最优化理论与应用课程报告

# 拟牛顿法实验报告


学　校：　南京航空航天大学

院　系：　计算机科学与技术学院

专　业：　计算机技术

姓　名：　林国瑞

学　号：　SF1916009

教　师：　朱琨


日　期：　2019 年 1 月 10 日

# 目录

# Chapter 1

# 算法实现与求解

## 1.1 一般的非线性函数（非二次函数）

```
#coding:UTF-8

from numpy import *

#fun  f(x)=100*(x1^2-x2^2)+(x1-1)^2
def fun(x):
    return 100 * (x[0,0] ** 2 - x[1,0]) ** 2 + (x[0,0] - 1) ** 2

#gfun g(x) 是一个 2*1 矩阵，第一行第一列是对 x1 求偏导，第二行第一列是对 x2 求偏导
def gfun(x):
    result = zeros((2, 1))
    result[0, 0] = 400 * x[0,0] * (x[0,0] ** 2 - x[1,0]) + 2 * (x[0,0] - 1)
    result[1, 0] = -200 * (x[0,0] ** 2 - x[1,0])
    return result
```

$$min \quad f(x) = 100(x_1^2 - x_2)^2 + (x_1 - 1)^2$$

$$g(x) = Df(x) = \begin{bmatrix} 400x_1(x_1^2 - x_2) + 2(x_1 - 1) \\ -200(x_1^2 - x_2) \end{bmatrix}$$

## 1.2 rank1 算法

rank1 算法流程图近似矩阵迭代公式：

$$H_{k+1} = H_k + \frac{(\Delta x^{(k)} - H_k \Delta g^{(k)})(\Delta x^{(k)} - H_k \Delta g^{(k)})^T}{(\Delta x^{(k)} - H_k \Delta g^{(k)})^T \Delta g^{(k)}}$$

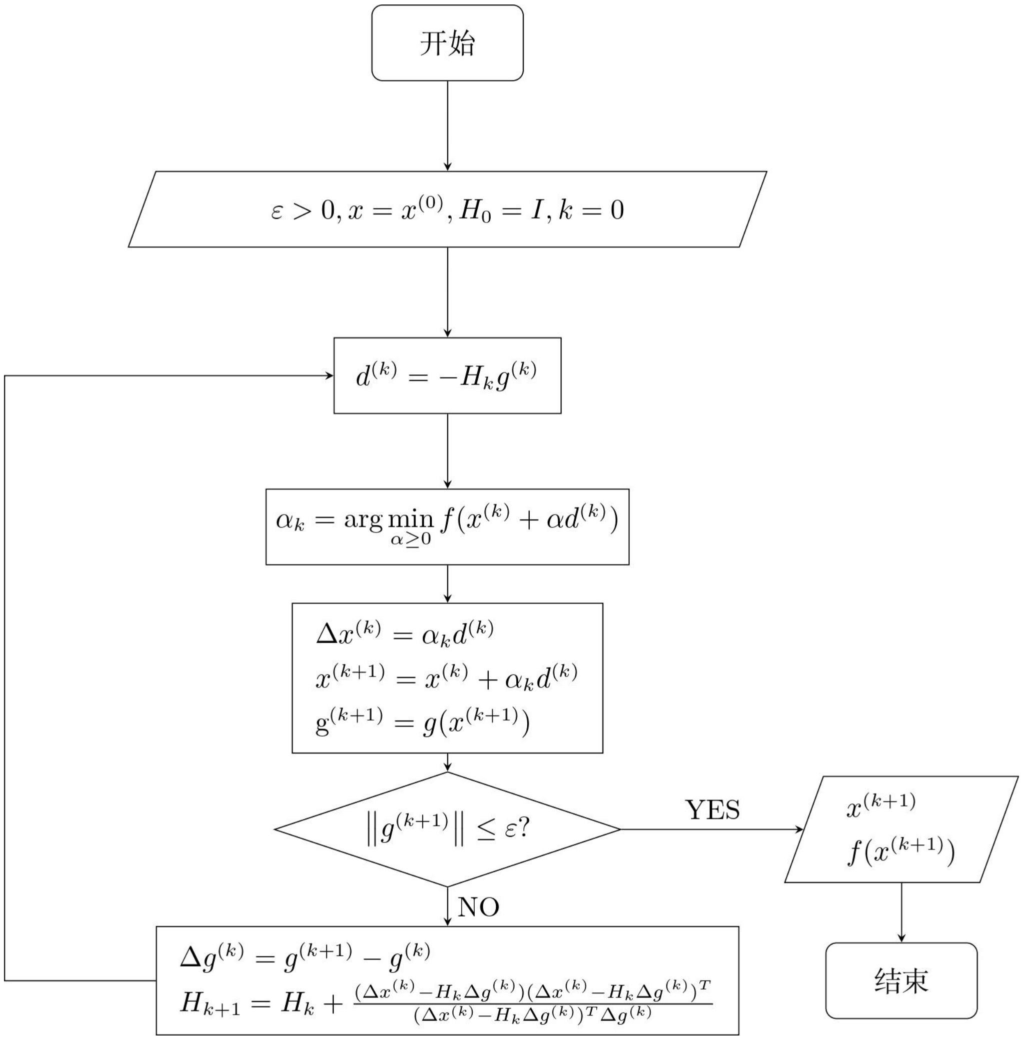



图 1: 算法流程图

```
def rank1(fun, gfun, x0):
    result = []
    maxk = 500  # 最大迭代次数
    rho = 0.55
    sigma = 0.4
    epsilon=1e-5;
    m = shape(x0)[0]
    Hk = eye(m)
    k = 0
    while (k < maxk):
        gk = mat(gfun(x0))# 计算梯度
        dk = -mat(Hk)*gk  # 计算搜索方向
        if(np.linalg.norm(gk)<epsilon): # 检验终止准则
            break
        m = 0
        mk = 0
        while (m < 20): # 用 Armijo 搜索求步长
```

