Machine Intelligence II - Team MensaNord

Sheet 11

- Nikolai Zaki
- Alexander Moore
- Johannes Rieke
- Georg Hoelger
- Oliver Atanaszov

In [1]:
```
from __future__ import division, print_function
import matplotlib.pyplot as plt
%matplotlib inline
import scipy.stats
import numpy as np
from scipy.ndimage import imread
import sys
```

Exercise 1

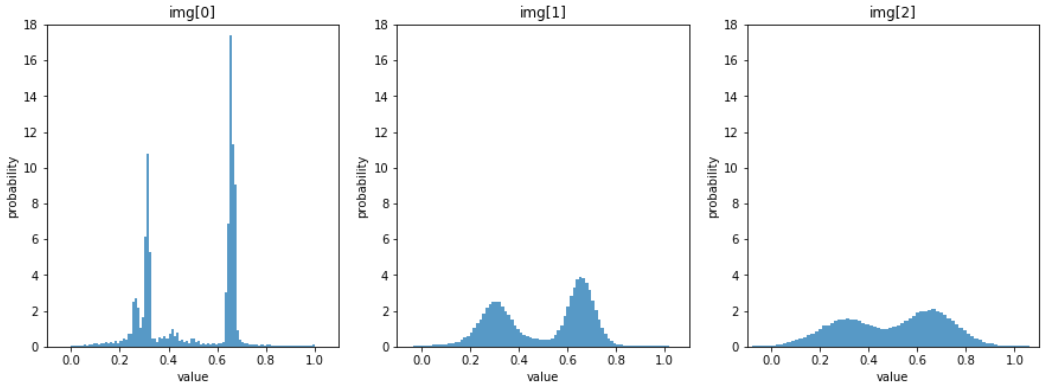
- Load the data into a vector and normalize it such that the values are between 0 and 1.
- Create two new datasets by adding Gaussian noise with zero mean and standard deviation σ N ∈ {0.05, 0.1}.

In [2]:
```
# import image
img_orig = imread('testimg.jpg').flatten()
print("$img_orig")
print("shape: \t\t", img_orig.shape) # = vector
print("values: \t from ", img_orig.min(), " to ", img_orig.max(), "\n")

# "img" holds 3 vectors
img = np.zeros((3,img_orig.shape[0]))
print("$img")
print("shape: \t\t",img.shape)

std = [0, 0.05, 0.1]
for i in range(img.shape[1]):
    # normalize => img[0]
    img[0][i] = img_orig[i] / 255
    # gaussian noise => img[1] img[2]
    img[1][i] = img[0][i] + np.random.normal(0, std[1])
    img[2][i] = img[0][i] + np.random.normal(0, std[2])

print(img[:, 0:4])
```

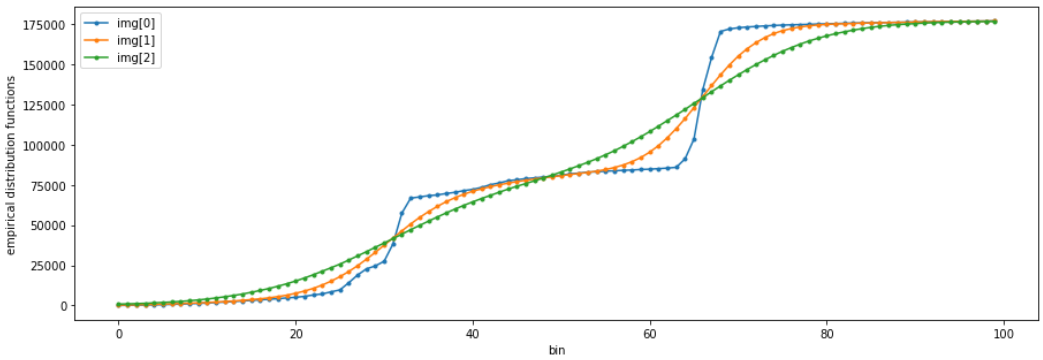
```
$img_orig
shape:          (177500,)
values:         from  0  to  255

$img
shape:          (3, 177500)
[[ 0.63529412  0.63137255  0.62745098  0.63137255]
 [ 0.67858136  0.63816685  0.69517821  0.6407592 ]
 [ 0.56691858  0.57284359  0.62174947  0.46852629]]
```

- Create a figure showing the 3 histograms (original & 2 sets of noise corrupted data – use enough bins!). In an additional figure, show the three corresponding empirical distribution functions in one plot.

