Practical Optimization Method: Homework 2

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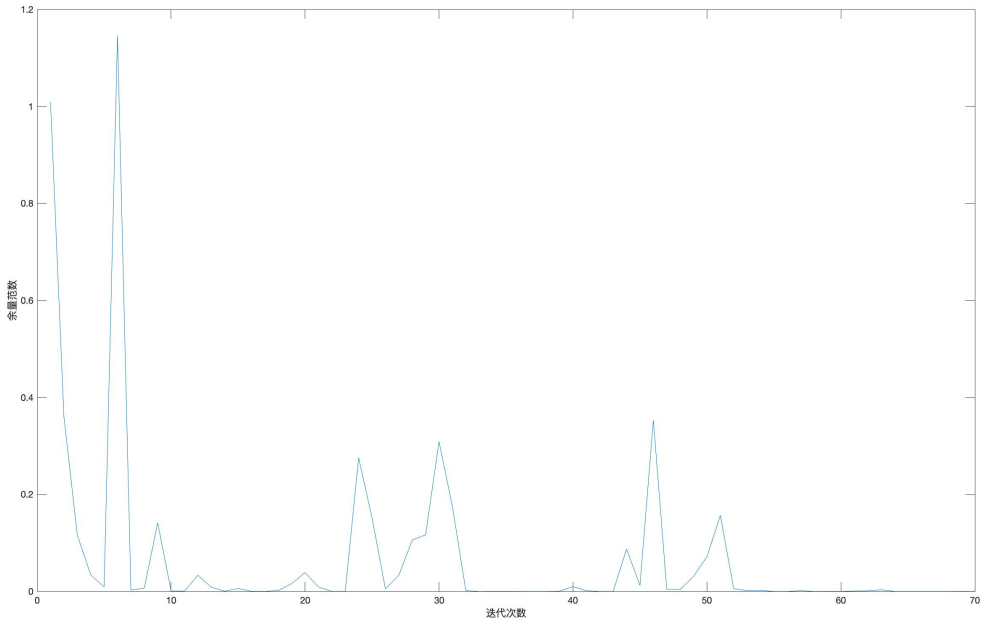
Question 1

利用 CG 法课件 P25 所给出的算法，设置 $A(i,j) = \frac{1}{i+j-1}$，初始值 $x_0 = 0$，$r_0 = Ax_0 - b$，$p_0 = -r_0$，迭代次数 $k = 0$，通过共轭梯度法迭代使 r_k 下降到 10^{-6} 以下，运行结果如下。

n	迭代次数	迭代结束时的余量
5	6	$7.25 * 10^{-8}$
8	19	$8.63 * 10^{-9}$
12	39	$7.02 * 10^{-7}$
20	71	$8.95 * 10^{-7}$

下图以 $n = 20$ 为例，可以发现在 CG 算法运算过程中，随着迭代次数的增加，余量会出现较大幅度的波动，但最终趋于平稳。



Question 2&3

2. 将 $\hat{x} = Cx$ 代入 ϕ 得 $\hat{\phi}(\hat{x}) = \frac{1}{2}\hat{x}^T(C^{-T}AC^{-1})^{-1}\hat{x} - (C^{-T}b)^T\hat{x}$

即解 $(C^{-T}AC^{-1})\hat{x} = C^{-T}b$

∴原算法变为：

Given $\hat{x}_0$;

Set $\hat{r}_0 \leftarrow C^{-T}AC^{-1}\hat{x}_0 - C^{-T}b$, $\hat{p}_0 \leftarrow -\hat{r}_0$, $k \leftarrow 0$

while $\hat{r}_k \neq 0$ do

$\hat{\alpha}_k \leftarrow -\frac{\hat{r}_k^T p_k}{\hat{p}_k^T C^{-T}AC^{-1}p_k}$;

$\hat{x}_{k+1} \leftarrow \hat{x}_k + \hat{\alpha}_k \hat{p}_k$;

