Python 的数值计算

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1 定积分

1.0.1 一元定积分

[1]:
```
# 导入积分模块
import scipy.integrate as integrate
# 导入基础计算库
import numpy as np
```

[2]:
```
result = integrate.quad(lambda x: np.sin(x)+3*x**2-3*x, 0, 4.5)
result
```

[2]: (61.960795799430784, 6.912907000856692e-13)

1.0.2 一元定积分，给定参数

[1]:
```
# 导入积分模块
import scipy.integrate as integrate
# 导入基础计算库
import numpy as np
```

[2]:
```
# 定义函数
def integrand(x, a, b):
    return a*x**2 + b


a = 2
b = 1
```

[3]:
```
I = integrate.quad(integrand, 0, 1, args=(a,b))
I
```

[3]: (1.6666666666666667, 1.8503717077085944e-14)

1.0.3 二元重积分

[1]:
```
# 导入积分
from scipy.integrate import dblquad
# 导入基础计算库
import numpy as np
# 二重积分
def I(n):
    return dblquad(
        lambda t, x: np.exp(-x*t)/t**n,
        0,
        np.inf,
        lambda x: 1,
        lambda x: np.inf
    )
```

[2]:
```
print(I(4))
```

```
(0.2500000000043577, 1.298303346936809e-08)
```

[3]:
```
print(I(3))
```

```
(0.33333333325010883, 1.3888461883425516e-08)
```

[4]:
```
print(I(2))
```

```
(0.4999999999985751, 1.3894083651858995e-08)
```

[5]:
```
area = dblquad(
    lambda x, y: x*y,
    0,
    0.5,
    lambda x: 0,
    lambda x: 1-2*x
)
area
```

[5]:
```
(0.010416666666666668, 4.101620128472366e-16)
```

1.0.4 辛普森法计算积分

[1]:
```
# 导入积分模块
import scipy.integrate as integrate
# 导入基础计算库
import numpy as np
```

[2]:
```
def f1(x):
   return x**2


def f2(x):
   return x**3
```

[3]:
```
x = np.array([1,3,4])
y1 = f1(x)
# 辛普森数值计算积分
I1 = integrate.simpson(y1, x)
print(I1)
```

```
21.0
```

[4]:
```
y2 = f2(x)
I2 = integrate.simpson(y2, x)
print(I2)
```

```
61.5
```

2 最优化

2.0.1 多元函数无约束的最优化问题

[1]:
```
# 导入基础计算库
import numpy as np
# 导入最优化库
from scipy.optimize import minimize
```

[2]:
```
def rosen(x):
    """The Rosenbrock function"""
    return sum(100.0*(x[1:]-x[:-1]**2.0)**2.0 + (1-x[:-1])**2.0)
```

[3]:
```
# 初始值
x0 = np.array([1.3, 0.7, 0.8, 1.9, 1.2])
res = minimize(
    rosen, x0, method="nelder-mead",
    options={"xatol": 1e-8, "disp": True}
)
print(res)
```

```
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 339
         Function evaluations: 571
       message: Optimization terminated successfully.
       success: True
        status: 0
           fun: 4.861153433422115e-17
             x: [ 1.000e+00  1.000e+00  1.000e+00  1.000e+00  1.000e+00]
           nit: 339
          nfev: 571
 final_simplex: (array([[ 1.000e+00,  1.000e+00, …,  1.000e+00,
                          1.000e+00],
                        [ 1.000e+00,  1.000e+00, …,  1.000e+00,
                          1.000e+00],
                        …,
                        [ 1.000e+00,  1.000e+00, …,  1.000e+00,
                          1.000e+00],
```

```
                    [ 1.000e+00,  1.000e+00, …,  1.000e+00,
                      1.000e+00]]), array([ 4.861e-17,  7.652e-17,
8.114e-17,  8.633e-17,
                     8.641e-17,  2.179e-16]))
```

[4]:
```
# 最小值点
print(res.x)
```

```
[1. 1. 1. 1. 1.]
```

[5]:
```
# 目标函数的梯度
def rosen_der(x):
    xm = x[1:-1]
    xm_m1 = x[:-2]
    xm_p1 = x[2:]
    der = np.zeros_like(x)
    der[1:-1] = 200*(xm-xm_m1**2) - 400*(xm_p1 - xm**2)*xm - 2*(1-xm)
    der[0] = -400*x[0]*(x[1]-x[0]**2) - 2*(1-x[0])
    der[-1] = 200*(x[-1]-x[-2]**2)
    return der
```

[6]:
```
res = minimize(
    rosen, x0, method="BFGS", jac=rosen_der,
    options={"disp": True}
)
print(res)
```

```
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 25
         Function evaluations: 30
         Gradient evaluations: 30
  message: Optimization terminated successfully.
  success: True
   status: 0
      fun: 4.0130879949972905e-13
        x: [ 1.000e+00  1.000e+00  1.000e+00  1.000e+00  1.000e+00]
      nit: 25
      jac: [-5.690e-06 -2.733e-06 -2.545e-06 -7.735e-06  5.781e-06]
 hess_inv: [[ 7.588e-03  1.244e-02 …  4.615e-02  9.222e-02]
            [ 1.244e-02  2.482e-02 …  9.299e-02  1.857e-01]
            …
            [ 4.615e-02  9.299e-02 …  3.738e-01  7.462e-01]
            [ 9.222e-02  1.857e-01 …  7.462e-01  1.494e+00]]
     nfev: 30
     njev: 30
```

[7]:
```python
# 最小值点
print(res.x)
```

```
[1.00000004 1.0000001  1.00000021 1.00000044 1.00000092]
```

[8]:
```python
# 目标函数的黑塞矩阵
def rosen_hess(x):
    x = np.asarray(x)
    H = np.diag(-400*x[:-1],1) - np.diag(400*x[:-1],-1)
    diagonal = np.zeros_like(x)
    diagonal[0] = 1200*x[0]**2-400*x[1]+2
    diagonal[-1] = 200
    diagonal[1:-1] = 202 + 1200*x[1:-1]**2 - 400*x[2:]
    H = H + np.diag(diagonal)
    return H
```

[9]:
```python
res = minimize(
    rosen, x0, method="Newton-CG",
    jac=rosen_der, hess=rosen_hess,
    options={"xtol": 1e-8, "disp": True}
)
print(res)
```

```
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 24
         Function evaluations: 33
         Gradient evaluations: 33
         Hessian evaluations: 24
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 3.5306674342205174e-17
       x: [ 1.000e+00  1.000e+00  1.000e+00  1.000e+00  1.000e+00]
     nit: 24
     jac: [ 2.687e-08  9.267e-08  3.701e-07  1.485e-06 -8.526e-07]
    nfev: 33
    njev: 33
    nhev: 24
```

[10]:
```python
# 最小值点
print(res.x)
```

```
[1.         1.         1.         0.99999999 0.99999999]
```

[11]:
```python
res = minimize(
    rosen, x0, method="trust-ncg",
    jac=rosen_der, hess=rosen_hess,
    options={"gtol": 1e-8, "disp": True}
)
print(res)
```

```
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 20
         Function evaluations: 21
         Gradient evaluations: 20
         Hessian evaluations: 19
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 1.232595164407831e-30
       x: [ 1.000e+00  1.000e+00  1.000e+00  1.000e+00  1.000e+00]
     nit: 20
     jac: [-0.000e+00  0.000e+00  0.000e+00  4.441e-14 -2.220e-14]
    nfev: 21
    njev: 20
    nhev: 19
    hess: [[ 8.020e+02 -4.000e+02 ...  0.000e+00  0.000e+00]
           [-4.000e+02  1.002e+03 ...  0.000e+00  0.000e+00]
           ...
           [ 0.000e+00  0.000e+00 ...  1.002e+03 -4.000e+02]
           [ 0.000e+00  0.000e+00 ... -4.000e+02  2.000e+02]]
```