In [3]:
```
# histograms
fig, axes = plt.subplots(1, 3, figsize=(15, 5))
for i, ax in enumerate(axes.flatten()):
    plt.sca(ax)
    plt.hist(img[i], 100, normed=1, alpha=0.75)
    plt.xlim(-0.1, 1.1)
    plt.ylim(0, 18)
    plt.xlabel("value")
    plt.ylabel("probability")
    plt.title('img[{}]'.format(i))
```



In [4]:
```
# divide probablity space in 100 bins
nbins = 100
bins = np.linspace(0, 1, nbins+1)

# holds data equivalent to shown histograms (but cutted from 0 to 1)
elementsPerBin = np.zeros((3,nbins))
for i in range(3):
    ind = np.digitize(img[i], bins)
    elementsPerBin[i] = [len(img[i][ind == j]) for j in range(nbins)]

# counts number of elements from bin '0' to bin 'j'
sumUptoBinJ = np.asarray([[0 for i in range(nbins)] for i in range(3)])
for i in range(3):
    for j in range(nbins):
        sumUptoBinJ[i][j] = np.sum(elementsPerBin[i][0:j+1])

# plot
plt.figure(figsize=(15, 5))
for i in range(3):
    plt.plot(sumUptoBinJ[i], '.-')
plt.legend(['img[0]', 'img[1]', 'img[2]'])
plt.xlabel('bin')
plt.ylabel('empirical distribution functions');
```



- Take a subset of P = 100 observations and estimate the probability density p̂ of intensities with a rectangular kernel (“gliding window”) parametrized by window width h.
- Plot the estimates p̂ resulting for (e.g. 10) different samples of size P

In [5]:
```
def H(vec, h):
    """
    (rectangular) histogram kernel function
    """
    vec = np.asarray(vec)
    return np.asarray([1 if abs(x)<.5 else 0 for x in vec])
```

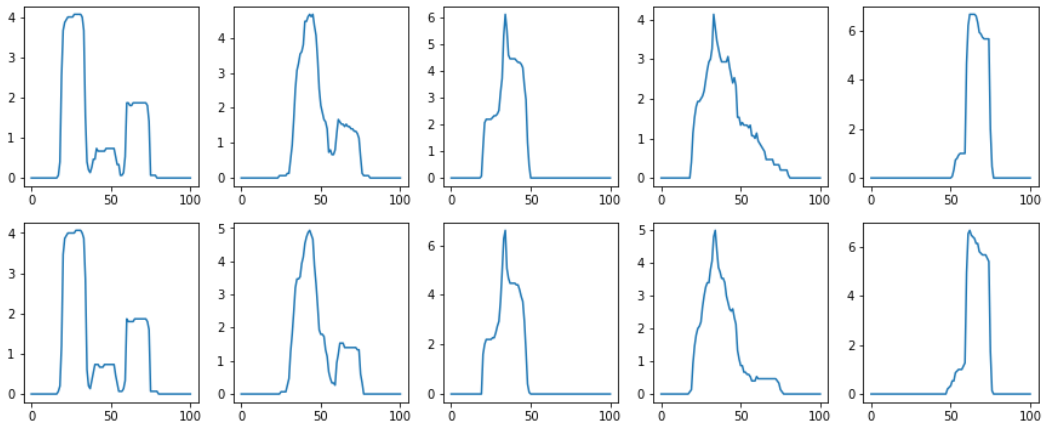
$$P(\underline{x}) = \frac{1}{h^n}\frac{1}{p}\Sigma_{\alpha=1}^{p} H(\frac{\underline{x}-\underline{x}^{(\alpha)}}{h})$$