$\hat{r}_{k+1} \leftarrow \hat{r}_k + \hat{\alpha}_k C^{-T}AC^{-1}\hat{p}_k$;

$\hat{\beta}_{k+1} \leftarrow \frac{\hat{r}_{k+1}^T \hat{r}_{k+1}}{\hat{r}_k^T \hat{r}_k}$;

$\hat{p}_{k+1} \leftarrow -\hat{r}_{k+1} + \hat{\beta}_{k+1}\hat{p}_k$;

$k \leftarrow k+1$;

End (while)

其中，$\hat{r}_0 = C^{-T}AC^{-1}\hat{x}_0 - C^{-T}b = C^{-T}(A(C^{-1}\hat{x}_0) - b) = C^{-T}(Ax_0 - b) = C^{-T}r_0$

$\hat{p}_0 = -\hat{r}_0 = -C^{-T}r_0$

令 $My_0 = r_0$ $\hat{\alpha}_0 = -\frac{(C^{-T}r_0)^T (-C^{-T}r_0)}{(C^{-1}\hat{p}_0)^T A (C^{-1}\hat{p}_0)}$

$= \frac{r_0^T C^{-1}C^{-T}r_0}{(C^{-1}\hat{p}_0)^T A (C^{-1}\hat{p}_0)} = -\frac{r_0^T y_0}{p_0^T A p_0}$

∵ $C^{-1}C^{-T}r_0 = y_0 = M^{-1}r_0$

$\Rightarrow M = C^TC$.

$C^{-1}\hat{p}_0 = -C^{-1}C^{-T}r_0 = p_0 = -M^{-1}r_0$

且 $\hat{p}_k = Cp_k$ ∴ $\hat{\alpha}_k = -\frac{\hat{r}_k^T p_k}{\hat{p}_k^T C^{-T}AC^{-1}\hat{p}_k} = \frac{r_k^T C^{-1}C^{-T}r_k}{(C^{-1}\hat{p}_k)^T A (C^{-1}\hat{p}_k)} = \frac{r_k^T y_k}{p_k^T A p_k}$

$x_{k+1} = C^{-1}\hat{x}_{k+1} = C^{-1}(Cx_k + \hat{\alpha}_k Cp_k) = x_k + \hat{\alpha}_k p_k$

$r_{k+1} = C^T\hat{r}_{k+1} = C^T(\hat{r}_k + \hat{\alpha}_k C^{-T}AC^{-1}\hat{p}_k) = r_k + \hat{\alpha}_k A p_k$

$\hat{\beta}_{k+1} = \frac{(C^{-T}r_{k+1})^T (C^{-T}r_{k+1})}{(C^{-T}r_k)^T (C^{-T}r_k)} = \frac{r_{k+1}^T y_{k+1}}{r_k^T y_k}$

$p_{k+1} = C^{-1}\hat{p}_k = C^{-1}(-C^{-T}r_{k+1} + \hat{\beta}_{k+1}(Cp_k)) = -y_{k+1} + \hat{\beta}_{k+1}p_k$

∴ 经简化后的算法为：

Given x_0, preconditioner M ($M = C^TC$)

Set $r_0 \leftarrow Ax_0 - b$

Solve $My_0 = r_0$, $p_0 \leftarrow -y_0$, $k \leftarrow 0$

while $r_k \neq 0$, do

$\alpha_k \leftarrow -\frac{r_k^T y_k}{p_k^T A p_k}$;

$x_{k+1} \leftarrow x_k + \alpha_k p_k$;

$r_{k+1} \leftarrow r_k + \alpha_k A p_k$;

Solve $My_{k+1} = r_{k+1}$;

$\beta_{k+1} \leftarrow \frac{r_{k+1}^T y_{k+1}}{r_k^T y_k}$;

$p_{k+1} \leftarrow -y_{k+1} + \beta_{k+1} p_k$;

$k \leftarrow k+1$;

End (while)