[12]:
```python
# 最小值点
print(res.x)
```

```
[1. 1. 1. 1. 1.]
```

[13]:
```python
res = minimize(
    rosen, x0, method="trust-krylov",
    jac=rosen_der, hess=rosen_hess,
    options={"gtol": 1e-8, "disp": True}
)
print(res)
```

```
 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
     0      0  cg_i -6.273083e+02  4.029038e+02  0.000000e+00  0.000000e+00
```

```
2.246107e+03  4.021147e+03  2.486853e-04  3.217671e-02

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -9.528585e+01  1.478412e+02  0.000000e+00  0.000000e+00
6.001708e+02  1.890129e+03  5.290645e-04  6.067939e-02

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -8.662599e+00  5.824611e+01  0.000000e+00  0.000000e+00
1.285783e+02  9.542387e+02  1.047956e-03  2.052100e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -1.798598e+00  3.481545e+01  0.000000e+00  0.000000e+00
5.168333e+01  7.425689e+02  1.346676e-03  4.537776e-01

    1     0  cg_i -2.721261e+00  1.426076e+01  0.000000e+00  0.000000e+00
5.002168e+02  9.938183e+02  1.522401e-03  1.677804e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -7.242386e-02  4.575385e+00  0.000000e+00  0.000000e+00
1.400669e+01  1.354439e+03  7.383128e-04  1.067048e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -8.331939e-03  2.017934e+00  0.000000e+00  0.000000e+00
4.550681e+00  1.242730e+03  8.046802e-04  1.966351e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -1.639774e-03  1.039910e+00  0.000000e+00  0.000000e+00
2.017620e+00  1.241266e+03  8.056290e-04  2.656515e-01

    1     0  cg_i -2.362748e-03  4.063620e-01  0.000000e+00  0.000000e+00
6.397659e+02  1.077635e+03  1.337094e-03  1.526986e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -1.218928e-04  2.280362e-01  0.000000e+00  0.000000e+00
4.066296e-01  6.782503e+02  1.474382e-03  3.144920e-01

    1     0  cg_i -1.746236e-04  3.200387e-01  0.000000e+00  0.000000e+00
3.803600e+02  7.063791e+02  2.028090e-03  1.969687e+00
```

```
    2     0  cg_i -3.519759e-04  3.984883e-01  0.000000e+00  0.000000e+00
6.920085e+02  1.259964e+03  3.463074e-03  1.550338e+00

    3     0  cg_i -5.758296e-03  3.569591e+00  0.000000e+00  0.000000e+00
3.595435e+02  4.623626e+02  6.809270e-02  8.024274e+01

 TR Solving trust region problem, radius 2.500000e-01; starting on first
irreducible block
 TR Coldstart. Seeking suitable initial Î»â , starting with 0
 TR Starting Newton iteration for Î»â  with initial choice 0.000000e+00
 TR  iter        Î»            dÎ»       â hâ (Î»)â -radius
 TR      1  2.943145e-01  2.943145e-01  3.059076e-07
 TR      2  2.943152e-01  7.617834e-07 -1.912359e-14

 iter inewton type    objective     Î³áµ¢â â |háµ¢|      leftmost         Î»
Î³             Î´
    4     2   hot -2.875301e-02  0.000000e+00  0.000000e+00  2.943152e-01
1.315535e+02  1.382362e+03

Early exit as hotstart with early termination on

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost         Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -7.518233e-03  1.522235e+00  0.000000e+00  0.000000e+00
4.090478e+00  1.112762e+03  8.986647e-04  1.384891e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost         Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -1.096841e-03  8.409536e-01  0.000000e+00  0.000000e+00
1.518407e+00  1.051001e+03  9.514742e-04  3.067379e-01

    1     0  cg_i -1.570721e-03  3.392978e-01  0.000000e+00  0.000000e+00
5.820853e+02  1.068564e+03  1.340154e-03  1.627863e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost         Î»
Î³             Î´             Î±             Î²
    0     0  cg_i -6.479100e-05  1.641071e-01  0.000000e+00  0.000000e+00
3.391135e-01  8.874534e+02  1.126820e-03  2.341879e-01

    1     0  cg_i -8.150449e-05  1.044376e-01  0.000000e+00  0.000000e+00
4.294650e+02  1.013502e+03  1.241202e-03  4.050039e-01

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost         Î»
Î³             Î´             Î±             Î²
```

```
     0     0  cg_i -6.864955e-06  9.214155e-02  0.000000e+00  0.000000e+00
1.044215e-01  7.941673e+02  1.259181e-03  7.786304e-01

     1     0  cg_i -1.991674e-05  1.301343e-01  0.000000e+00  0.000000e+00
7.007735e+02  9.436083e+02  3.074601e-03  1.994676e+00

     2     0  cg_i -1.195321e-04  3.179941e-01  0.000000e+00  0.000000e+00
4.593539e+02  7.337610e+02  1.176448e-02  5.971103e+00

     3     0  cg_i -4.188868e-04  7.535566e-01  0.000000e+00  0.000000e+00
2.077086e+02  6.764504e+02  5.920769e-03  5.615569e+00

 iter inewton type    objective      â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
     0     0  cg_i -8.816451e-04  5.184366e-01  0.000000e+00  0.000000e+00
1.324450e+00  9.948272e+02  1.005200e-03  1.532216e-01

 iter inewton type    objective      â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
     0     0  cg_i -1.332921e-04  2.868284e-01  0.000000e+00  0.000000e+00
5.178932e-01  1.006112e+03  9.939256e-04  3.067355e-01

     1     0  cg_i -1.931659e-04  1.227712e-01  0.000000e+00  0.000000e+00
5.572219e+02  9.956424e+02  1.455536e-03  1.832097e-01

 iter inewton type    objective      â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
     0     0  cg_i -7.494787e-06  5.036955e-02  0.000000e+00  0.000000e+00
1.227312e-01  1.004896e+03  9.951282e-04  1.684325e-01

     1     0  cg_i -9.038951e-06  2.464230e-02  0.000000e+00  0.000000e+00
4.124145e+02  9.907665e+02  1.217272e-03  2.393460e-01

     2     0  cg_i -9.419876e-06  1.237374e-02  0.000000e+00  0.000000e+00
4.019071e+02  9.936897e+02  1.254603e-03  2.521387e-01

 iter inewton type    objective      â gâ â _Mâ »Â¹      leftmost          Î»
Î³             Î´             Î±             Î²
     0     0  cg_i -8.123315e-08  6.017427e-03  0.000000e+00  0.000000e+00
1.237352e-02  9.423732e+02  1.061151e-03  2.365023e-01

     1     0  cg_i -1.141577e-07  5.764425e-03  0.000000e+00  0.000000e+00
4.582903e+02  7.727586e+02  1.818562e-03  9.176781e-01

     2     0  cg_i -1.714596e-07  9.206608e-03  0.000000e+00  0.000000e+00
```

```
5.267653e+02  7.945608e+02  3.448951e-03  2.550864e+00

     3      0  cg_i -3.626456e-07  1.409674e-02  0.000000e+00  0.000000e+00
4.630807e+02  9.612789e+02  4.511145e-03  2.344434e+00

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost         Î»
Î³             Î´             Î±             Î²
     0      0  cg_i -7.032046e-09  1.474521e-03  0.000000e+00  0.000000e+00
3.727647e-03  9.880023e+02  1.012143e-03  1.564705e-01

     1      0  cg_i -8.304899e-09  6.906989e-04  0.000000e+00  0.000000e+00
3.908177e+02  1.008664e+03  1.170863e-03  2.194196e-01

     2      0  cg_i -8.600911e-09  3.514945e-04  0.000000e+00  0.000000e+00
4.000658e+02  9.932200e+02  1.240972e-03  2.589760e-01

     3      0  cg_i -8.677805e-09  2.907239e-05  0.000000e+00  0.000000e+00
4.100794e+02  1.012058e+03  1.244756e-03  6.841074e-03

 iter inewton type    objective     â gâ â _Mâ »Â¹      leftmost         Î»
Î³             Î´             Î±             Î²
     0      0  cg_i -1.065816e-17  7.061929e-08  0.000000e+00  0.000000e+00
1.369755e-07  8.801844e+02  1.136126e-03  2.658036e-01

     1      0  cg_i -1.488030e-17  6.089564e-08  0.000000e+00  0.000000e+00
4.537891e+02  8.245442e+02  1.693228e-03  7.435764e-01

     2      0  cg_i -2.014909e-17  8.298704e-08  0.000000e+00  0.000000e+00
5.092692e+02  7.910571e+02  2.841638e-03  1.857155e+00

     3      0  cg_i -3.327619e-17  1.245258e-07  0.000000e+00  0.000000e+00
4.795737e+02  9.158651e+02  3.812224e-03  2.251637e+00

Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 19
         Function evaluations: 20
         Gradient evaluations: 20
         Hessian evaluations: 18
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 1.1618442019708214e-28
       x: [ 1.000e+00  1.000e+00  1.000e+00  1.000e+00  1.000e+00]
     nit: 19
```

```
     jac: [ 4.396e-14  2.109e-14  6.417e-14  3.499e-13 -1.998e-13]
    nfev: 20
    njev: 20
    nhev: 18
    hess: [[ 8.020e+02 -4.000e+02 ...  0.000e+00  0.000e+00]
           [-4.000e+02  1.002e+03 ...  0.000e+00  0.000e+00]
           ...
           [ 0.000e+00  0.000e+00 ...  1.002e+03 -4.000e+02]
           [ 0.000e+00  0.000e+00 ... -4.000e+02  2.000e+02]]
```