In [6]:
```
def P_est(x, h, data, kernel = H):
    """
    returns the probability that data contains values @ (x +- h/2)
    """
    n = 1 #= data.shape[1] #number of dimensions (for multidmensional da
ta)
    p = len(data)
    return 1/(h**n)/p*np.sum(kernel((data - x)/h, h))
```

In [7]:
```
# take 10 data sets with 100 observations (indexes 100k to 101k)
# nomenclature: data_3(3, 10, 100) holds 3 times data(10, 100)
P = 100
offset = int(100000)
data_3 = np.zeros((3, 10,P))
for j in range(3):
    for i in range(10):
        data_3[j][i] = img[j][offset+i*P:offset+(i+1)*P]
print(data_3.shape)
```

```
(3, 10, 100)
```

In [8]:
```
# calculate probability estimation for (center +- h/2) on the 10 data se
ts
h = .15
nCenters = 101
Centers = np.linspace(0,1,nCenters)

fig, ax = plt.subplots(2,5,figsize=(15,6))
ax = ax.ravel()
for i in range(10):
    ax[i].plot([P_est(center,h,data_3[0][i]) for center in Centers])
```



- Calculate the negative log-likelihood per datapoint of your estimator using 5000 samples from the data not used for the density estimation (i.e. the “test-set”). Get the average of the negative log-likelihood over the 10 samples.

$$P(\{\underline{x}^{(\alpha)}\};\underline{w}) = -\Sigma_{\alpha=1}^{p} lnP(\underline{x}^{(\alpha)};\underline{w})$$

In [9]:
```
testdata = img[0][50000:55000]

# calculate average negative log likelihood for
def avg_NegLL(data, h, kernel=H):
    sys.stdout.write(".")
    average = 0
    for i in range(10):
        L_prob = [np.log(P_est(x,h,data[i],kernel)) for x in testdata]
        negLL = -1*np.sum(L_prob)
        average += negLL
    average /= 10
    return average
```

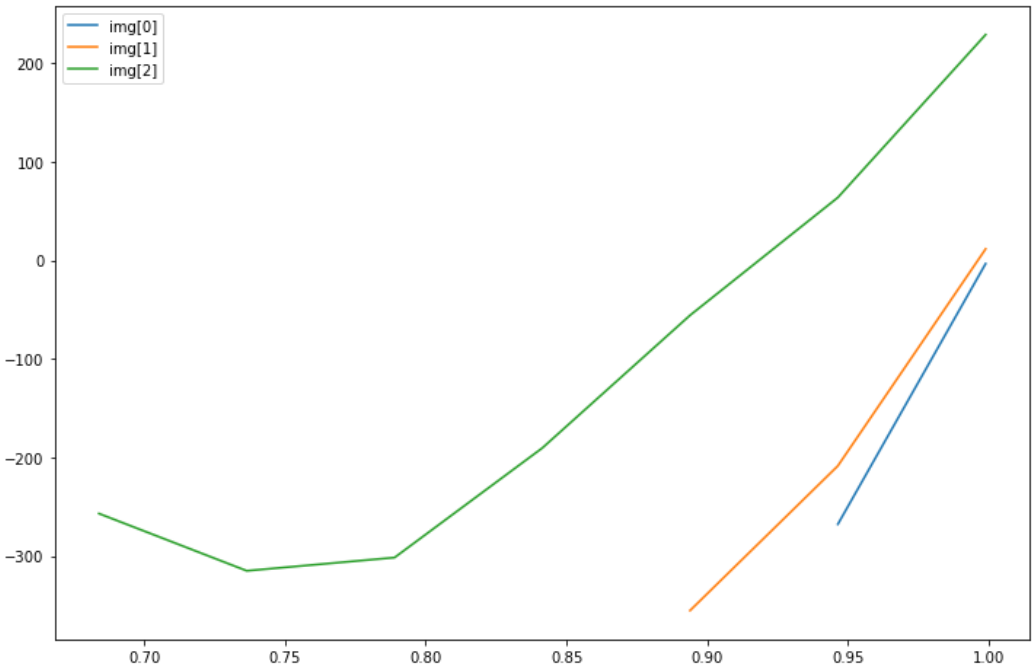
2) Repeat this procedure (without plotting) for a sequence of kernel widths h to get the mean log likelihood (averaged over the different samples) resulting for each value of h.