3. 证明：$\det(B_{k+1}) = \det\left(B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} + \phi_k (s_k^T B_k s_k) v_k v_k^T\right)$

$= \det\left(B_{k+1}^{(BFGS)} + \phi_k (s_k^T B_k s_k) v_k v_k^T\right)$

$= \det(B_{k+1}^{(BFGS)}) \det(I + \phi_k (s_k^T B_k s_k) H_{k+1}^{(BFGS)} v_k v_k^T)$

下证明对 AVV^T 的矩阵等价秩一矩阵 ($A, V \neq 0$)

$$VV^T = \begin{pmatrix} v_1^2 & v_1 v_2 & \cdots & v_1 v_n \\ v_1 v_2 & v_2^2 & \cdots & v_2 v_n \\ \vdots & \vdots & \ddots & \vdots \\ v_1 v_n & v_2 v_n & \cdots & v_n^2 \end{pmatrix}$$

$$AVV^T = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} v_1^2 & v_1 v_2 & \cdots & v_1 v_n \\ v_1 v_2 & v_2^2 & \cdots & v_2 v_n \\ \vdots & \vdots & \ddots & \vdots \\ v_1 v_n & v_2 v_n & \cdots & v_n^2 \end{pmatrix}$$

$\because (AVV^T)_{i,j} = v_j(a_{i1} v_1 + a_{i2} v_2 + \cdots + a_{in} v_n)$

$\therefore AVV^T$ 秩为 1

$\therefore H_{k+1}^{(BFGS)} v_k v_k^T$ 秩为 1

$$\therefore \det\left(I+\phi_k(s_k^T B_k s_k) H_{k+1}^{(BFGS)} v_k v_k^T\right)$$

$$= 1+\phi_k(s_k^T B_k s_k)\, v_k^T (H_{k+1}^{(BFGS)})^T v_k$$

$$\phi_k(s_k^T B_k s_k)\, v_k^T (H_{k+1}^{(BFGS)})^T v_k$$

$$= \frac{(s_k^T y_k)^2}{(s_k^T y_k)^2 - (s_k^T B_k s_k)(y_k^T H_k y_k)} (s_k^T B_k s_k)\, v_k^T \left[I-\frac{s_k y_k^T}{s_k^T y_k}\right] H_k \left(I-\frac{y_k s_k^T}{s_k^T y_k}\right) + \frac{s_k s_k^T}{s_k^T y_k} \Big] v_k$$

$$s_k^T v_k = s_k^T\left(\frac{y_k}{y_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k}\right) = \frac{s_k^T y_k}{y_k^T s_k} - \frac{s_k^T B_k s_k}{s_k^T B_k s_k} = 1-1 = 0$$

$$\therefore v_k^T s_k = s_k^T v_k = 0$$

$$\therefore \phi_k(s_k^T B_k s_k)\, v_k^T (H_{k+1}^{(BFGS)})^T v_k$$

$$= \frac{(s_k^T y_k)^2}{(s_k^T y_k)^2 - (s_k^T B_k s_k)(y_k^T H_k y_k)} (s_k^T B_k s_k)\, v_k^T H_k v_k$$

$$= \frac{(s_k^T y_k)^2}{(s_k^T y_k)^2 - (s_k^T B_k s_k)(y_k^T H_k y_k)} (s_k^T B_k s_k) \left(\frac{y_k^T}{y_k^T s_k} - \frac{s_k^T B_k}{s_k^T B_k s_k}\right) H_k \left(\frac{y_k}{y_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k}\right)$$

$$= \frac{(s_k^T y_k)^2}{(s_k^T y_k)^2 - (s_k^T B_k s_k)(y_k^T H_k y_k)} (s_k^T B_k s_k) \cdot \frac{(s_k^T B_k s_k)(y_k^T H_k y_k) - (y_k^T s_k)^2}{(y_k^T s_k)^2 (s_k^T B_k s_k)}$$

$$= -1$$

$$\therefore \det\left(I+\phi_k(s_k^T B_k s_k) H_{k+1}^{(BFGS)} v_k v_k^T\right) = 1-1 = 0$$

$$\therefore \det(B_{k+1}) = 0$$

$\therefore B_{k+1}$ 是奇异矩阵.