(下页继续)

(续上页)

```
            newf = fun(x0 + rho ** m * dk)
            oldf = fun(x0)
            if (newf < oldf + sigma * (rho ** m) * (gk.T * dk)[0,0]):
                mk = m
                break
            m = m + 1

        #rank1 校正
        x = x0 + rho ** mk * dk
        sk = x - x0
        yk = gfun(x) - gk
        Hk = Hk + (sk-Hk*yk) * (sk-Hk*yk).T / ((sk-Hk*yk).T * yk)

        k = k + 1
        x0 = x
        result.append(fun(x0))

    return result
```

## 1.3 DFP 算法

DFP 算法流程图近似矩阵迭代公式：$H_{k+1} = H_k + \frac{\Delta x^{(k)} \Delta x^{(k)T}}{\Delta x^{(k)T} \Delta g^{(k)}} - \frac{\left[H_k \Delta g^{(k)}\right]\left[H_k \Delta g^{(k)}\right]^T}{\Delta g^{(k)T} H_k \Delta g^{(k)}}$

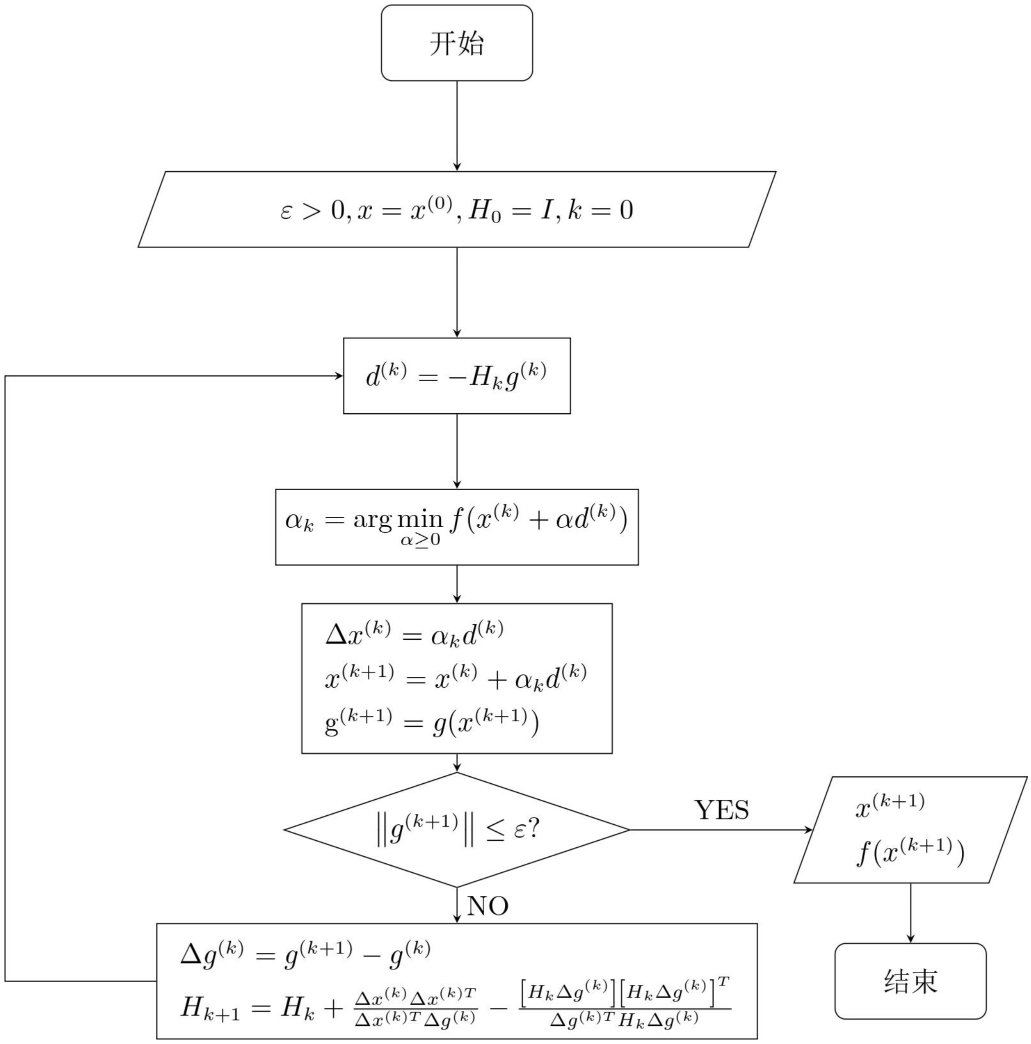



图 2: 算法流程图

```
def dfp(fun, gfun, x0):
    result = []
    maxk = 500  # 最大迭代次数
    rho = 0.55
    sigma = 0.4
    epsilon=1e-5;
    m = shape(x0)[0]
    Hk = eye(m)
    k = 0
    while (k < maxk):
        gk = mat(gfun(x0))# 计算梯度
        dk = -mat(Hk)*gk
        if(np.linalg.norm(gk)<epsilon): # 检验终止准则
            break
        m = 0
        mk = 0
        while (m < 20):
```