[14]:
```python
# 最小值点
print(res.x)
```

```
[1. 1. 1. 1. 1.]
```

[15]:
```python
res = minimize(
    rosen, x0, method="trust-exact",
    jac=rosen_der, hess=rosen_hess,
    options={"gtol": 1e-8, "disp": True}
)
print(res)
```

```
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 13
         Function evaluations: 14
         Gradient evaluations: 13
         Hessian evaluations: 14
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 1.5343031448490 83e-22
       x: [ 1.000e+00  1.000e+00  1.000e+00  1.000e+00  1.000e+00]
     nit: 13
     jac: [ 7.503e-12  2.589e-11  1.048e-10  4.210e-10 -2.398e-10]
    nfev: 14
    njev: 13
    nhev: 14
    hess: [[ 8.020e+02 -4.000e+02 ...  0.000e+00  0.000e+00]
           [-4.000e+02  1.002e+03 ...  0.000e+00  0.000e+00]
           ...
           [ 0.000e+00  0.000e+00 ...  1.002e+03 -4.000e+02]
           [ 0.000e+00  0.000e+00 ... -4.000e+02  2.000e+02]]
```

[16]:
```
# 最小值点
print(res.x)
```

```
[1. 1. 1. 1. 1.]
```

2.0.2 多元函数有约束的最优化问题

求解约束问题如下

$$
\begin{aligned}
\min_{x_0,x_1} \ 100(x_1 - x_0^2)^2 + (1 - x_0)^2 \\
\text{subject to:} \\
x_0 + 2x_1 \leq 1 \\
x_0^2 + x_1 \leq 1 \\
x_0^2 - x_1 \leq 1 \\
2x_0 + x_1 = 1 \\
0 \leq x_0 \leq 1 \\
-0.5 \leq x_1 \leq 2
\end{aligned}
$$

[1]:
```
import numpy as np
```

[2]:
```
from scipy.optimize import Bounds
# 定义变量的边界
bounds = Bounds(
    [0, -0.5], # 下界
    [1.0, 2.0] # 上界
)
```

[3]:
```
from scipy.optimize import LinearConstraint
# 定义线性约束
linear_constraint = LinearConstraint(
    [
        [1, 2],
        [2, 1]
    ],
    [-np.inf, 1], # 下界
    [1, 1] # 上界
)
```

[4]:
```
# 非线性约束
def cons_f(x):
    return [
        x[0]**2 + x[1],
        x[0]**2 - x[1]
    ]
# 非线性约束的雅可比形式
```

```
def cons_J(x):
    return [
        [2*x[0], 1],
        [2*x[0], -1]
    ]
# 黑塞矩阵的线性组合
def cons_H(x, v):
    return v[0]*np.array(
        [
            [2, 0],
            [0, 0]
        ]
    ) + v[1]*np.array(
        [
            [2, 0],
            [0, 0]
        ]
    )
from scipy.optimize import NonlinearConstraint
# 构造非线性约束
nonlinear_constraint = NonlinearConstraint(
    cons_f,
    -np.inf, # 下界
    1, # 上界
    jac=cons_J,
    hess=cons_H
)
```

[5]:

```
from scipy.optimize import minimize
# 初始值
x0 = np.array([0.5, 0])
# 最优化目标函数
def rosen(x):
    """The Rosenbrock function"""
    return sum(100.0*(x[1:]-x[:-1]**2.0)**2.0 + (1-x[:-1])**2.0)
# 目标函数的导数
def rosen_der(x):
    xm = x[1:-1]
    xm_m1 = x[:-2]
    xm_p1 = x[2:]
    der = np.zeros_like(x)
    der[1:-1] = 200*(xm-xm_m1**2) - 400*(xm_p1 - xm**2)*xm - 2*(1-xm)
    der[0] = -400*x[0]*(x[1]-x[0]**2) - 2*(1-x[0])
    der[-1] = 200*(x[-1]-x[-2]**2)
```

```
    return der
# 目标函数的黑塞矩阵
def rosen_hess(x):
    x = np.asarray(x)
    H = np.diag(-400*x[:-1],1) - np.diag(400*x[:-1],-1)
    diagonal = np.zeros_like(x)
    diagonal[0] = 1200*x[0]**2-400*x[1]+2
    diagonal[-1] = 200
    diagonal[1:-1] = 202 + 1200*x[1:-1]**2 - 400*x[2:]
    H = H + np.diag(diagonal)
    return H
```

