# sheet02

November 11, 2016

## 1 Sheet 2: Maximum Likelihood Estimation

In this exercise sheet, we will look at various properties of maximum-likelihood estimation, and how to find maximum-likelihood parameters.

#### 1.0.1 ML vs. James Stein Estimator (15 P)

Let $X_1, \ldots, X_n \in \mathbb{R}^d$ be independent draws from a multivariate Gaussian distribution with mean vector $\mu$ and covariance matrix $\Sigma = \sigma^2 I$. It can be shown that the maximum-likelihood estimator of the mean parameter $\mu$ is the empirical mean given by:

$$\hat{\mu}_{\text{ML}} = \frac{1}{N} \sum_{i=1}^{N} X_i$$

It was once believed that the maximum-likelihood estimator was the most accurate possible (i.e. the one with the smallest Euclidean distance from the true mean). However, it was later demonstrated that the following estimator

$$\hat{\mu}_{JS} = \Big(1 - \frac{(d-2)\cdot\sigma^2}{n \cdot \|\mu_{\text{ML}}\|^2}\Big)\hat{\mu}_{\text{ML}}$$

(a shrinked version of the maximum-likelihood estimator towards the origin) has actually a smaller distance from the true mean when $d \geq 3$. This however assumes knowledge of the variance of the distribution for which the mean is estimated. This estimator is called the James-Stein estimator. While the proof is a bit involved, this fact can be easily demonstrated empirically through simulation. This is the object of this exercise.

The code below draws ten 50-dimensional points from a normal distribution with mean vector $\mu = (1, \ldots, 1)$ and covariance $\Sigma = I$.

```
In [439]: def getdata(seed):

              n = 10               # data points
              d = 50               # dimensionality of data
              m = numpy.ones([d])  # true mean
              s = 1.0              # true standard deviation

              rstate = numpy.random.mtrand.RandomState(seed)
              X = rstate.normal(0,1,[n,d])*s+m

              return X,m,s
```

The following function computes the maximum likelihood estimator from a sample of the data assumed to be generated by a Gaussian distribution:

```
In [440]: import numpy
          def ML(X):
              X_ml = numpy.mean(X,axis=0)
              return X_ml
```

- **Based on the ML estimator function, write a function that receives as input the data $(X_i)_{i=1}^n$ and the (known) variance $\sigma^2$ of the generating distribution, and computes the James-Stein estimator**

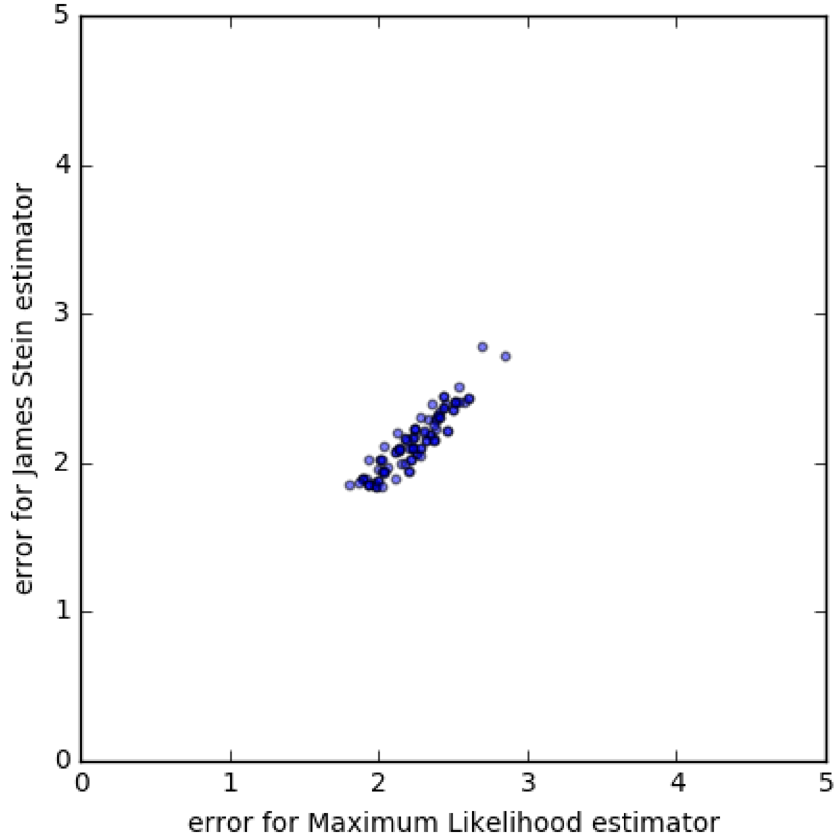
```
In [441]: import numpy
          import random
          def JS(X,s):
              n = 10
              d = 50
              num = (d-2)*(s*s)
              X_ml = ML(X)

              X_sq = numpy.square(X_ml)

              X_sqsum = numpy.sum(X_sq)
              den = n*X_sqsum
              res1 = num/den
              res2 = 1 - res1
              m_js = res2*X_ml
              return m_js
          seed = random.randint(0,99)

          X,m,s = getdata(seed)
          result = JS(X,s)

          print(result)

[ 0.91462639  1.23948138  0.83374761  0.88665586  0.65344909  0.88448107
  0.98149717  0.70146071  0.45072473  1.21575437  1.36499062  0.76018241
  0.60000665  0.8125837   1.2248957   0.53373545  0.73633746  0.81641188
  1.4498917   1.15303948  1.28698031  0.4451644   1.35592865  0.67715367
  1.43926955  0.532079    1.10380603  1.06916496  0.25293176  0.7045336
  0.96147557  0.84081484  1.01017597  1.16098146  1.00983296  0.7433361
  1.43645628  1.04301823  0.30578041  1.11197288  0.80106805  0.79281338
  0.8230307   0.573341    1.03353905  0.67921304  1.29873171  0.66972837
  0.70860476  0.73915327]
```