(下页继续)

(续上页)

```
            newf = fun(x0 + rho ** m * dk)
            oldf = fun(x0)
            if (newf < oldf + sigma * (rho ** m) * (gk.T * dk)[0,0]):
                mk = m
                break
            m = m + 1

        #DFP 校正
        x = x0 + rho ** mk * dk
        sk = x - x0
        yk = gfun(x) - gk
        if (sk.T * yk > 0):
            Hk = Hk - (Hk * yk * yk.T * Hk) / (yk.T * Hk * yk) + (sk * sk.T) / (sk.T * yk)

        k = k + 1
        x0 = x
        result.append(fun(x0))

    return result
```

## 1.4 BFGS 算法

BFGS 算法流程图近似矩阵迭代公式; $H_{k+1} = H_k - \frac{H_k \Delta x^{(k)} \Delta x^{(k)T} H_k}{\Delta x^{(k)T} H_k \Delta x^{(k)}} + \frac{\left[\Delta g^{(k)}\right]\left[\Delta g^{(k)}\right]^T}{\Delta g^{(k)T} \Delta x^{(k)}}$

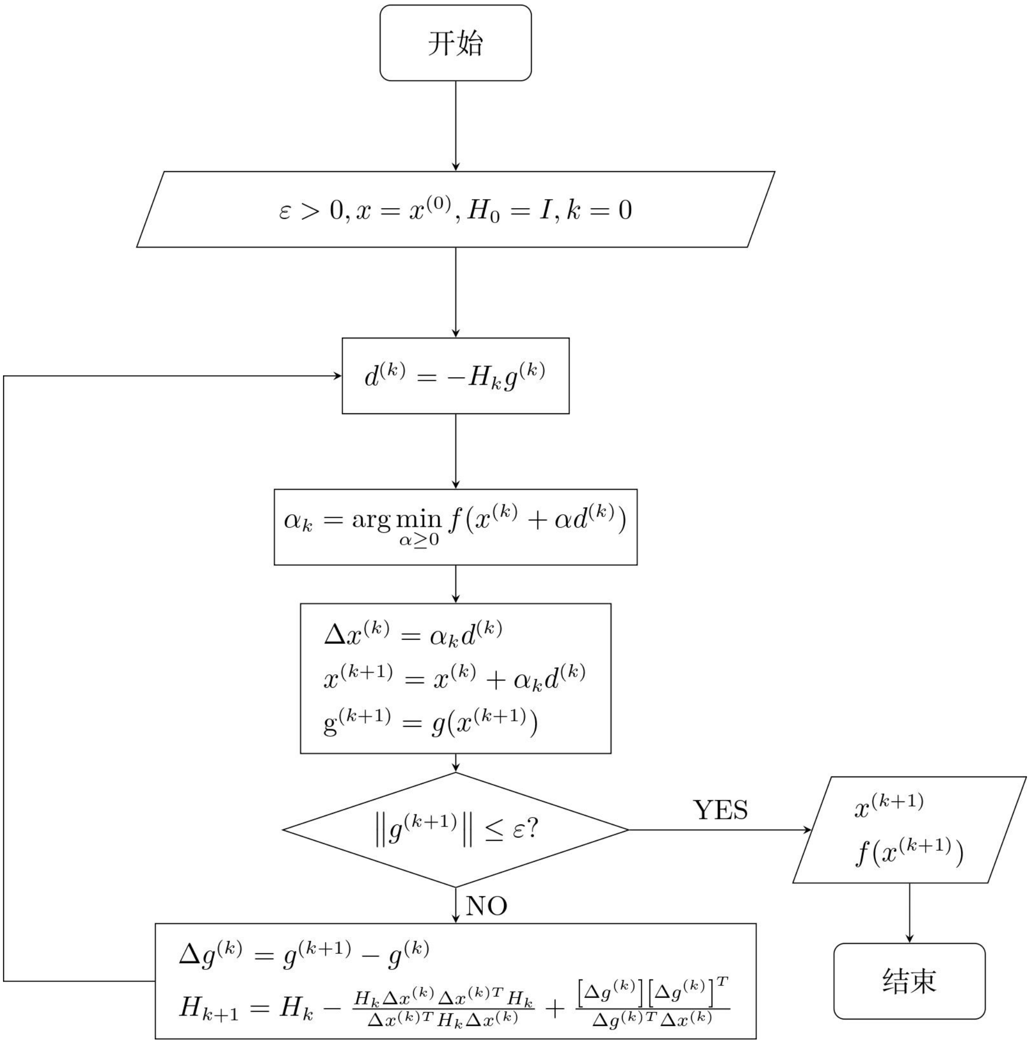



图 3: 算法流程图

```
def bfgs(fun, gfun, x0):
    result = []
    maxk = 500 # 最大迭代次数
    rho = 0.55
    sigma = 0.4
    epsilon=1e-5;
    m = shape(x0)[0]
    Bk = eye(m)
    k = 0
    while (k < maxk):
        gk = mat(gfun(x0)) # 计算梯度
        dk = mat(-linalg.solve(Bk, gk))
        if(np.linalg.norm(gk)<epsilon): # 检验终止准则
            break
        m = 0
        mk = 0
        while (m < 20):   # 用 Armijo 搜索求步长
```