[6]:
```
res = minimize(
    rosen, # 目标函数
    x0, # 初始值
    method="trust-constr", # 求解算法
    jac=rosen_der, # 梯度
    hess=rosen_hess, # 黑塞矩阵
    constraints=[linear_constraint, nonlinear_constraint], # 约束
    options={"verbose": 1},
    bounds=bounds # 变量范围
)
print(res)
```

```
`gtol` termination condition is satisfied.
Number of iterations: 12, function evaluations: 8, CG iterations: 7, optimality:
2.99e-09, constraint violation: 0.00e+00, execution time: 0.047 s.
           message: `gtol` termination condition is satisfied.
           success: True
            status: 1
               fun: 0.3427175756422305
                 x: [ 4.149e-01  1.701e-01]
               nit: 12
              nfev: 8
              njev: 8
              nhev: 8
          cg_niter: 7
      cg_stop_cond: 1
              grad: [-8.265e-01 -4.140e-01]
   lagrangian_grad: [ 1.495e-09 -2.990e-09]
            constr: [array([ 7.552e-01,  1.000e+00]), array([ 3.423e-01,
2.070e-03]), array([ 4.149e-01,  1.701e-01])]
               jac: [array([[ 1.000e+00,  2.000e+00],
                            [ 2.000e+00,  1.000e+00]]), array([[ 8.299e-01,
1.000e+00],
```

```
                                [ 8.299e-01, -1.000e+00]]), array([[ 1.000e+00,
0.000e+00],
                                [ 0.000e+00,  1.000e+00]])]
        constr_nfev: [0, 8, 0]
        constr_njev: [0, 8, 0]
        constr_nhev: [0, 13, 0]
                  v: [array([ 6.536e-04,  4.128e-01]), array([ 2.433e-04,
1.603e-04]), array([-1.121e-04, -1.513e-04])]
             method: tr_interior_point
         optimality: 2.989621706689068e-09
   constr_violation: 0.0
     execution_time: 0.046998023986816406
          tr_radius: 3834.1597660672387
     constr_penalty: 1.0
  barrier_parameter: 0.00016000000000000007
  barrier_tolerance: 0.00016000000000000007
              niter: 12
```

[7]:
```
# 最优化的点
print(res.x)
```

```
[0.41494531 0.17010937]
```

[8]:
```
# 定义不等式约束
ineq_cons = {
    "type": "ineq", # 不等式约束
    "fun" : lambda x: np.array(
        [
            1 - x[0] - 2*x[1],
            1 - x[0]**2 - x[1],
            1 - x[0]**2 + x[1]
        ]
    ),
    "jac" : lambda x: np.array(
        [
            [-1.0, -2.0],
            [-2*x[0], -1.0],
            [-2*x[0], 1.0]
        ]
    )
}
# 定义等式约束
eq_cons = {
    "type": "eq",
    "fun" : lambda x: np.array([2*x[0] + x[1] - 1]),
```

```
    "jac" : lambda x: np.array([2.0, 1.0])
}
```

[9]:
```
x0 = np.array([0.5, 0])
res = minimize(
    rosen,
    x0,
    method="SLSQP",
    jac=rosen_der,
    constraints=[eq_cons, ineq_cons],
    options={"ftol": 1e-9, "disp": True},
    bounds=bounds
)
print(res)
```

```
Optimization terminated successfully    (Exit mode 0)
            Current function value: 0.34271757499419825
            Iterations: 4
            Function evaluations: 5
            Gradient evaluations: 4
 message: Optimization terminated successfully
 success: True
  status: 0
     fun: 0.34271757499419825
       x: [ 4.149e-01  1.701e-01]
     nit: 4
     jac: [-8.268e-01 -4.137e-01]
    nfev: 5
    njev: 4
```

[10]:
```
# 最优化的点
print(res.x)
```

```
[0.41494475 0.1701105 ]
```

2.0.3 带约束的最小二乘优化问题

这种问题在 Python 中计算的一般形式如下

$$\min_{\mathbf{x}} \frac{1}{2}\sum_{i=1}^{n}\rho(f_i(\mathbf{x})^2)\text{subject to:}\mathbf{lb} \leq \mathbf{x} \leq \mathbf{ub}$$

其中的 $f_i(\mathbf{x})$ 表示残差函数，一般是 $y_i - \hat{y}_i$。

这里假设 $f_i(\mathbf{x})$ 的形式如下

$$f_i(\mathbf{x}) = \frac{x_0(u_i^2 + u_i x_1)}{u_i^2 + u_i x_2 + x_3} - y_i, \qquad i = 1, 2, \cdots, 11$$

这里的 x_1, x_2, x_3, x_0 是要求解的参数，其中的 u_i, y_i 是已知的数据。

[1]:
```python
import numpy as np
from scipy.optimize import least_squares
```

[2]:
```python
# 定义模型
def model(x, u):
    return x[0] * (u ** 2 + x[1] * u) / (u ** 2 + x[2] * u + x[3])
# 定义损失函数 f_i(x)
def fun(x, u, y):
    return model(x, u) - y
# 损失函数的雅可比矩阵
def jac(x, u, y):
    J = np.empty((u.size, x.size))
    den = u ** 2 + x[2] * u + x[3]
    num = u ** 2 + x[1] * u
    J[:, 0] = num / den
    J[:, 1] = x[0] * u / den
    J[:, 2] = -x[0] * num * u / den ** 2
    J[:, 3] = -x[0] * num / den ** 2
    return J
```

[3]:
```python
# 数据样本
u = np.array(
    [
        4.0, 2.0, 1.0, 5.0e-1, 2.5e-1, 1.67e-1, 1.25e-1,
        1.0e-1, 8.33e-2, 7.14e-2, 6.25e-2
    ]
)
y = np.array(
    [
        1.957e-1, 1.947e-1, 1.735e-1, 1.6e-1, 8.44e-2, 6.27e-2,
        4.56e-2, 3.42e-2, 3.23e-2, 2.35e-2, 2.46e-2
    ]
)
# 初始值
x0 = np.array([2.5, 3.9, 4.15, 3.9])
res = least_squares(
    fun, # 损失函数 f_i(x)
    x0, # 初始值
    jac=jac, # 雅可比矩阵
    bounds=(0, 100), # 变量范围
    args=(u, y), # fun 中的参数
    verbose=1
)
print(res)
```

```
`ftol` termination condition is satisfied.
```

```
Function evaluations 131, initial cost 4.4383e+00, final cost 1.5375e-04, first-
order optimality 4.52e-08.
     message: `ftol` termination condition is satisfied.
     success: True
      status: 2
         fun: [-1.307e-03 -1.876e-03  8.920e-03 -1.111e-02  8.352e-03
               -1.737e-04  2.584e-05  1.263e-03 -3.524e-03  6.168e-04
               -3.889e-03]
           x: [ 1.928e-01  1.913e-01  1.231e-01  1.361e-01]
        cost: 0.00015375280234150847
         jac: [[ 1.008e+00  4.638e-02 -4.676e-02 -1.169e-02]
               [ 1.000e+00  8.800e-02 -8.800e-02 -4.400e-02]
               …
               [ 1.251e-01  9.180e-02 -1.148e-02 -1.608e-01]
               [ 1.074e-01  8.160e-02 -8.766e-03 -1.403e-01]]
        grad: [-4.526e-10 -1.445e-10  1.552e-09  8.542e-08]
  optimality: 4.516919346939224e-08
 active_mask: [0 0 0 0]
        nfev: 131
        njev: 104
```

[4]:
```python
# 最优点
print(res.x)
```

```
[0.192806   0.19130332 0.12306046 0.13607205]
```

2.0.4 一元函数无约束最优化问题

[1]:
```python
from scipy.optimize import minimize_scalar
# 定义函数
f = lambda x: (x - 2) * (x + 1)**2
res = minimize_scalar(f, method="brent")
print(res)
```

```
 message:
          Optimization terminated successfully;
          The returned value satisfies the termination criteria
          (using xtol = 1.48e-08 )
 success: True
     fun: -4.0
       x: 1.0
     nit: 7
    nfev: 10
```