We would like to compute the error of the maximum likelihood estimator and the James-Stein estimator for 100 different samples (where each sample consists of 10 draws generated by the function `getdata` with a different random seed). Here, for reproducibility, we use seeds from 0 to 99. The error should be measured as the Euclidean distance between the true mean vector and the estimated mean vector.

- **Compute the maximum-likelihood and James-Stein estimations.**
- **Measure the error of these estimations.**
- **Build a scatter plot comparing these errors for different samples.**

In [446]:
```
import matplotlib
%matplotlib inline
from matplotlib import pyplot as plt
mlList = []
jsList = []
d=50
seeds = numpy.random.randint(100,size=100)
true_mean_vector = numpy.ones([d])
for x in numpy.nditer(seeds):
    X,m,s = getdata(x)
    m_ml = ML(X)
    m_ml_estimate_vector = numpy.sqrt(numpy.sum((true_mean_vector-m_ml)**
    #print(m_ml_estimate_vector.shape)
    mlList.append([m_ml_estimate_vector])

    m_js = JS(X,s)
    m_js_estimate_vector = numpy.sqrt(numpy.sum((true_mean_vector-m_js)**
    jsList.append([m_js_estimate_vector])

fig = plt.figure(figsize=(5,5))
plt.xlim(0, 5)
plt.ylim(0, 5)
plt.xlabel('error for Maximum Likelihood estimator')
plt.ylabel('error for James Stein estimator')
plt.scatter(mlList,jsList,s=10,alpha=0.5)
#plt.figure(figsize=(5,5))
#plt.plot(mlList,jsList,'-o')
#plt.xscale('log');plt.yscale('log'); plt.xlabel('error for Maximum Like
```

Out[446]:
```
<matplotlib.collections.PathCollection at 0x1117f8450>
```




### 1.0.2 Parameters of a mixture of exponentials (15 P)

We consider the following "mixture of exponentials" distribution supported on $\mathbb{R}^+$, that we use to generate data, but whose parameters $\alpha$ and $\beta$ are unknown.

$$p(x;\alpha,\beta) = 0.5 \cdot \left[\alpha e^{-\alpha x} + \beta e^{-\beta x}\right]$$

