sheet02_T

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 $X_1, \dots, X_n \in \mathbb{R}^d$ be independent draws from a multivariate Gaussian distribution with mean vector μ and covariance matrix $\Sigma = \sigma^2 I$. It can be shown that the maximum-likelihood estimator of the mean parameter μ 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 $\mu = (1, \dots, 1)$ and covariance $\Sigma = I$.

```
In [2]: import numpy
        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 [3]: def ML(X):
            return X.mean(axis=0)
```

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

```
In [4]: def JS(X,s):
            n = len(X)
            d = 50
            m_JS = (1 - ((d -2)*s**2)/(n*(numpy.linalg.norm(ML(X))**2)))*ML(X)
            return m_JS
```

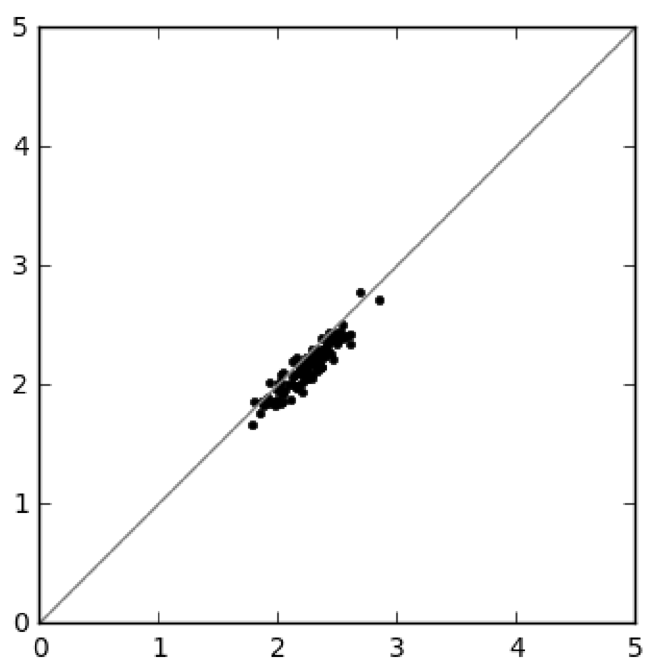
We would like to compute the error of the maximum likelihood estimator and the James-Stein estimator for 100 different samples (where each sample consists of 10 draws generated by the function `getdata` with a different random seed). Here, for reproducibility, we use seeds from 0 to 99. The error should 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 [5]: def MLerror(X, m):
            return numpy.sqrt(sum(((ML(X) - m)**2)))
        def JSerror(X, m):
            return numpy.sqrt(sum(((JS(X, s) - m)**2)))
        MLmeanEr = 0
        JSmeanEr = 0

        for i in range(0,100):
                X, m, s =  getdata(i)
                n = len(range(0,100))+1
                MLmeanEr +=  + MLerror(X, m)
                JSmeanEr += JSerror(X, m)

        print(MLmeanEr/n)
        print(JSmeanEr/n)

2.20849175392
2.11899418995
```

```
In [6]: MLlist = []
        JSlist = []
        MLmeanEr = 0
```

```
JSmeanEr = 0
for i in range(0,100):
        X, m, s =  getdata(i)
        n = len(range(0,100))+1
        MLlist.append(MLerror(X, m))
        JSlist.append(JSerror(X, m))
#print(MLlist)
#print(JSlist)
#error = numpy.matrix(MLlist)- numpy.matrix(JSlist)
#print(error)