[2]:
```
# 最优点
print(res.x)
```

```
1.0
```

2.0.5 一元函数有界约束最优化问题

[1]:
```
from scipy.optimize import minimize_scalar
# 定义函数
f = lambda x: (x - 2) * (x + 1)**2
res = minimize_scalar(f, bounds=(1,10), method="bounded")
print(res)
```

```
 message: Solution found.
 success: True
  status: 0
     fun: -3.999999999953027
       x: 1.0000039570068944
     nit: 20
    nfev: 20
```

[2]:
```
# 最优点
print(res.x)
```

```
1.0000039570068944
```

2.0.6 一元函数求根

[1]:
```
from scipy import optimize
# 定义目标函数
def f(x):
    return (x**3 - 1)  # only one real root at x = 1
# 导数
def fprime(x):
    return 3*x**2
```

[2]:
```
sol = optimize.root_scalar(
    f, # 目标函数
    bracket=[0, 3], # 寻根区间
    method="brentq"
)
print(sol.root, sol.iterations, sol.function_calls)
```

```
1.0 10 11
```

[3]:
```
sol = optimize.root_scalar(
    f,
    x0=0.2, # 初始值
    fprime=fprime, # 导数
    method="newton"
)
print(sol.root, sol.iterations, sol.function_calls)
```

```
1.0 11 22
```

2.0.7 线性规划

线性规划的数学表达如下

$$\begin{aligned}\min_x c^T x\\ \text{subject to:}\\ A_{ub}x \le b_{ub}\\ A_{eq}x \le b_{eq}\\ l \le x \le u\end{aligned}$$

下面求解一个实际例子

$$\begin{aligned}\max_{x_1,x_2,x_3,x_4} \quad 29x_1 + 45x_2\\ x_1 - x_2 - 3x_3 \le 5\\ 2x_1 - 3x_2 - 7x_3 + 3x_4 \ge 10\\ 2x_1 + 8x_2 + x_3 = 60\\ 4x_1 + 4x_2 + x_4 = 60\\ 0 \le x_1\\ 0 \le x_2 \le 5\\ x_3 \le 0.5\\ -3 \le x_4\end{aligned}$$

[1]:
```
import numpy as np
from scipy.optimize import linprog
# 价值系数，最大值需要将 c 的系数变号
c = np.array([-29.0, -45.0, 0.0, 0.0])
A_ub = np.array(
    [
        [1.0, -1.0, -3.0, 0.0],
        [-2.0, 3.0, 7.0, -3.0]
    ]
)
b_ub = np.array([5.0, -10.0])
A_eq = np.array(
    [
```

```
        [2.0, 8.0, 1.0, 0.0],
        [4.0, 4.0, 0.0, 1.0]
    ]
)
b_eq = np.array([60.0, 60.0])
# 变量范围
x0_bounds = (0, None)
x1_bounds = (0, 5.0)
x2_bounds = (-np.inf, 0.5)  # +/- np.inf can be used instead of None
x3_bounds = (-3.0, None)
# 构造变量界
bounds = [x0_bounds, x1_bounds, x2_bounds, x3_bounds]
# 线性规划
result = linprog(
    c,
    A_ub=A_ub,
    b_ub=b_ub,
    A_eq=A_eq,
    b_eq=b_eq,
    bounds=bounds
)
print(result)
```

```
       message: The problem is infeasible. (HiGHS Status 8: model_status is
Infeasible; primal_status is At lower/fixed bound)
       success: False
        status: 2
           fun: None
             x: None
           nit: 3
         lower:  residual: None
                marginals: None
         upper:  residual: None
                marginals: None
         eqlin:  residual: None
                marginals: None
       ineqlin:  residual: None
                marginals: None
```

这个线性规划无最优解，改变一下条件

[2]:
```
x1_bounds = (0, 6)
bounds = [x0_bounds, x1_bounds, x2_bounds, x3_bounds]
result = linprog(c, A_ub=A_ub, b_ub=b_ub, A_eq=A_eq, b_eq=b_eq, bounds=bounds)
print(result)
```

```
        message: Optimization terminated successfully. (HiGHS Status 7: Optimal)
        success: True
         status: 0
            fun: -505.974358974359
              x: [ 9.410e+00  5.179e+00 -2.564e-01  1.641e+00]
            nit: 3
          lower:  residual: [ 9.410e+00  5.179e+00        inf  4.641e+00]
                 marginals: [ 0.000e+00  0.000e+00  0.000e+00  0.000e+00]
          upper:  residual: [       inf  8.205e-01  7.564e-01        inf]
                 marginals: [ 0.000e+00  0.000e+00  0.000e+00  0.000e+00]
          eqlin:  residual: [ 0.000e+00  0.000e+00]
                 marginals: [-2.887e+00 -5.415e+00]
        ineqlin:  residual: [ 0.000e+00  0.000e+00]
                 marginals: [-5.174e+00 -1.805e+00]
 mip_node_count: 0
 mip_dual_bound: 0.0
        mip_gap: 0.0
```

[3]:
```python
# 最优点
print(result.x)
# 最优值
print(result.fun)
```

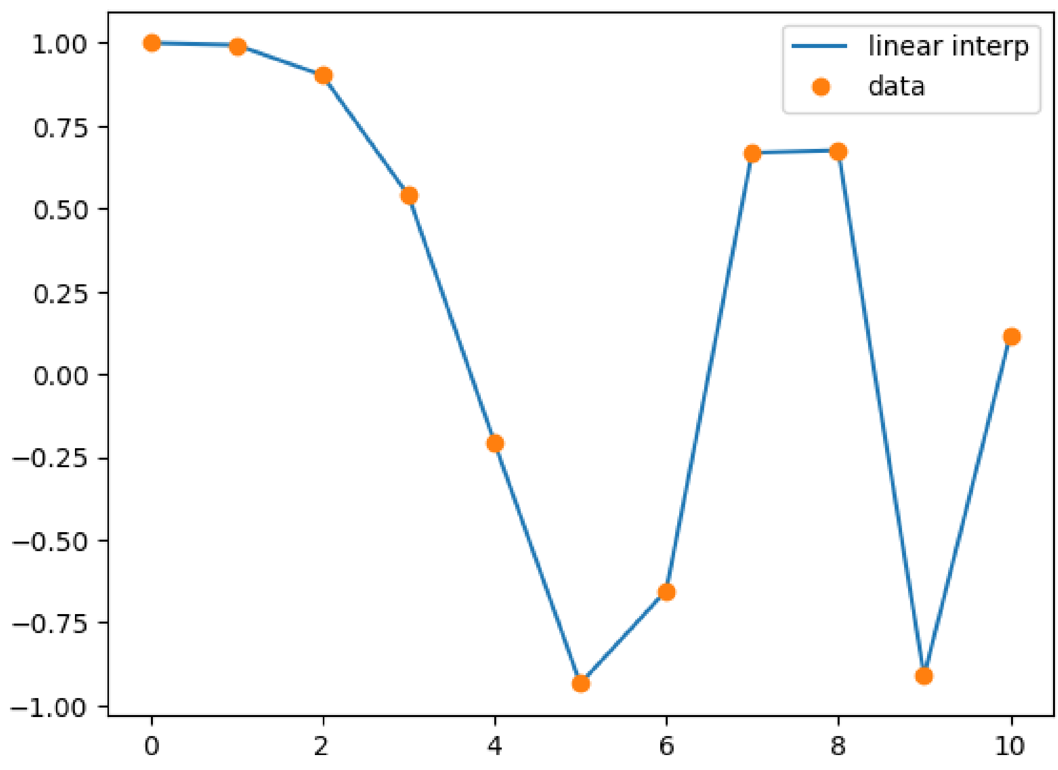
```
[ 9.41025641  5.17948718 -0.25641026  1.64102564]
-505.974358974359
```