Question 4

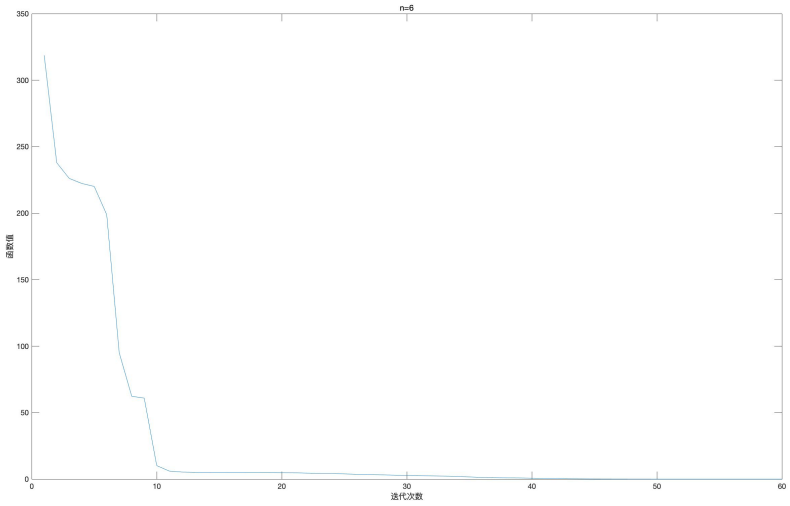
利用拟牛顿法课件 P23 所给出的算法，依次求解 Rosenbrock 函数和 Powell singular 函数求最小值，两者除了给定函数和初值不同外，其余算法流程均相同。

算法细节方面，对于 α 的选取，本代码中采用了满足 Wolfe 条件的不精确求解，设置 $c_1 = 10^{-4}$，$c_2 = 0.9$，在不满足 $f(x_k + \alpha_k p_k) \le f(x_k) + c_1 \alpha_k (\nabla f(x_k))^T p_k$ 时进行 $\alpha = \alpha * 0.5$ 的操作，若已满足，在 $(\nabla f(x_k + \alpha_k p_k))^T p_k \ge c_2 (\nabla f(x_k))^T p_k$ 时采用对前一取值和后一取值取平均的方式得到迭代的 α_k，再次进入上述判断，直至满足 Wolfe 条件，运行结果如下，可以看到，在拟牛顿法 BFGS 迭代过程中，函数值持续下降，且存在下降速率突然增加的拐点。具体代码见于附录。

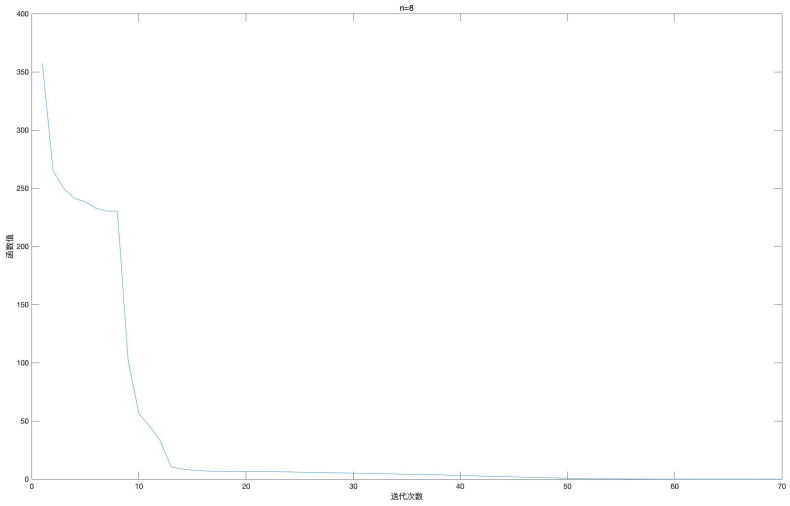
4.1 Rosenbrock 函数

n	迭代次数	x^*	$f(x^*)$
6	60	$(1,1,1,1,1,1)^T$	$2.48 * 10^{-17}$
8	70	$(1,1,1,1,1,1,1,1)^T$	$6.96 * 10^{-15}$
10	81	$(1,1,1,1,1,1,1,1,1,1)^T$	$2.48 * 10^{-15}$