(a) Apply this procedure to all 3 datasets (original and the two noise-corruped ones) to make a plot showing the obtained likelihoods (y-axis) vs. kernel width h (x-axis) as one line for each dataset.

In [10]:
```
hs = np.linspace(0.001, 0.999, 20)

def plot_negLL(data_3=data_3, kernel=H):
    fig = plt.figure(figsize=(12,8))
    for j in range(3):
        print("calc data[{}]".format(j))
        LLs = [avg_NegLL(data_3[j],h,kernel=kernel) for h in hs]
        plt.plot(hs,LLs)
        print()
    plt.legend(['img[0]', 'img[1]', 'img[2]'])
    plt.show()
```

In [18]:
```
plot_negLL()
```

```
calc data[0]
.
/home/georg/anaconda3/lib/python3.6/site-packages/ipykernel/__main__.py:8
: RuntimeWarning: divide by zero encountered in log

..................
calc data[1]
..................
calc data[2]
..................
```



not plotted points have value = inf because:

$negLL = -log(\Pi_\alpha P(x^\alpha, w))$

so if one single $P(x^\alpha, w) = 0$ occurs (x has 5000 elements)

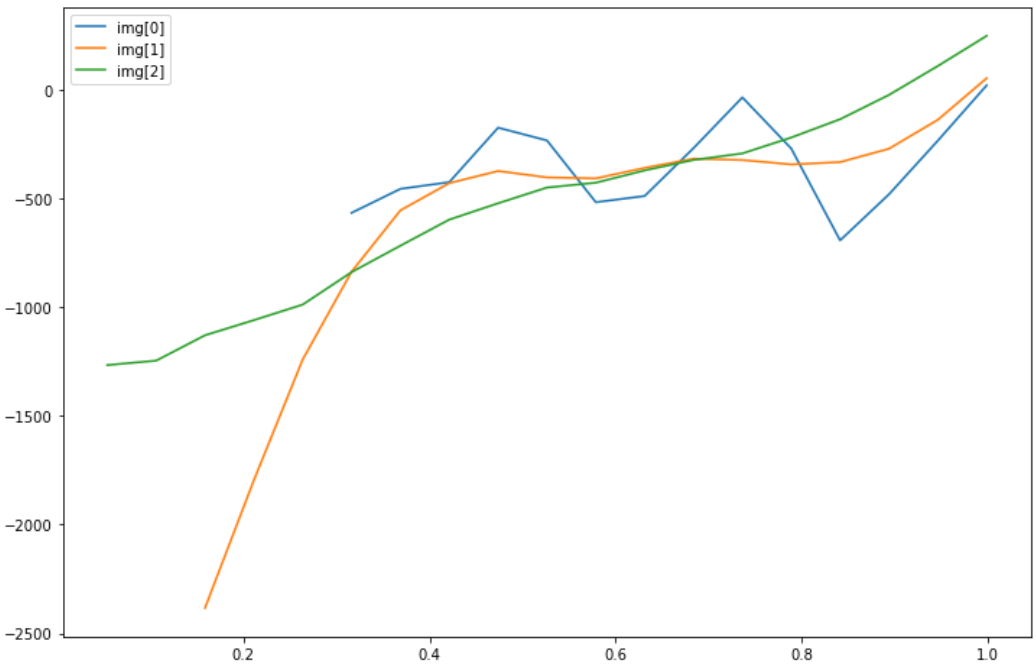
the result is -log(0)=inf (not defined)

this only occurs with the histogram kernel.

