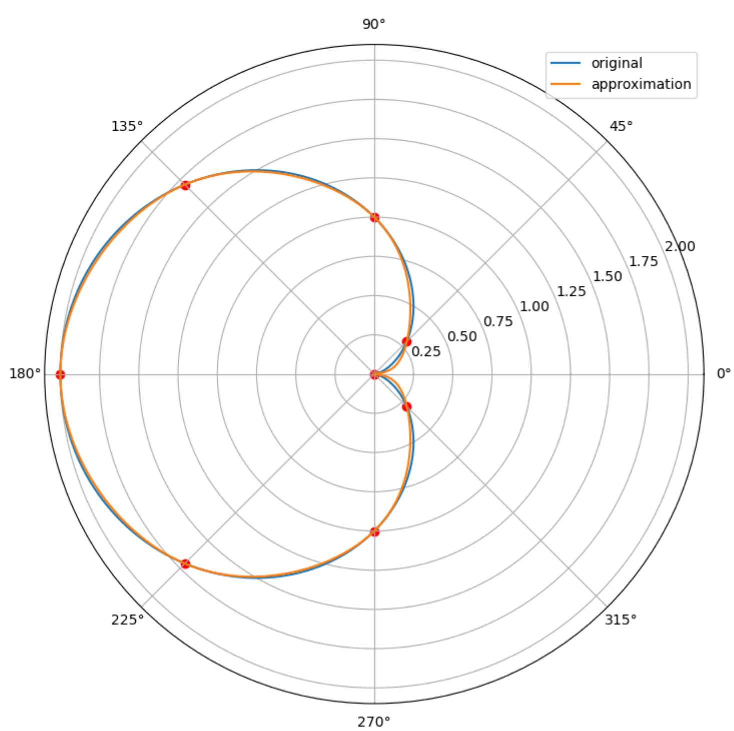
两个样条函数的表达式比较繁琐，各段的系数a,b,c,d请通过运行T5.ipynb获得，从而可以写出其分段表达式：

$$S_\Delta(X,t)=a_t+b_t(x-x_t)+c_t(x-x_t)^2+d_t(x-x_t)^3,\ \ x\in[x_t,x_{t+1}]$$

$$S_\Delta(Y,t)=a_t+b_t(y-y_t)+c_t(y-y_t)^2+d_t(y-y_t)^3,\ \ y\in[y_t,y_{t+1}]$$

(c)画出曲线，比较

作图如下所示。插值点已经在图中标出。



(d)

该算法可以平滑连接所有点，是因为在该算法中，x和y都是关于参数t的三次样条插值函数，三次样条插值是二阶导数连续的，因此当参数t连续变化时，它们形成的点$(x(t), y(t))$也将构成一条平滑曲线。