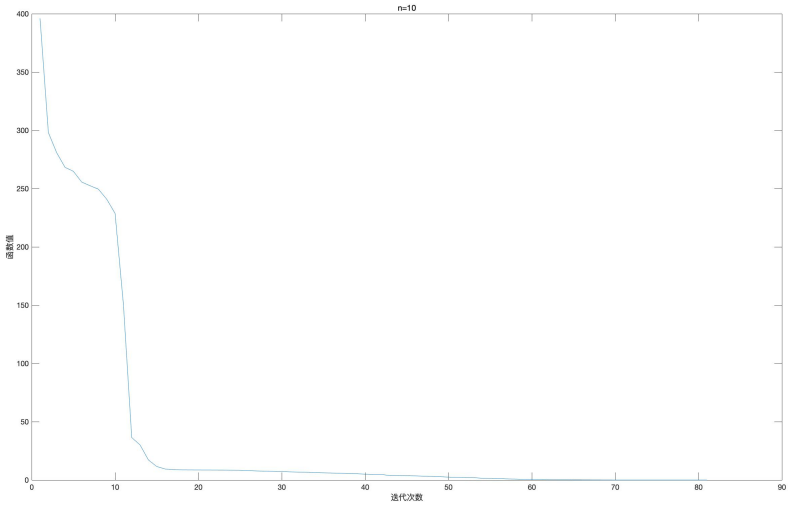
4.1.1 n=6



4.1.2 n=8



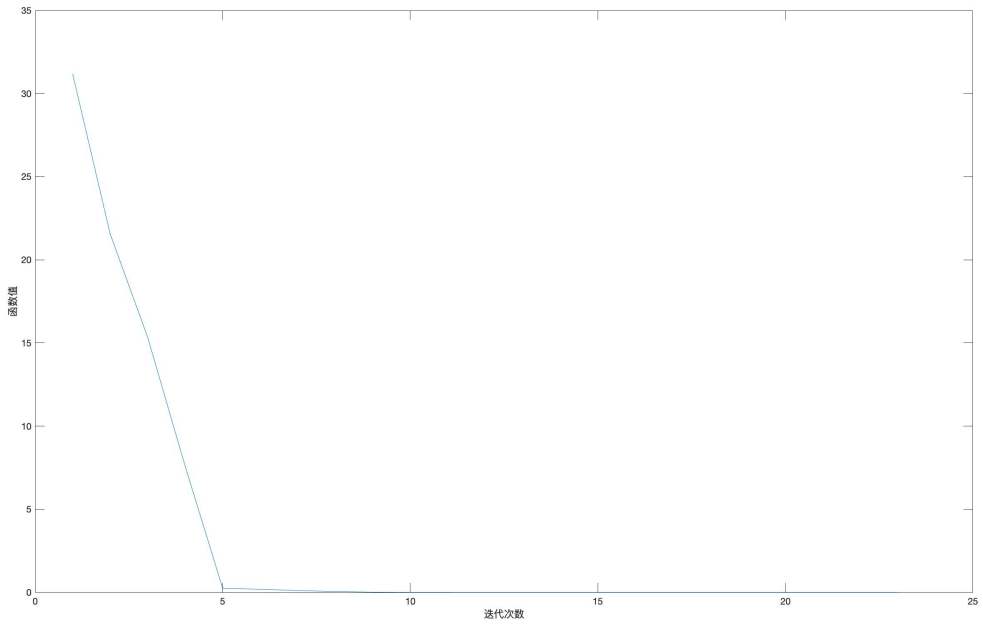
4.1.3 n=10



4.2 Powell singular 函数

改变函数值，其余结构均不变，当迭代次数大于 10 次时函数值便趋于稳定，迭代 23 次后运行结束，接近理论值 $x^* = (0, 0, 0, 0)^T$ 以及 $f(x^*) = 0$，具体运行结果如下：