(下页继续)

(续上页)

```
            newf = fun(x0 + rho ** m * dk)
            oldf = fun(x0)
            if (newf < oldf + sigma * (rho ** m) * (gk.T * dk)[0,0]):
                mk = m
                break
            m = m + 1

        #BFGS 校正
        x = x0 + rho ** mk * dk
        sk = x - x0
        yk = gfun(x) - gk
        if (yk.T * sk > 0):
            Bk = Bk - (Bk * sk * sk.T * Bk) / (sk.T * Bk * sk) + (yk * yk.T) / (yk.T * sk)

        k = k + 1
        x0 = x
        result.append(fun(x0))

    return result
```

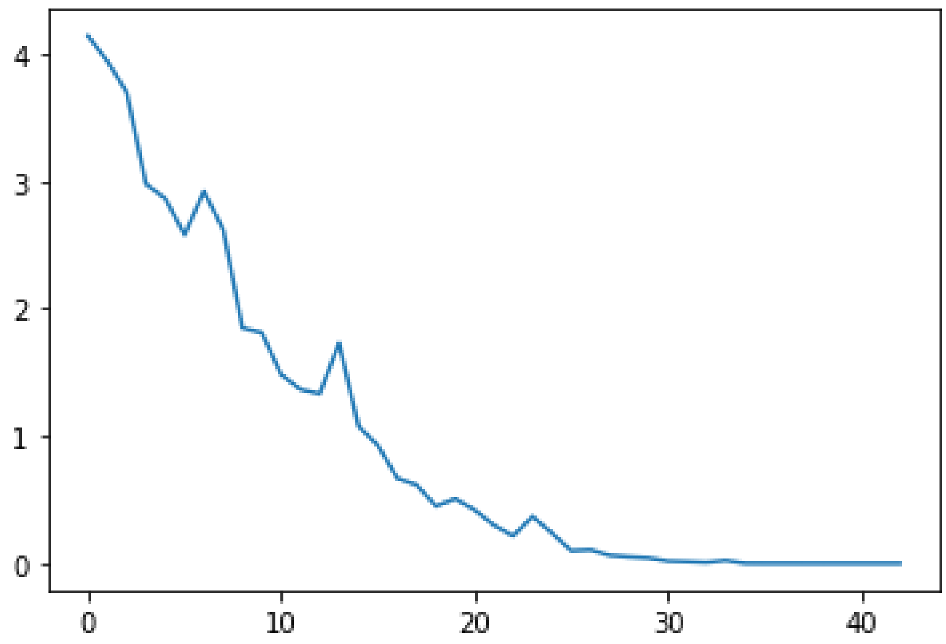
`result` 中记录了每一次迭代的 `x` 的函数值。`result` 中元素的数量即迭代总次数。

# Chapter 2

# 算法收敛速度

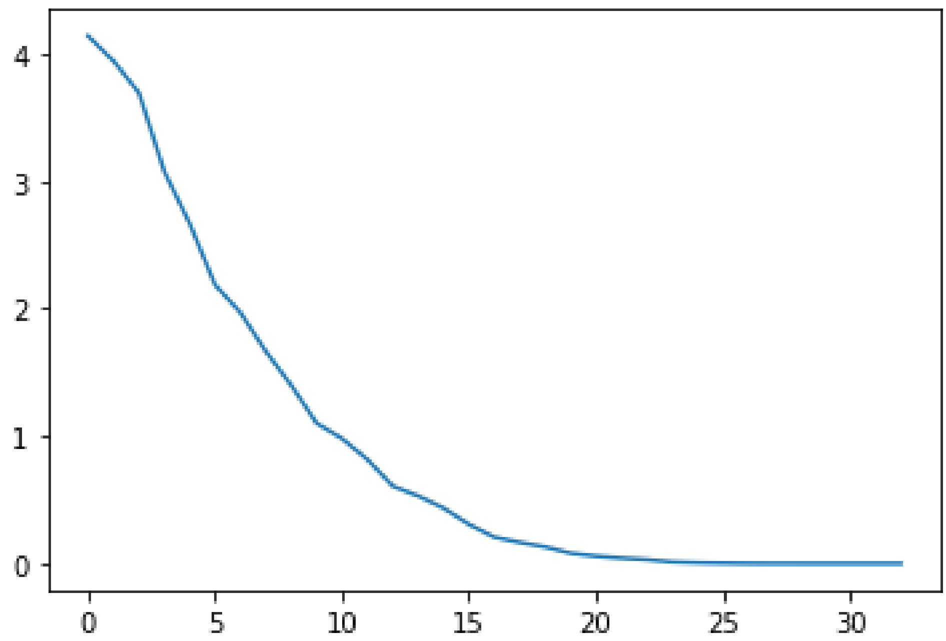
```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[-1.2], [1]])
result = rank1(fun, gfun, x0)

n = len(result)
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
plt.show()
```

```
43
6.469347536626816e-19
```