3 插值

3.0.1 分段线性插值

[1]:
```python
import numpy as np
import matplotlib.pyplot as plt
```

[2]:
```python
# 插值点
x = np.linspace(0, 10, num=11)
y = np.cos(-x**2 / 9.0)
# 新的插值点
xnew = np.linspace(0, 10, num=1001)
# 插值结果
ynew = np.interp(xnew, x, y)
plt.plot(xnew, ynew, "-", label="linear interp")
plt.plot(x, y, "o", label="data")
plt.legend(loc="best")
plt.show()
```

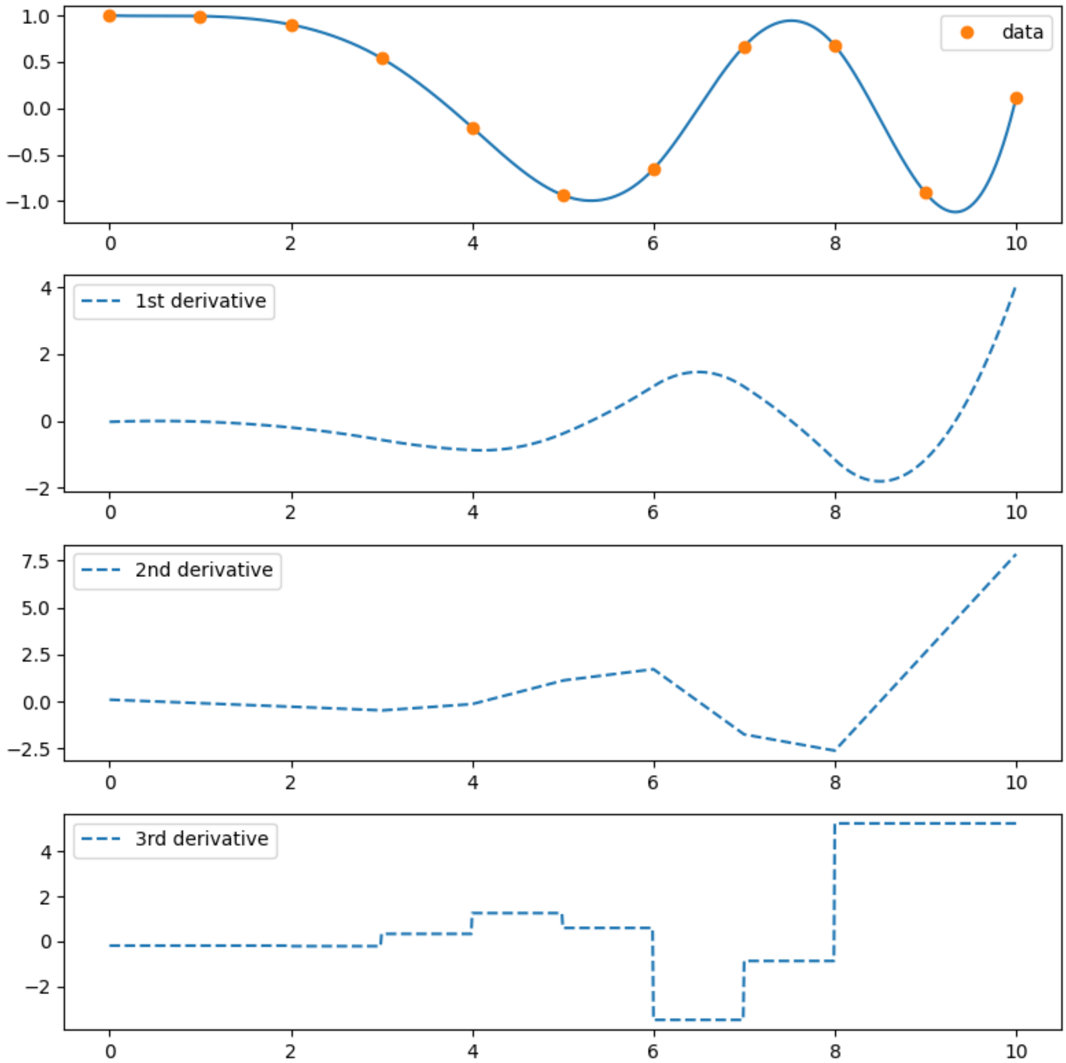


3.0.2 三次样条插值

[1]:
```
import numpy as np
from scipy.interpolate import CubicSpline
import matplotlib.pyplot as plt
```

[2]:
```
# 插值点
x = np.linspace(0, 10, num=11)
y = np.cos(-x**2 / 9.)
# 构造插值函数
spl = CubicSpline(x, y)
# 绘图
fig, ax = plt.subplots(4, 1, figsize=(8, 8))
# 新的插值点
xnew = np.linspace(0, 10, num=1001)
# 新插值点
ax[0].plot(xnew, spl(xnew))
# 原始数据
ax[0].plot(x, y, "o", label="data")
# 插值函数的一阶导
ax[1].plot(xnew, spl(xnew, nu=1), "--", label="1st derivative")
# 插值函数的二阶导
ax[2].plot(xnew, spl(xnew, nu=2), "--", label="2nd derivative")
```

```
# 插值函数的三阶导
ax[3].plot(xnew, spl(xnew, nu=3), "--", label="3rd derivative")
for j in range(4):
    ax[j].legend(loc="best")
plt.tight_layout()
plt.show()
```