# Plot and embed in ipython notebook!
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
#import plotly.plotly as py


axes = plt.gca()
axes.set_xlim([0,5])
axes.set_ylim([0,5])
axes.set_aspect('equal')
plt.plot(MLlist, JSlist, "o", color = "black", ms=3)
plt.plot([0,5], [0,5], 'k-', color = "grey")
plt.show()
```



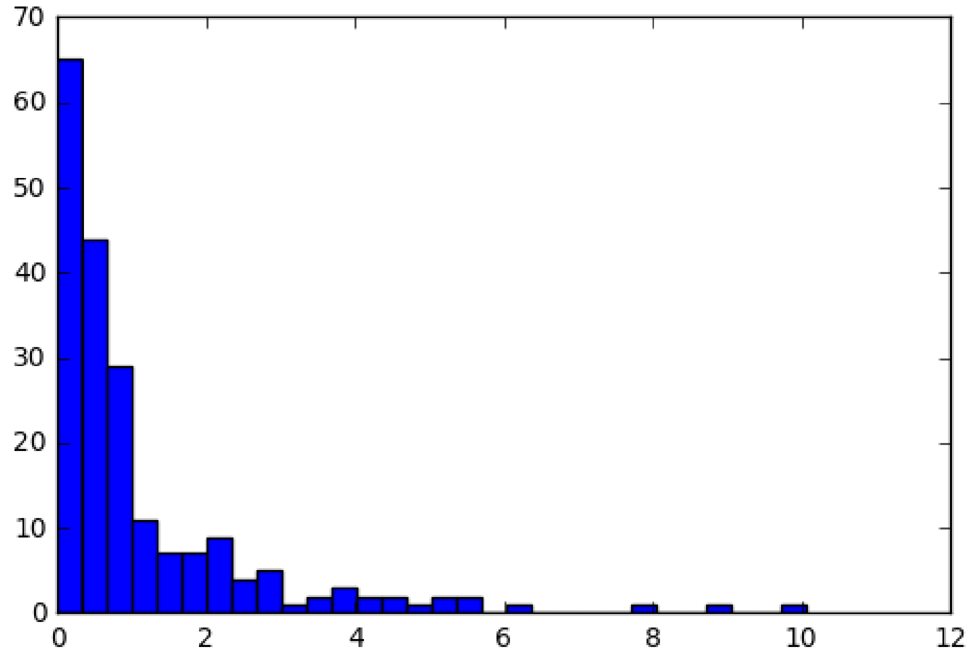
1.0.2 Parameters of a mixture of exponentials (15 P)

We consider the following "mixture of exponentials" distribution supported on $\mathbb{R}^+$, that we use to generate data, but whose parameters α and β 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 [7]:
```
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 α, β analytically by solving directly the equation $\nabla \ell = 0$. Instead, we will analyze the function over a grid of parameters α, β. We know a priori that parameters α and β 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.**

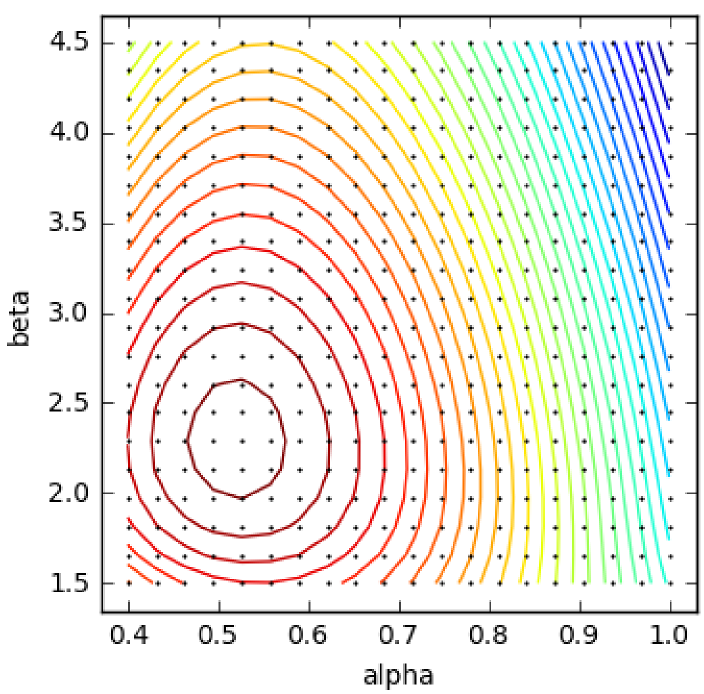
Highest log-likelihood values (i.e. most probable parameters) should appear in red, and lowest values should be plotted in blue. Two adjacent lines of the contour plot should represent a log-likelihood difference of 1.0. In your code, favor numpy array operations over Python loops.