迭代次数	x^*	$f(x^*)$
23	$(0.0021, -0.0002, 0.0034, 0.0034)^T$	$2.48 * 10^{-9}$



A 附录

A.1 Question 1 CG 法代码

```
#include <iostream>
#include <Eigen/Dense>

using namespace std;
using namespace Eigen;

void CG(MatrixXd A, VectorXd b, VectorXd& x, double e){
    VectorXd r=A*x-b,r_pre;
    VectorXd p=-1.0*r;
    int iter=0;
    while(iter<=100000&&r.norm()>=e){
        double alpha=-1.0*(r.dot(p))/(p.dot(A*p));
        x=x+alpha*p;
        r_pre=r;
        r+=alpha*A*p;
        cout<<iter<<":"<<r.norm()<<endl;
        double beta=r.dot(r)/r_pre.dot(r_pre);
        p=-1*r+beta*p;
        iter++;
    }
    cout<<"total iteration times:"<<iter<<endl;
}

int main() {
    int size=20;
    double e=1e-6;
    MatrixXd A(size,size);
    VectorXd b(size);
    for(int i=0;i<size;i++){
        for(int j=0;j<size;j++){
            A(i,j)=1.0/(i+j+1);
        }
        b(i)=1;
    }

    VectorXd x = VectorXd::Zero(size);

    CG(A,b,x,e);
```

```
    std::cout << "Solution x:\n" << x << std::endl;
    return 0;
}
```

A.2 Question 4 BFGS 求解 Rosenbrock 函数代码

```
#include <iostream>
#include <Eigen/Dense>
#include <cmath>

using namespace std;
using namespace Eigen;

double f(VectorXd x){
    double ans=0,a,b;
    for(int i=0;i<x.size()-1;i++){
        a=x(i+1)-x(i)*x(i);
        b=1-x(i);
        ans+=100*a*a+b*b;
    }
    return ans;
}

VectorXd gradient(VectorXd x){
    VectorXd ans(x.size());
    for(int i=0;i<x.size();i++){
        if(i==0){
            ans(i)=-400*(x(i+1)-x(i)*x(i))*x(i)-2+2*x(i);
        }else if(i<x.size()-1){
            ans(i)=200*(x(i)-x(i-1)*x(i-1))-400*(x(i+1)-x(i)*x(i))*x(i)-2+2*x(
    i);
        }else{
            ans(i)=200*(x(i)-x(i-1)*x(i-1));
        }
    }
    return ans;
}

double LineSearch(VectorXd x,VectorXd p){
    double alpha=1,c1=1e-4,c2=0.9;
    double alpha_min=0,alpha_max=1;
    for(int i=0;i<10000;i++){
```

```
36          VectorXd y=x+alpha*p;
37          VectorXd grad=gradient(x);
38          if(f(y)>f(x)+c1*alpha*grad.dot(p)){
39              alpha*=0.5;
40              alpha_max=alpha;
41          }else if(gradient(y).dot(p)<c2*grad.dot(p)){
42              alpha_min=alpha;
43              alpha=(alpha_min+alpha_max)/2.0;
44          }else{
45              return alpha;
46          }
47      }
48      return alpha;
49  }
50
51  void bfgs(VectorXd x,double e){
52      int iter=0;
53      MatrixXd H=MatrixXd::Identity(x.size(),x.size());
54      MatrixXd In=MatrixXd::Identity(x.size(),x.size());
55      while(iter<1000000){
56          cout<<f(x)<<endl;
57          VectorXd p=-1*H*gradient(x);
58          double alpha=LineSearch(x,p);
59          VectorXd x_pre=x;
60          x+=alpha*p;
61          if(gradient(x).norm()<e){
62              break;
63          }
64          VectorXd s=x-x_pre;
65          VectorXd y=gradient(x)-gradient(x_pre);
66          double rho=s.dot(y);
67          MatrixXd A=In-s*y.transpose()/rho;
68          MatrixXd B=In-y*s.transpose()/rho;
69          MatrixXd C=s*s.transpose()/rho;
70          H=A*H*B+C;
71          iter++;
72      }
73      cout<<iter<<endl;
74      cout<<"Solution x:\n"<<x<<endl;
75      cout<<"Function Value:\n"<<f(x)<<endl;
76  }
77
78  int main(){
```

```
    int size=6;
    double e=1e-5;
    VectorXd x(size);
    for(int i=0;i<size;i++){
        if(i%2==0){
            x(i)=-1.2;
        }else{
            x(i)=1;
        }
    }
    bfgs(x,e);
}
```