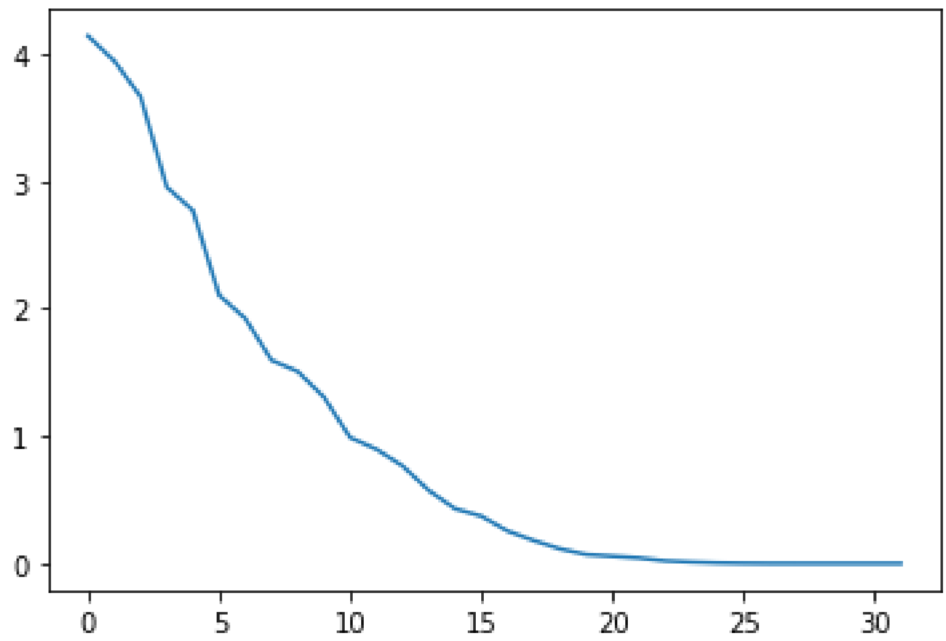

```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[-1.2], [1]])
result = dfp(fun, gfun, x0)

n = len(result)
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
plt.show()
```

```
33
2.1896368842271688e-16
```




```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[-1.2], [1]])
result = bfgs(fun, gfun, x0)

n = len(result)
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
plt.show()
```

```
32
6.753896559404069e-16
```




| 初始点 | 算法 | 迭代次数 | 目标函数值 |
|---|---|---|---|
| [-1.2,0] | rank1 | 43 | 6.469347536626816e-19 |
| [-1.2,0] | DFP | 33 | 2.1896368842271688e-16 |
| [-1.2,0] | BFGS | 32 | 6.753896559404069e-16 |

```
function [x,val,k]=sr1(fun,gfun, x0)
% 功能: 用对称秩 1 算法求解无约束问题:  min f(x)
% 输入: x0 是初始点, fun, gfun 分别是目标函数及其梯度
% 输出:  x, val 分别是近似最优点和最优值,  k 是迭代次数.
maxk=500;   % 给出最大迭代次数
rho=0.55;sigma=0.4; epsilon=1e-5;
k=0;   n=length(x0); Hk=eye(n);
while(k<maxk)
    gk=feval(gfun,x0); % 计算梯度
    dk=-Hk*gk; % 计算搜索方向
    if(norm(gk)<epsilon), break; end  % 检验终止准则
    m=0; mk=0;
    while(m<20)   % 用 Armijo 搜索求步长
        if(feval(fun,x0+rho^m*dk)<feval(fun,x0)+sigma*rho^m*gk'*dk)
            mk=m; break;
        end
        m=m+1;
    end
    x=x0+rho^mk*dk;
    sk=x-x0;  yk=feval(gfun,x)-gk;
    Hk=Hk+(sk-Hk*yk)*(sk-Hk*yk)'/((sk-Hk*yk)'*yk); % 秩 1 校正
    k=k+1;     x0=x;
end
```

(下页继续)

(续上页)

```
val=feval(fun,x0);
```

# Chapter 3

# 算法的不同

秩 1 算法的近似矩阵 $H_k$ 不都是正定的。秩 2 算法可以保证在任意第 k 步迭代下，只要一维搜索是精确的，近似矩阵 $H_k$ 就都是正定的。如 DFP 算法和 BFGS 算法。

# Chapter 4

# 利用三种算法求解二次型函数

$$min \quad f(x) = \frac{1}{2}x^T Qx - x^T b + log(\pi)$$

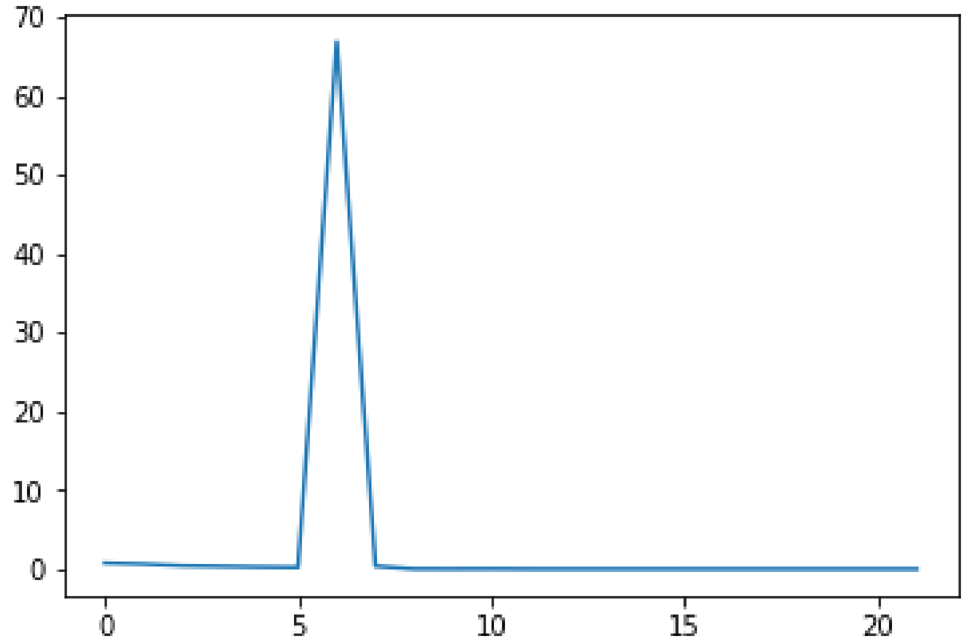
$$Q = \begin{bmatrix} 5 & -3 \\ -3 & 2 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