(b) Repeat the previous step (LL & plot) for samples of size P = 500.

In [17]:
```
P = 500
data_3b = np.zeros((3, 10,P))
for j in range(3):
    for i in range(10):
        data_3b[j][i] = img[j][offset+i*P:offset+(i+1)*P]

plot_negLL(data_3=data_3b)
```

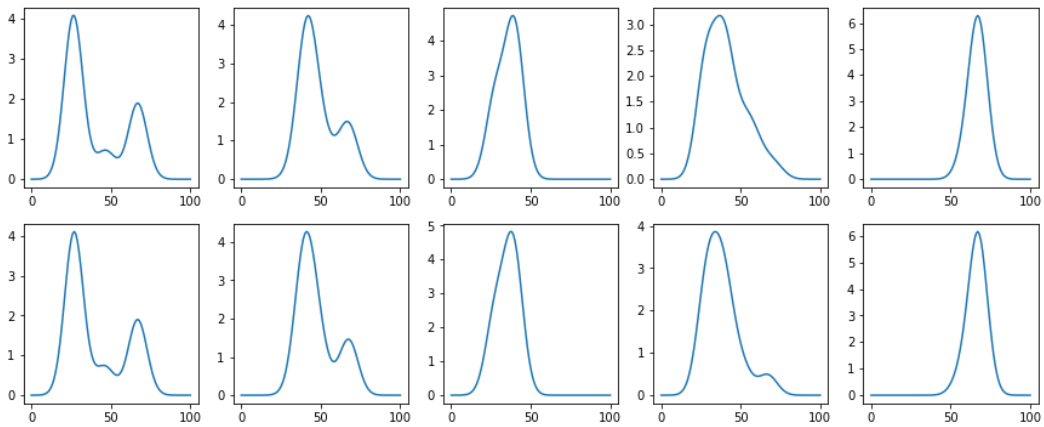
```
calc data[0]
.
/home/georg/anaconda3/lib/python3.6/site-packages/ipykernel/__main__.py:8
: RuntimeWarning: divide by zero encountered in log

..................
calc data[1]
..................
calc data[2]
..................
```



(c) Repeat the previous steps (a & b) for the Gaussian kernel with σ^2 = h.

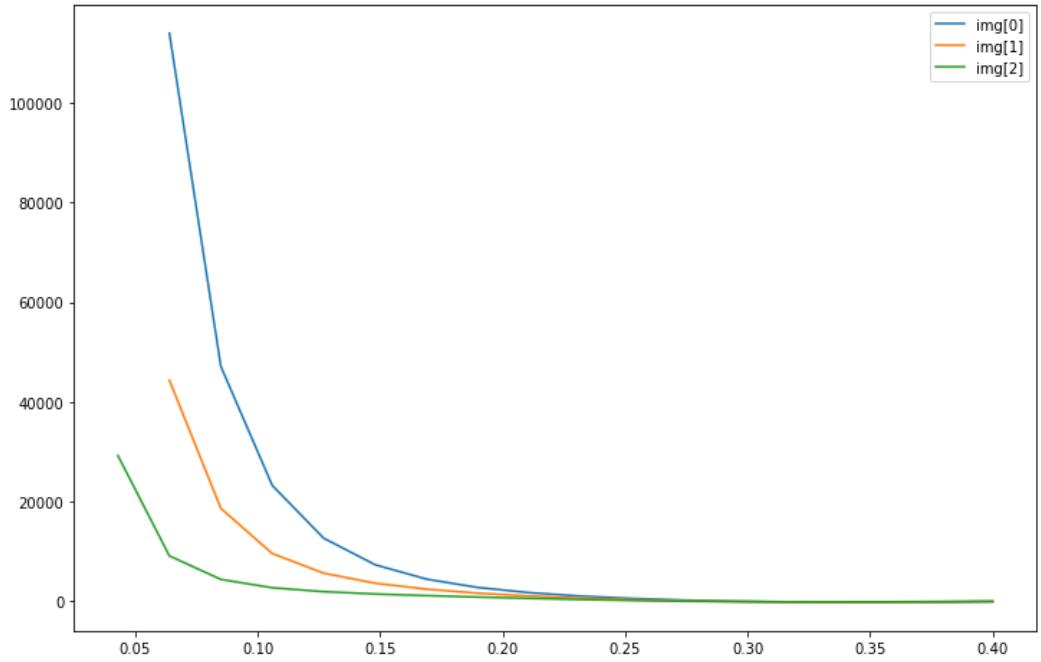
In [12]:
```
def Gaussian(x,h):
    """
    gaussian kernel function
    """

    return np.exp(-x**2/h/2)/np.sqrt(2*np.pi*h)
```