A dataset $\mathcal{D} = x_1, \ldots, x_N$ with $N = 200$ has been generated from that distribution. It is given below and plotted as a histogram.

```
In [ ]: D=[ 0.74,  0.20,  0.56,  0.05,  0.67,  0.41,  0.74,  4.63,  0.59,  0.39,
            0.71,  0.17,  5.34,  0.33,  0.01,  1.11,  0.60,  0.41,  0.65,  1.97,
            0.19,  0.80,  0.04,  0.48,  0.54,  0.59,  0.31,  1.40,  0.63,  0.38,
            0.36,  0.02,  0.68,  0.72,  0.84,  0.30,  0.01,  1.37,  0.89,  0.10,
            0.21,  0.68,  0.14,  0.10,  0.11,  0.01,  0.09,  0.50,  0.34,  0.30,
            1.22, 10.05,  0.19,  0.04,  0.13,  1.53,  2.28,  1.76,  0.03,  0.31,
            0.37,  0.50,  0.05,  0.30,  0.53,  0.63,  4.20,  0.86,  0.29,  1.98,
            1.27,  0.35,  0.43,  0.35,  0.75,  0.25,  1.15,  1.65,  0.82,  0.37,
            2.55,  2.75,  3.06,  0.97,  2.65,  8.97,  0.04,  2.98,  0.36,  0.01,
            0.85,  0.90,  0.09,  0.01,  0.82,  2.30,  2.09,  0.29,  0.16,  2.12,
```

```
     5.28,  0.27,  0.15,  1.02,  0.51,  0.02,  1.72,  1.35,  0.51,  0.27,
     1.05,  2.24,  3.93,  0.62,  3.38,  0.56,  0.49,  2.84,  0.27,  0.12,
     3.99,  0.16,  0.09,  3.61,  0.54,  0.08,  0.31,  1.38,  0.63,  0.61,
     0.21,  0.13,  2.28,  2.61,  4.60,  0.02,  0.34,  0.15,  0.07,  2.44,
     0.86,  0.73,  2.01,  0.26,  0.72,  1.56,  0.09,  0.97,  0.24,  0.92,
     1.05,  0.71,  1.28,  3.79,  1.32,  0.17,  0.39,  2.82,  0.12,  2.06,
     2.04,  0.00,  1.94,  0.27,  0.91,  0.36,  0.92,  5.69,  0.33,  0.69,
     1.00,  2.19,  0.01,  0.08,  1.16,  0.31,  0.83,  0.41,  1.27,  0.08,
     4.69,  0.65,  0.43,  0.10,  2.92,  0.06,  6.21,  0.90,  0.00,  0.52,
     0.65,  0.26,  1.94,  0.37,  0.50,  5.66,  4.24,  0.40,  0.39,  7.89]

%matplotlib inline
from matplotlib import pyplot as plt
plt.hist(D,bins=30)
plt.show()
```

For this dataset, the log-likelihood function is given by

$$\ell(\alpha,\beta) = \log \prod_{i=1}^{N} p(x_i;\alpha,\beta) = \sum_{i=1}^{N} \log(e^{-\alpha x_i} + \beta e^{-\beta x_i}) - \log(2)$$

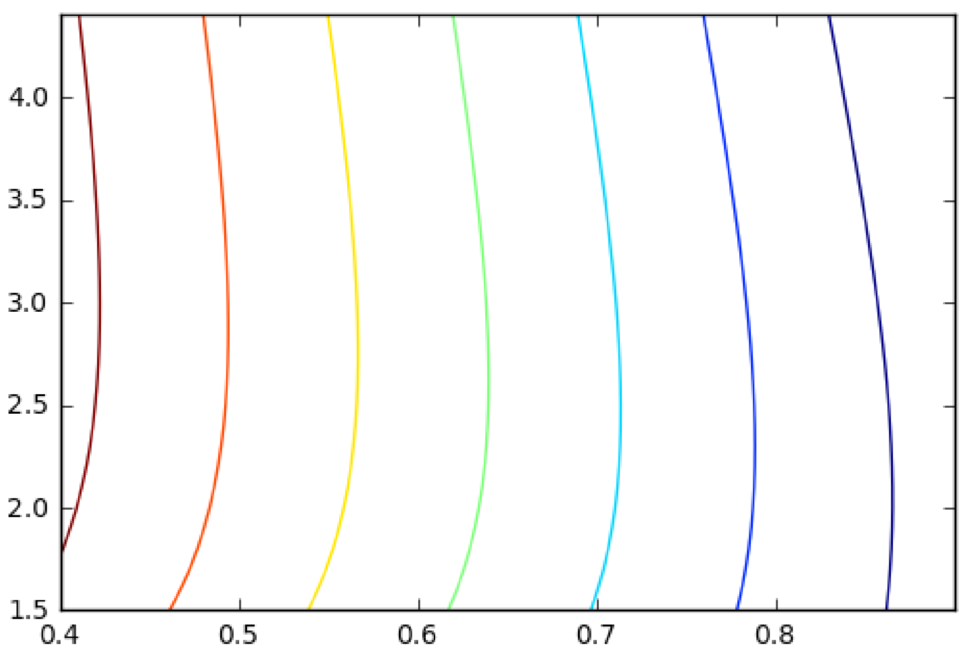
Unfortunately, it is difficult to extract the parameters $\alpha, \beta$ analytically by solving directly the equation $\nabla \ell = 0$. Instead, we will analyze the function over a grid of parameters $\alpha, \beta$. We know a priori that parameters $\alpha$ and $\beta$ are in the intervals $[0.4, 1.0]$ and $[1.5, 4.5]$ respectively.