初始点 $x^(0) = [0,0]^T$

## 4.1 rank1 算法

```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[0], [0]])
result = rank1(fun, gfun, x0)
n = len(result)
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
print (result)   # 迭代中间结果
plt.show()
```

```
22
7.03038991702876e-19
[0.7796505328309867, 0.647903329132764, 0.43174864447002853, 0.35395519320995333, 0.
↪2790157858586189, 0.2301727452032303, 66.8551930552344, 0.3803419443079954, 0.
↪01919688557291296, 0.014493403655030242, 0.0243827267616587, 0.006523531618577661, 0.
↪004711909032094199, 0.003938932709861242, 0.005944832855606774, 0.00013813269252629403, 2.
↪7062473522404853e-05, 1.1753584996447982e-06, 1.7974047514389684e-07, 4.12580600588475e-11,␣
↪4.2697255197291215e-13, 7.03038991702876e-19]
```



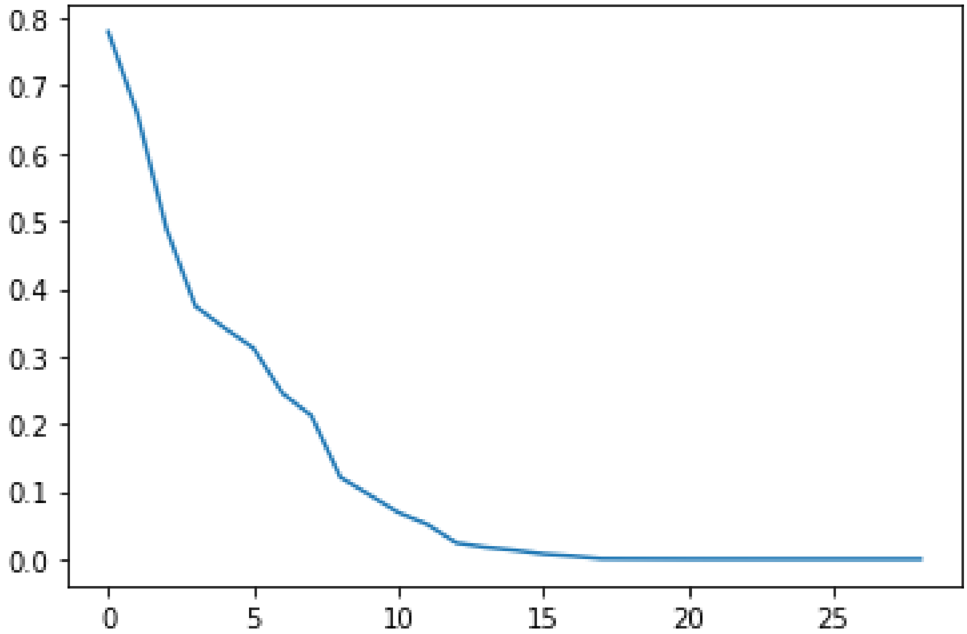

## 4.2 DFP 算法

```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[0], [0]])
result = dfp(fun, gfun, x0)

n = len(result)
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
print (result)   # 迭代中间结果
plt.show()
```

```
29
7.19219715138461e-17
[0.7796505328309867, 0.6594092966734678, 0.4884649661302388, 0.37412962490090296, 0.
↪34187217174408696, 0.3120357733196676, 0.2452711477829217, 0.2122170971698485, 0.
↪12114855860725816, 0.09503104273020731, 0.06883922226115423, 0.051367526656193756, 0.
↪023795380641520036, 0.017416572210177308, 0.012996917660099784, 0.007397028905316069, 0.
↪004372484396145824, 0.00047420975648178657, 0.00030087781694019037, 0.00017741503728331413,␣
↪6.025114908106955e-05, 2.4188348072428142e-05, 2.6128936793145394e-06, 4.7596994547672995e-
↪07, 4.256328564678119e-08, 1.4857356731312556e-09, 1.8314208202538454e-11, 7.56977430809567e-
↪14, 7.19219715138461e-17]
```

(下页继续)