In [13]:
```
fig, ax = plt.subplots(2,5,figsize=(15,6))
h = .15

ax = ax.ravel()
for i in range(10):
    ax[i].plot([P_est(center,h,data_3[0][i],kernel=Gaussian) for center
in Centers])
```



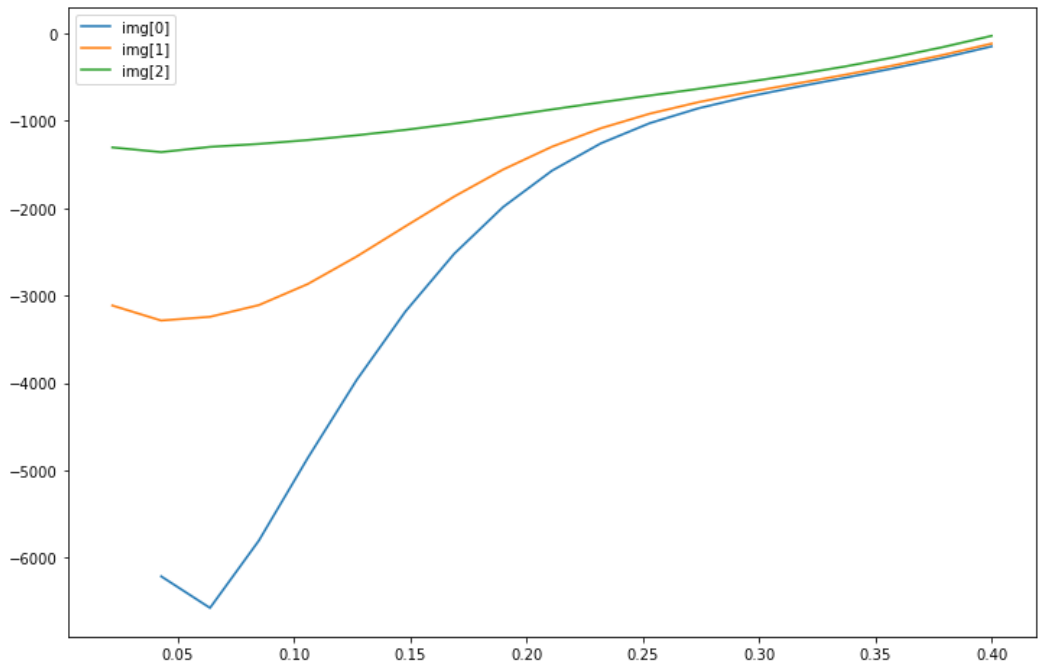
In [13]:
```
hs = np.linspace(0.001, 0.4, 20)
plot_negLL(kernel=Gaussian)
```

```
calc data[0]
.

/home/georg/anaconda3/lib/python3.6/site-packages/ipykernel/__main__.py:8
: RuntimeWarning: divide by zero encountered in log

..................
calc data[1]
..................
calc data[2]
..................
```



In [22]:
```
plot_negLL(data_3=data_3b, kernel=Gaussian)
```

```
calc data[0]
.

/home/georg/anaconda3/lib/python3.6/site-packages/ipykernel/__main__.py:8
: RuntimeWarning: divide by zero encountered in log

..................
calc data[1]
..................
calc data[2]
..................
```