A.3 Question 4 BFGS 求解 Powell singular 函数代码

```
#include <iostream>
#include <Eigen/Dense>
#include <cmath>

using namespace std;
using namespace Eigen;

double f(VectorXd x){
    double ans=0,a,b,c,d;
    a=x(0)+10*x(1);
    b=x(2)-x(3);
    c=x(1)-2*x(2);
    d=x(0)-x(3);
    ans=a*a+5*b*b+c*c*c*c+10*d*d*d*d;
    return ans;
}

VectorXd gradient(VectorXd x){
    VectorXd ans(x.size());
    double a,b,c,d;
    a=x(0)+10*x(1);
    b=x(2)-x(3);
    c=x(1)-2*x(2);
    d=x(0)-x(3);
    ans(0)=2*a+40*d*d*d;
    ans(1)=20*a+4*c*c*c;
    ans(2)=10*b-8*c*c*c;
```

```
    ans(3)=-10*b-40*d*d*d;
    return ans;
}

double LineSearch(VectorXd x,VectorXd p){
    double alpha=1,c1=1e-4,c2=0.9;
    double alpha_min=0,alpha_max=1;
    for(int i=0;i<10000;i++){
        VectorXd y=x+alpha*p;
        VectorXd grad=gradient(x);
        if(f(y)>f(x)+c1*alpha*grad.dot(p)){
            alpha*=0.5;
            alpha_max=alpha;
        }else if(gradient(y).dot(p)<c2*grad.dot(p)){
            alpha_min=alpha;
            alpha=(alpha_min+alpha_max)/2.0;
        }else{
            return alpha;
        }
    }
    return alpha;
}

void bfgs(VectorXd x,double e){
    int iter=0;
    MatrixXd H=MatrixXd::Identity(x.size(),x.size());
    MatrixXd In=MatrixXd::Identity(x.size(),x.size());
    while(iter<1000000){
        cout<<f(x)<<endl;
        VectorXd p=-1*H*gradient(x);
        double alpha=LineSearch(x,p);
        VectorXd x_pre=x;
        x+=alpha*p;
        if(gradient(x).norm()<e){
            break;
        }
        VectorXd s=x-x_pre;
        VectorXd y=gradient(x)-gradient(x_pre);
        double rho=s.dot(y);
        MatrixXd A=In-s*y.transpose()/rho;
        MatrixXd B=In-y*s.transpose()/rho;
        MatrixXd C=s*s.transpose()/rho;
        H=A*H*B+C;
```

```
71          iter++;
72      }
73      cout<<iter<<endl;
74      cout<<"Solution x:\n"<<x<<endl;
75      cout<<"Function Value:\n"<<f(x)<<endl;
76  }
77
78  int main(){
79      int size=4;
80      double e=1e-5;
81      VectorXd x(size);
82      x(0)=3;x(1)=-1;x(2)=0;x(3)=1;
83      bfgs(x,e);
84  }
```