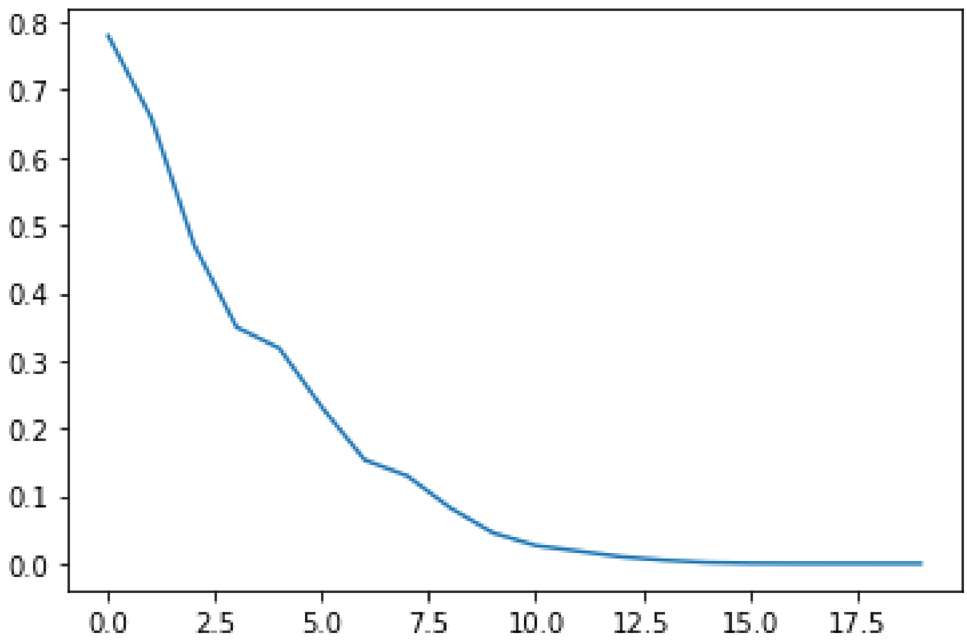
(续上页)




## 4.3 BFGS 算法

```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[0], [0]])
result = bfgs(fun, gfun, x0)

n = len(result)
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
print (result)   # 迭代中间结果
plt.show()
```

```
20
2.20047705066948e-11
[0.7796505328309867, 0.6595694253943865, 0.47152888012853705, 0.34924438689304865, 0.
↪3180704353850303, 0.23063472651536962, 0.15310047456201717, 0.12936214773849927, 0.
↪08232065702719052, 0.04522341147137615, 0.026501461178135587, 0.018220593494777646, 0.
↪009901412537376825, 0.00486909437034745, 0.0014634459405904923, 0.00033906943140043903, 5.
↪44227522716887e-05, 3.839876322272881e-06, 1.0573888624004621e-07, 2.20047705066948e-11]
```




| 初始点 | 算法 | 迭代次数 | 目标函数值 |
| --- | --- | --- | --- |
| [0,0] | rank1 | 22 | 7.03038991702876e-19 |
| [0,0] | DFP | 29 | 7.19219715138461e-17 |
| [0,0] | BFGS | 20 | 2.20047705066948e-11 |

从收敛的图形来看，rank1 算法随着迭代，函数值并没有正常减小，而是有一个突变，这可能是中间迭代矩阵不正定引起的。DFP 算法和 BFGS 算法收敛图形趋势比较正常。

针对 rank1 算法和 BFGS 算法的中间结果进行进一步分析。

得到这个异常是在第 5 次迭代产生的。

## 4.4 异常分析

```
def rank1_test(fun, gfun, x0):
    result = []
    maxk = 500   # 最大迭代次数
    rho = 0.55
    sigma = 0.4
    epsilon=1e-5
    m = shape(x0)[0]
    Hk = eye(m)
    print(Hk)
    k = 0
    while (k < maxk):
        gk = mat(gfun(x0))# 计算梯度
        dk = -mat(Hk)*gk  # 计算搜索方向
        if(np.linalg.norm(gk)<epsilon): # 检验终止准则
```

(下页继续)

(续上页)

```
            break
        m = 0
        mk = 0
        while (m < 20): # 用 Armijo 搜索求步长
            newf = fun(x0 + rho ** m * dk)
            oldf = fun(x0)
            if (newf < oldf + sigma * (rho ** m) * (gk.T * dk)[0,0]):
                mk = m
                break
            m = m + 1

        #rank1 校正
        x = x0 + rho ** mk * dk
        sk = x - x0
        yk = gfun(x) - gk
        Hk = Hk + (sk-Hk*yk) * (sk-Hk*yk).T / ((sk-Hk*yk).T * yk)
        print(Hk)
        print('这是第')
        print(k)
        print('次迭代生成的近似矩阵')
        if(k==5) :
            B=np.linalg.eigvals(Hk)
            print(B)
            if np.all(B>0):
                print ('正定')
            else:
                print ('非正定')
        if(k==9):
            B=np.linalg.eigvals(Hk)
            print(B)
            if np.all(B>0):
                print ('正定')
            else:
                print ('非正定')
        k = k + 1
        x0 = x
        result.append(fun(x0))

    return result
```

```
import matplotlib.pyplot as plt
import numpy as np

x0 = mat([[0], [0]])
result = rank1_test(fun, gfun, x0)
n = len(result)
```

(下页继续)

(续上页)

```
ax = plt.figure().add_subplot(111)
x = arange(0, n, 1)
y = result
ax.plot(x,y)
print (n)
print (result[n-1])
print (result)   # 迭代中间结果
plt.show()
```

```
[[1. 0.]
 [0. 1.]]
[[0.86724575 0.33750033]
 [0.33750033 0.14197494]]
这是第
0
次迭代生成的近似矩阵
[[0.05995369 0.03369757]
 [0.03369757 0.0276469 ]]
这是第
1
次迭代生成的近似矩阵
[[0.04723135 0.03268716]
 [0.03268716 0.02756666]]
这是第
2
次迭代生成的近似矩阵
[[0.28485643 0.21368771]
 [0.21368771 0.16543594]]
这是第
3
次迭代生成的近似矩阵
[[0.1220735  0.10383508]
 [0.10383508 0.09130286]]
这是第
4
次迭代生成的近似矩阵
[[ 0.09783395  0.15160711]
 [ 0.15160711 -0.0028477 ]]
这是第
5
次迭代生成的近似矩阵
[ 0.20723953 -0.11225328]
非正定
[[0.09789522 0.15556286]
 [0.15556286 0.25256117]]
这是第
```