In [8]:
```
import numpy as np

data = np.array(D)

#def func(a,b):
#    return sum(np.log(np.exp(-a*data) + b*np.exp(-b*data)) - np.log(2))

def func(a,b):
    temp = 0
    for d in D:
```

```
            temp += np.log(a*np.exp(-a*d) + b*np.exp(-b*d)) - np.log(2)
        return temp

    alphas = np.linspace(0.4, 1.0, 20)
    betas = np.linspace(1.5, 4.5, 20)
    alpha,beta = np.meshgrid(alphas, betas)

    result = func(alpha, beta)
    print("Range of result:", result.min(), result.max())
    print(alpha.shape, beta.shape, result.shape)
```

```
('Range of result:', -251.67826311342657, -218.22061393355011)
((20, 20), (20, 20), (20, 20))
```

```
In [9]: axes = plt.gca()
        axes.set_xlim([0.37,1.03])
        axes.set_ylim([1.35,4.65])
        levels = np.arange(result.min(), result.max(), 1)
        plt.xlabel('alpha')
        plt.ylabel('beta')
        axes.set_aspect(1./axes.get_data_ratio())
        plt.plot(alpha,beta,"o", color = "black", ms=1)
        plt.contour(alpha, beta, result, levels)
        plt.show()
```



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 α, β 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

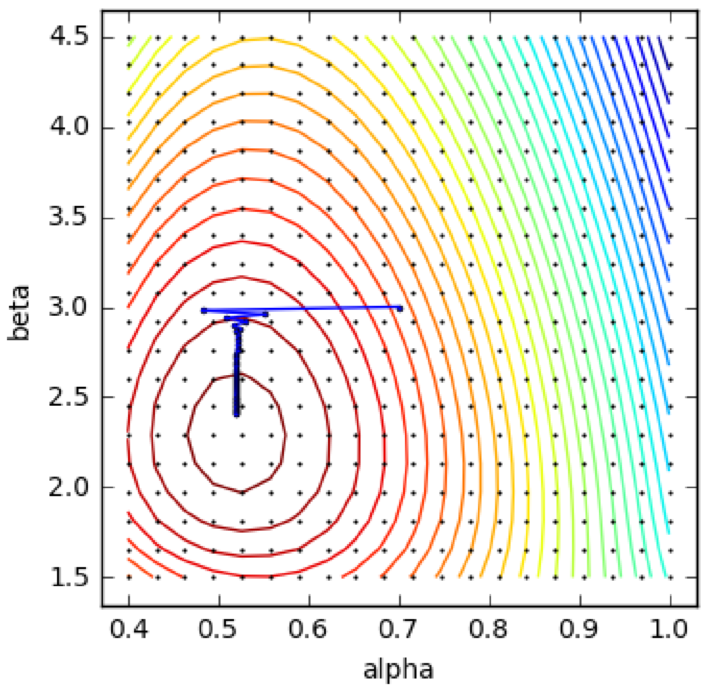
$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \leftarrow \begin{pmatrix}\alpha\\ \beta\end{pmatrix} + \gamma \nabla_{\alpha,\beta} \ell(\alpha,\beta)$$

where γ 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 [10]:
```
axes = plt.gca()
axes.set_xlim([0.37,1.03])
axes.set_ylim([1.35,4.65])
levels = np.arange(result.min(), result.max(), 1)
plt.xlabel('alpha')
plt.ylabel('beta')
axes.set_aspect(1./axes.get_data_ratio())
plt.plot(alpha,beta,"o", color = "black", ms=1)
plt.contour(alpha, beta, result, levels)

alpha_init = .7
beta_init = 3
gamma = .005
niter = 50

def der_a(a,b):
    temp = 0
    for d in D:
        temp += (np.exp(-a*d)*(1-a*d)) / (a*np.exp(-a*d) + b*np.exp(-b*d))
    return temp

def der_b(a,b):
    temp = 0
    for d in D:
        temp += (np.exp(-b*d)*(1-b*d)) / (a*np.exp(-a*d) + b*np.exp(-b*d))
```

```
        return temp

    def update(a,b, gamma):
        alpha = a + gamma*der_a(a,b)
        beta = b + gamma*der_b(a,b)
        return alpha, beta

    alist = [alpha_init]
    blist = [beta_init]

    for i in range(niter):
        a_upd, b_upd = update(alist[i], blist[i], gamma)
        alist.append(a_upd)
        blist.append(b_upd)
        plt.plot(alist[i],blist[i],"o", color = "b", ms=2)
        plt.plot([alist[i],alist[i+1]], [blist[i],blist[i+1]] , 'k-', color =
    plt.show()
```



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.**

This is a case of slow convergence. Maybe our step size should be adapted in later iterations as it is too small in the long run? Possibly perform line search to adjust γ at each iteration? Or scale the gradient by the inverse of the diagonal of the hessian? Cheat and use something from `scipy.optimize`?