- **Build a grid on this limited domain and evaluate log-likelihood at each point of the grid.**
- **Plot the log-likelihood function as a contour plot, and superpose the grid to it.**

Highest log-likelihood values (i.e. most probable parameters) should appear in red, and lowest values should be plotted in blue. Two adjacent lines of the contour plot should represent a log-likelihood difference of 1.0. In your code, favor numpy array operations over Python loops.

In [448]:
```
%matplotlib inline
from matplotlib import pyplot as plt

D=[ 0.74,  0.20,  0.56,  0.05,  0.67,  0.41,  0.74,  4.63,  0.59,  0.39,
    0.71,  0.17,  5.34,  0.33,  0.01,  1.11,  0.60,  0.41,  0.65,  1.97,
    0.19,  0.80,  0.04,  0.48,  0.54,  0.59,  0.31,  1.40,  0.63,  0.38,
    0.36,  0.02,  0.68,  0.72,  0.84,  0.30,  0.01,  1.37,  0.89,  0.10,
    0.21,  0.68,  0.14,  0.10,  0.11,  0.01,  0.09,  0.50,  0.34,  0.30,
    1.22, 10.05,  0.19,  0.04,  0.13,  1.53,  2.28,  1.76,  0.03,  0.31,
    0.37,  0.50,  0.05,  0.30,  0.53,  0.63,  4.20,  0.86,  0.29,  1.98,
    1.27,  0.35,  0.43,  0.35,  0.75,  0.25,  1.15,  1.65,  0.82,  0.37,
    2.55,  2.75,  3.06,  0.97,  2.65,  8.97,  0.04,  2.98,  0.36,  0.01,
    0.85,  0.90,  0.09,  0.01,  0.82,  2.30,  2.09,  0.29,  0.16,  2.12,
    5.28,  0.27,  0.15,  1.02,  0.51,  0.02,  1.72,  1.35,  0.51,  0.27,
    1.05,  2.24,  3.93,  0.62,  3.38,  0.56,  0.49,  2.84,  0.27,  0.12,
    3.99,  0.16,  0.09,  3.61,  0.54,  0.08,  0.31,  1.38,  0.63,  0.61,
```

```
    0.21,  0.13,  2.28,  2.61,  4.60,  0.02,  0.34,  0.15,  0.07,  2.44,
    0.86,  0.73,  2.01,  0.26,  0.72,  1.56,  0.09,  0.97,  0.24,  0.92,
    1.05,  0.71,  1.28,  3.79,  1.32,  0.17,  0.39,  2.82,  0.12,  2.06,
    2.04,  0.00,  1.94,  0.27,  0.91,  0.36,  0.92,  5.69,  0.33,  0.69,
    1.00,  2.19,  0.01,  0.08,  1.16,  0.31,  0.83,  0.41,  1.27,  0.08,
    4.69,  0.65,  0.43,  0.10,  2.92,  0.06,  6.21,  0.90,  0.00,  0.52,
    0.65,  0.26,  1.94,  0.37,  0.50,  5.66,  4.24,  0.40,  0.39,  7.89]

R = np.arange(0.4,1.0,0.1)
Q = np.arange(1.5,4.5,0.1)

X,Y = np.meshgrid(R,Q)


#plt.plot(X, Y)

#R = np.arange(0.4,1.0,0.1)
#Q = np.arange(1.5,4.5,0.1)
#X,Y = np.meshgrid(R,Q)

sample = np.array(D)
result = []
for k in np.nditer([D]):
    S += (np.log(np.exp(-X*k) + np.exp(-Y*k)*Y)) - np.log(2)

result = S
CS = plt.contour(X,Y,result)
```