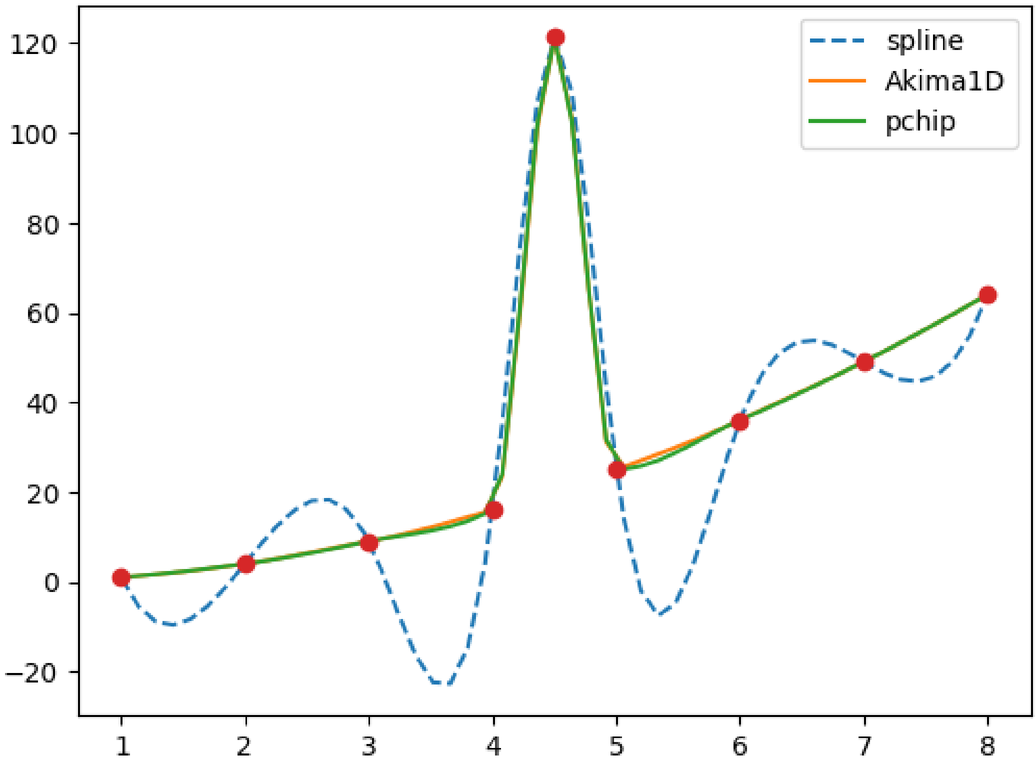


3.0.3 单调插值

[1]:
```
import numpy as np
from scipy.interpolate import CubicSpline, PchipInterpolator, Akima1DInterpolator
import matplotlib.pyplot as plt
```

[2]:
```
# 插值点
x = np.array([1., 2., 3., 4., 4.5, 5., 6., 7., 8])
y = x**2
```

```
# 异常点
y[4] += 101
# 新的插值点
xx = np.linspace(1, 8, 51)
# 三次样条插值
plt.plot(xx, CubicSpline(x, y)(xx), "--", label="spline")
# Akima 插值
plt.plot(xx, Akima1DInterpolator(x, y)(xx), "-", label="Akima1D")
# Pchip 插值
plt.plot(xx, PchipInterpolator(x, y)(xx), "-", label="pchip")
plt.plot(x, y, "o")
plt.legend()
plt.show()
```

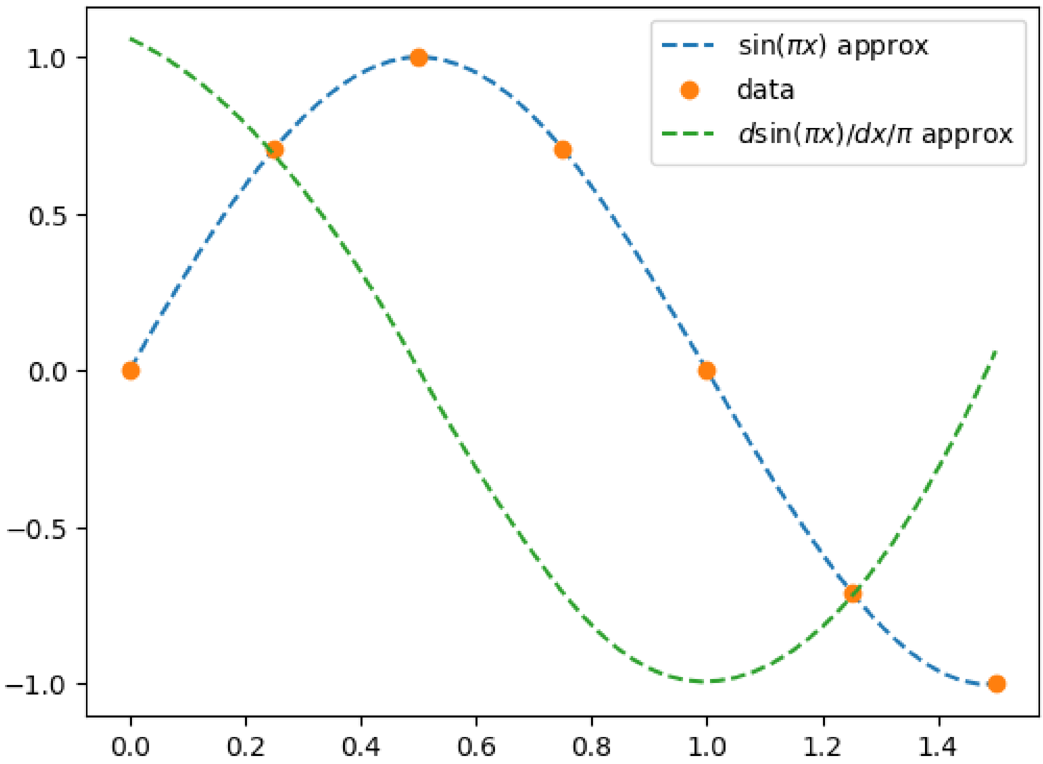


3.0.4 B 样条插值

[1]:
```
from scipy.interpolate import make_interp_spline
import matplotlib.pyplot as plt
import numpy as np
```

[2]:
```
# 插值点
x = np.linspace(0, 3/2, 7)
y = np.sin(np.pi*x)
```

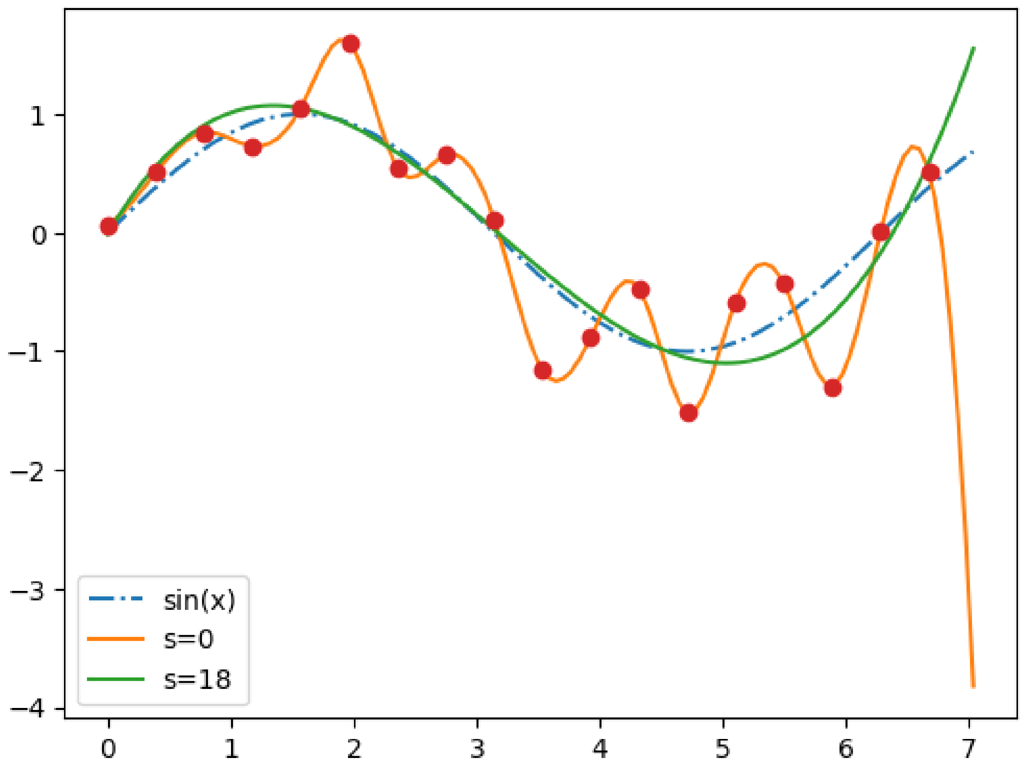
```
# 构造插值样本函数
bspl = make_interp_spline(x, y, k=3)
# 该样本函数的导数
der = bspl.derivative()
# 新的插值点
xx = np.linspace(0, 3/2, 51)
# 插值点函数
plt.plot(xx, bspl(xx), "--", label=r"$\sin(\pi x)$ approx")
# 原插值点数据
plt.plot(x, y, "o", label="data")
# 插值一阶导
plt.plot(xx, der(xx)/np.pi, "--", label="$d \sin(\pi x)/dx / \pi$ approx")
plt.legend()
plt.show()
```