(下页继续)

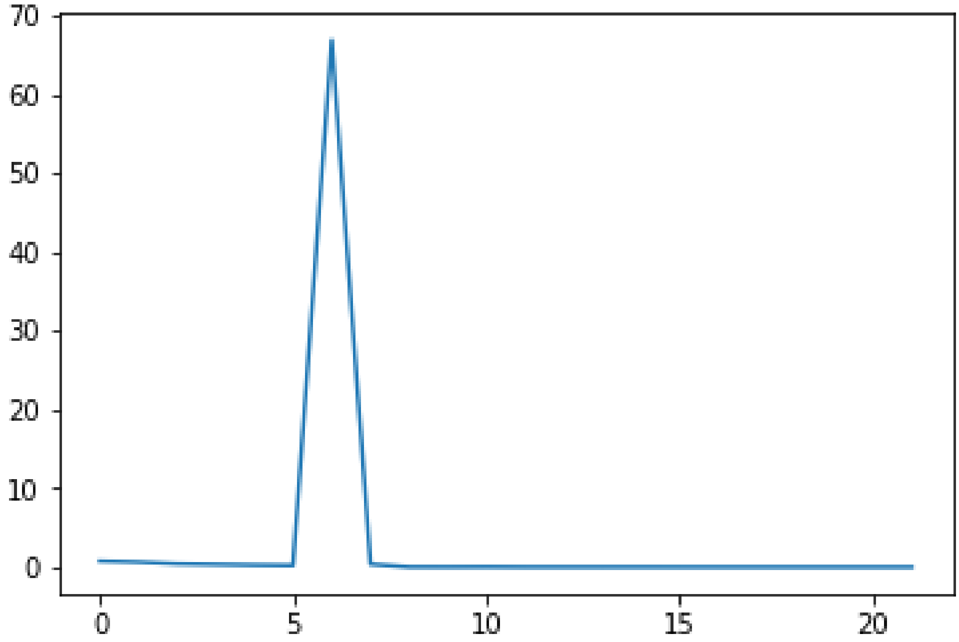
(续上页)

```
6
次迭代生成的近似矩阵
[[0.09743708 0.15523955]
 [0.15523955 0.252333  ]]
这是第
7
次迭代生成的近似矩阵
[[0.0970004  0.15408129]
 [0.15408129 0.2492608 ]]
这是第
8
次迭代生成的近似矩阵
[[-0.1639139  -0.27903183]
 [-0.27903183 -0.4696993 ]]
这是第
9
次迭代生成的近似矩阵
[ 0.00136778 -0.63498099]
非正定
[[0.48213674 0.83287166]
 [0.83287166 1.44397324]]
这是第
10
次迭代生成的近似矩阵
[[0.39264455 0.68923185]
 [0.68923185 1.21342355]]
这是第
11
次迭代生成的近似矩阵
[[0.25066573 0.45631128]
 [0.45631128 0.83131029]]
这是第
12
次迭代生成的近似矩阵
[[0.23548713 0.43465057]
 [0.43465057 0.80039925]]
这是第
13
次迭代生成的近似矩阵
[[0.31340729 0.60535568]
 [0.60535568 1.17437481]]
这是第
14
次迭代生成的近似矩阵
[[0.35368114 0.68572018]
 [0.68572018 1.33473825]]
这是第
```

(下页继续)

(续上页)

```
15
次迭代生成的近似矩阵
[[0.47146899 0.93304529]
 [0.93304529 1.85405927]]
这是第
16
次迭代生成的近似矩阵
[[0.38405497 0.77657038]
 [0.77657038 1.57396236]]
这是第
17
次迭代生成的近似矩阵
[[0.48106364 0.96051536]
 [0.96051536 1.9227534 ]]
这是第
18
次迭代生成的近似矩阵
[[0.47461    0.94648871]
 [0.94648871 1.89226724]]
这是第
19
次迭代生成的近似矩阵
[[0.50177928 1.00345234]
 [1.00345234 2.01169826]]
这是第
20
次迭代生成的近似矩阵
[[0.49983374 0.99968422]
 [0.99968422 2.00440016]]
这是第
21
次迭代生成的近似矩阵
22
7.03038991702876e-19
[0.7796505328309867, 0.647903329132764, 0.43174864447002853, 0.35395519320995333, 0.
↪2790157858586189, 0.2301727452032303, 66.8551930552344, 0.3803419443079954, 0.
↪01919688557291296, 0.014493403655030242, 0.0243827267616587, 0.006523531618577661, 0.
↪004711909032094199, 0.003938932709861242, 0.005944832855606774, 0.00013813269252629403, 2.
↪7062473522404853e-05, 1.1753584996447982e-06, 1.7974047514389684e-07, 4.12580600588475e-11,␣
↪4.2697255197291215e-13, 7.03038991702876e-19]
```




由上可知，第 5 次和第 9 次迭代产生的都不是正定矩阵。