### 1.0.3 Gradent-Based Optimization (10 P)

As an alternative to computing the log-likelihood for a whole grid, we would like to find the optimal parameters $\alpha, \beta$ by gradient-based optimization. The partial derivatives of the log-likelihood function are given by:

$$\frac{\partial \ell(\alpha,\beta)}{\partial \alpha} = \sum_{i=1}^{N} \frac{e^{-\alpha x_i}(1-\alpha x_i)}{\alpha e^{-\alpha x_i} + \beta e^{-\beta x_i}}$$
$$\frac{\partial \ell(\alpha,\beta)}{\partial \beta} = \sum_{i=1}^{N} \frac{e^{-\beta x_i}(1-\beta x_i)}{\alpha e^{-\alpha x_i} + \beta e^{-\beta x_i}}$$

A gradient ascent step of the log-likelihood function takes the form

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \leftarrow \begin{pmatrix}\alpha\\ \beta\end{pmatrix} + \gamma \nabla_{\alpha,\beta} \ell(\alpha,\beta)$$

where $\gamma$ is a learning rate to be defined. We start with initial parameters $\alpha = 0.7$ and $\beta = 3.0$.

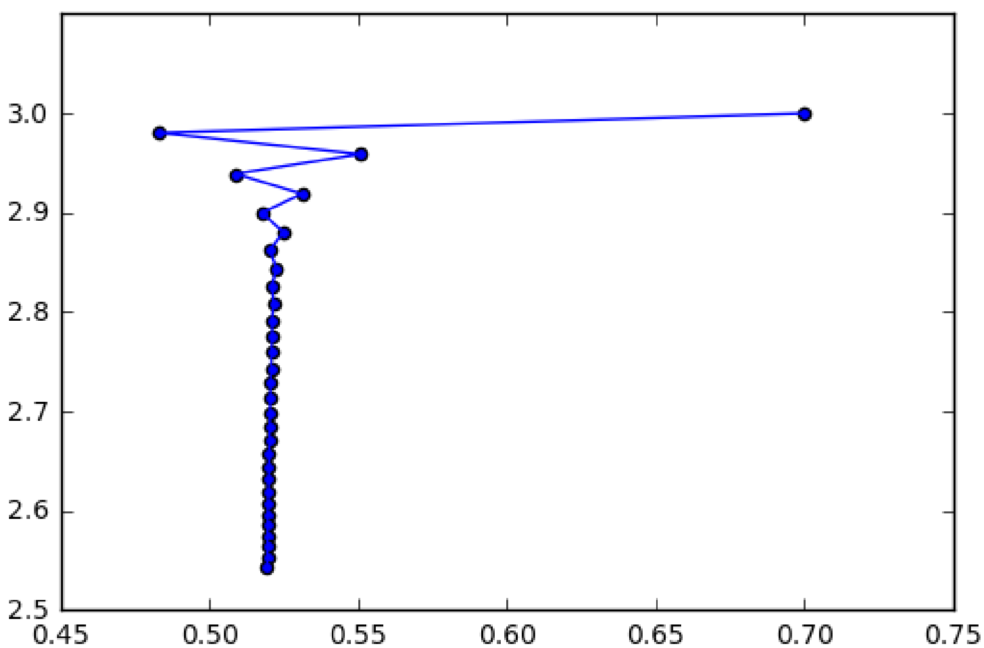
- **Implement the gradient ascent procedure.**
- **Run the gradient ascent with parameter $\gamma = 0.005$.**
- **Plot the trajectory of the gradient ascent in superposition to the contour plot of the previous exercise.**