3.0.5 样条平滑插值

```
[1]: import numpy as np
from scipy.interpolate import splrep, BSpline
import matplotlib.pyplot as plt
```

[2]:
```python
# 生成插值点数据，有噪声
x = np.arange(0, 2*np.pi+np.pi/4, 2*np.pi/16)
rng = np.random.default_rng()
y =  np.sin(x) + 0.4*rng.standard_normal(size=len(x))
# 构造插值点的样条表示方法
tck = splrep(x, y, s=0)
tck_s = splrep(x, y, s=len(x))
# 新的插值点
xnew = np.arange(0, 9/4, 1/50) * np.pi
plt.plot(xnew, np.sin(xnew), "-.", label="sin(x)")
plt.plot(xnew, BSpline(*tck)(xnew), "-", label="s=0")
plt.plot(xnew, BSpline(*tck_s)(xnew), "-", label=f"s={len(x)}")
plt.plot(x, y, "o")
plt.legend()
plt.show()
```



4 矩阵计算

4.0.1 矩阵的基本操作

[1]:
```
import numpy as np
from scipy import linalg
```

[2]:
```
# 定义矩阵
A = np.array([[1,2],[3,4]])
A
```

[2]:
```
array([[1, 2],
       [3, 4]])
```

[3]:
```
# 求逆
linalg.inv(A)
```

[3]:
```
array([[-2. ,  1. ],
       [ 1.5, -0.5]])
```

[4]:
```
b = np.array([[5,6]]) #2D array
b
```

[4]:
```
array([[5, 6]])
```

[5]:
```
# 转置
b.T
```

[5]:
```
array([[5],
       [6]])
```

[6]:
```
# 矩阵乘法
A*b
```

[6]:
```
array([[ 5, 12],
       [15, 24]])
```

[7]:
```
A.dot(b.T) #matrix multiplication
```

[7]:
```
array([[17],
       [39]])
```

4.0.2 矩阵求逆

[1]:
```
import numpy as np
from scipy import linalg
```

[2]:
```
A = np.array([[1,3,5],[2,5,1],[2,3,8]])
A
```

[2]:
```
array([[1, 3, 5],
       [2, 5, 1],
       [2, 3, 8]])
```

[3]:
```
# 逆矩阵
linalg.inv(A)
```

[3]:
```
array([[-1.48,  0.36,  0.88],
       [ 0.56,  0.08, -0.36],
       [ 0.16, -0.12,  0.04]])
```

[4]:
```
# 验证
A.dot(linalg.inv(A))
```

[4]:
```
array([[ 1.00000000e+00, -1.11022302e-16, -5.55111512e-17],
       [ 3.05311332e-16,  1.00000000e+00,  1.87350135e-16],
       [ 2.22044605e-16, -1.11022302e-16,  1.00000000e+00]])
```

4.0.3 求线性方程组

[1]:
```
import numpy as np
from scipy import linalg
```

[2]:
```
A = np.array([[1, 2], [3, 4]])
A
```

[2]:
```
array([[1, 2],
       [3, 4]])
```

[3]:
```
b = np.array([[5], [6]])
b
```

[3]:
```
array([[5],
       [6]])
```

[4]:
```
# 求解 Ax=b
linalg.inv(A).dot(b)  # slow
```

[4]:
```
array([[-4. ],
       [ 4.5]])
```

[5]:
```
# 检查
A.dot(linalg.inv(A).dot(b)) - b  # check
```

[5]:
```
array([[0.],
       [0.]])
```

[6]:
```
# 直接求解
np.linalg.solve(A, b)  # fast
```

[6]:
```
array([[-4. ],
       [ 4.5]])
```

[7]:
```
# 检验
A.dot(np.linalg.solve(A, b)) - b
```

[7]:
```
array([[0.],
       [0.]])
```

4.0.4 方阵行列式

[1]:
```
import numpy as np
from scipy import linalg
```

[2]:
```
A = np.array([[1,2],[3,4]])
A
```

[2]:
```
array([[1, 2],
       [3, 4]])
```

[3]:
```
linalg.det(A)
```

[3]:
```
-2.0
```

4.0.5 矩阵范数

[1]:
```
import numpy as np
from scipy import linalg
```

[2]:
```
A=np.array([[1,2],[3,4]])
A
```

[2]:
```
array([[1, 2],
       [3, 4]])
```

[3]:
```
linalg.norm(A)
```

[3]:
```
5.477225575051661
```

[4]:
```
linalg.norm(A,"fro")
```

[4]:
```
5.477225575051661
```

[5]:
```
# L1 norm (max column sum)
linalg.norm(A,1)
```

[5]:
```
6.0
```

[6]:
```
# L1 norm (min column sum)
linalg.norm(A,-1)
```

[6]: 4.0

[7]:
```
# max row sum
linalg.norm(A,np.inf)
```

[7]: 7.0

4.0.6 矩阵特征分解（特征值和特征向量）

[1]:
```
import numpy as np
from scipy import linalg
```

[2]:
```
A = np.array([[1, 2], [3, 4]])
A
```

[2]:
```
array([[1, 2],
       [3, 4]])
```

[3]:
```
# 求解特征值和特征向量
la, v = linalg.eig(A)
l1, l2 = la
# 特征值
print(l1, l2)
```

```
(-0.3722813232690143+0j) (5.372281323269014+0j)
```

[4]:
```
# 第一个特征向量
print(v[:, 0])
```

```
[-0.82456484  0.56576746]
```

[5]:
```
# 第二个特征向量
print(v[:, 1])
```

```
[-0.41597356 -0.90937671]
```

[6]:
```
print(np.sum(abs(v**2), axis=0))
```

```
[1. 1.]
```

[7]:
```
v1 = np.array(v[:, 0]).T
print(linalg.norm(A.dot(v1) - l1*v1))
```

```
5.551115123125783e-17
```

4.0.7 矩阵奇异值分解

[1]:
```python
import numpy as np
from scipy import linalg
```

[2]:
```python
A = np.array([[1,2,3],[4,5,6]])
A
```

[2]:
```
array([[1, 2, 3],
       [4, 5, 6]])
```

[3]:
```python
M,N = A.shape
# 奇异值分解
U,s,Vh = linalg.svd(A)
print(U)
print(s)
print(Vh)
```

```
[[-0.3863177  -0.92236578]
 [-0.92236578  0.3863177 ]]
[9.508032   0.77286964]
[[-0.42866713 -0.56630692 -0.7039467 ]
 [ 0.80596391  0.11238241 -0.58119908]
 [ 0.40824829 -0.81649658  0.40824829]]
```

[4]:
```python
# 奇异值分解 对角矩阵
Sig = linalg.diagsvd(s,M,N)
print(Sig)
```

```
[[9.508032   0.         0.        ]
 [0.         0.77286964 0.        ]]
```

[5]:
```python
print(U.dot(Sig.dot(Vh)))
```

```
[[1. 2. 3.]
 [4. 5. 6.]]
```