In [447]:
```
D=[ 0.74,  0.20,  0.56,  0.05,  0.67,  0.41,  0.74,  4.63,  0.59,  0.39,
    0.71,  0.17,  5.34,  0.33,  0.01,  1.11,  0.60,  0.41,  0.65,  1.97,
    0.19,  0.80,  0.04,  0.48,  0.54,  0.59,  0.31,  1.40,  0.63,  0.38,
    0.36,  0.02,  0.68,  0.72,  0.84,  0.30,  0.01,  1.37,  0.89,  0.10,
    0.21,  0.68,  0.14,  0.10,  0.11,  0.01,  0.09,  0.50,  0.34,  0.30,
    1.22, 10.05,  0.19,  0.04,  0.13,  1.53,  2.28,  1.76,  0.03,  0.31,
    0.37,  0.50,  0.05,  0.30,  0.53,  0.63,  4.20,  0.86,  0.29,  1.98,
    1.27,  0.35,  0.43,  0.35,  0.75,  0.25,  1.15,  1.65,  0.82,  0.37,
    2.55,  2.75,  3.06,  0.97,  2.65,  8.97,  0.04,  2.98,  0.36,  0.01,
    0.85,  0.90,  0.09,  0.01,  0.82,  2.30,  2.09,  0.29,  0.16,  2.12,
    5.28,  0.27,  0.15,  1.02,  0.51,  0.02,  1.72,  1.35,  0.51,  0.27,
    1.05,  2.24,  3.93,  0.62,  3.38,  0.56,  0.49,  2.84,  0.27,  0.12,
    3.99,  0.16,  0.09,  3.61,  0.54,  0.08,  0.31,  1.38,  0.63,  0.61,
    0.21,  0.13,  2.28,  2.61,  4.60,  0.02,  0.34,  0.15,  0.07,  2.44,
    0.86,  0.73,  2.01,  0.26,  0.72,  1.56,  0.09,  0.97,  0.24,  0.92,
    1.05,  0.71,  1.28,  3.79,  1.32,  0.17,  0.39,  2.82,  0.12,  2.06,
    2.04,  0.00,  1.94,  0.27,  0.91,  0.36,  0.92,  5.69,  0.33,  0.69,
    1.00,  2.19,  0.01,  0.08,  1.16,  0.31,  0.83,  0.41,  1.27,  0.08,
    4.69,  0.65,  0.43,  0.10,  2.92,  0.06,  6.21,  0.90,  0.00,  0.52,
    0.65,  0.26,  1.94,  0.37,  0.50,  5.66,  4.24,  0.40,  0.39,  7.89]
%matplotlib inline
#import solution
import numpy as np
```

```python
import matplotlib.pyplot as plt
from scipy import stats
import pylab

#solution.s2b(D)
gamma = 0.005
alpha = 0.7
beta = 3.0
a=[]
b=[]
a.append(alpha)
b.append(beta)

def gradient_ascent(alpha, beta, D, ep, max_iter):
    converged = False
    iter = 0
    num = len(D) # number of samples

    # Iterate Loop
    while not converged:
        # for each training sample, compute the gradient learning
        update_a = 0
        update_b = 0
        for i in D:
            derq = alpha*np.exp(-alpha*i)+beta*np.exp(-beta*i)
            dera = np.exp(-alpha*i)*(1-alpha*i)
            derb = np.exp(-beta*i)*(1-beta*i)
            update_a += dera/derq
            update_b += derb/derq

        # update alpha and beta
        alpha += gamma*update_a
        a.append(alpha)
        beta += gamma*update_b
        b.append(beta)

        # mean squared error
        e = np.sqrt(np.square(update_a*gamma)+np.square(update_b*gamma))

        if e <= ep:
            print 'Converged, iterations: ', iter, '!!!'
            converged = True

        iter += 1  # update iter

        if iter == max_iter:
            print 'Max interactions exceeded!'
```

```
                converged = True

        return a,b

    if __name__ == '__main__':

        # call gredient ascent, and get intercept(=theta0) and slope(=theta1)
        a, b = gradient_ascent(alpha, beta, D, ep=0.01, max_iter=3000)

        # plot
        plt.scatter(a, b)
        line, = plt.plot(a, b, '-')
        plt.show()
        print "Done!"
```

```
Converged, iterations:  29 !!!
```




```
Done!
```

As it can be seen, the optimization procedure does not converge in reasonable time and seems to oscillate.

- **Explain the problem(s) with this approach. Propose a simple improvement of the optimization technique and apply it.**

The partial derivative is not orthogonal to the real gradient contour. To solve this problem, we should compute the gradient vector of alpha and beta with repect to the log-likelihood function in prevoius work, and shrink the learning rate step by step to approach local minimum

In [ ]:
```
### REPLACE BY YOUR CODE
import solution
solution.s2c(D)
###
```