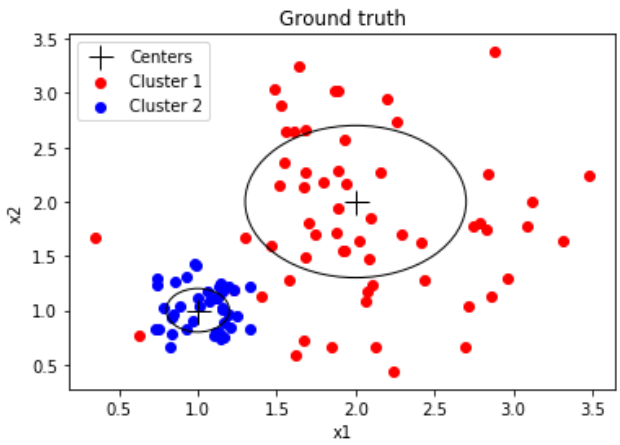
Exercise 2

1.1 Create dataset

In [6]:
```
M = 2
w1, w2 = [2,2], [1,1]  # means
sigma2 = 0.2  # standard deviations
N = 100
P1, P2 = 2/3, 1/3

def create_data(sigma1=0.7):
    X = np.zeros((N, 2))
    which_gaussian = np.zeros(N)

    for n in range(N):
        if np.random.rand() < P1:  # sample from first Gaussian
            X[n] = np.random.multivariate_normal(w1, np.eye(len(w1)) * s
igma1**2)
            which_gaussian[n] = 0
        else:  # sample from second Gaussian
            X[n] = np.random.multivariate_normal(w2, np.eye(len(w2)) * s
igma2**2)
            which_gaussian[n] = 1

    return X, which_gaussian

sigma1 = 0.7
X, which_gaussian = create_data(sigma1)
```

In [7]:
```
def plot_data(X, which_gaussian, centers, stds):
    plt.scatter(*X[which_gaussian == 0].T, c='r', label='Cluster 1')
    plt.scatter(*X[which_gaussian == 1].T, c='b', label='Cluster 2')
    plt.plot(centers[0][0], centers[0][1], 'k+', markersize=15, label='C
enters')
    plt.plot(centers[1][0], centers[1][1], 'k+', markersize=15)
    plt.gca().add_artist(plt.Circle(centers[0], stds[0], ec='k', fc='non
e'))
    plt.gca().add_artist(plt.Circle(centers[1], stds[1], ec='k', fc='non
e'))
    plt.xlabel('x1')
    plt.ylabel('x2')
    plt.legend()

plot_data(X, which_gaussian, [w1, w2], [sigma1, sigma2])
plt.title('Ground truth')
```

Out[7]: <matplotlib.text.Text at 0x7f14e6371198>



1.2 Run Expectation-Maximization algorithm

See slide 18 of the lecture for an outline of the algorithm.

In [8]:
```
from scipy.stats import multivariate_normal

def variance(X):
    """Calculate a single variance value for the vectors in X."""
    mu = X.mean(axis=0)
    return np.mean([np.linalg.norm(x - mu)**2 for x in X])

def run_expectation_maximization(X, w=None, sigma_squared=None, verbose=
False):
    # Initialization.
    P_prior = np.ones(2) * 1 / M
    P_likelihood = np.zeros((N, M))
    P_posterior = np.zeros((M, N))

    mu = X.mean(axis=0)  # mean of the original data
    var = variance(X)  # variance of the original data

    if w is None:
        w = np.array([mu + np.random.rand(M) - 0.5, mu + np.random.rand(
M) - 0.5])

    if sigma_squared is None:
        sigma_squared = np.array([var + np.random.rand() - 0.5,var + np.
random.rand() - 0.5])
        #sigma_squared = np.array([var, var])

    if verbose:
        print('Initial centers:', w)
        print('Initial variances:', sigma_squared)
        print()
        print()


    theta = 0.001
    distance = np.inf
    step = 0


    # Optimization loop.
    while distance > theta:
    #for i in range(1):
        step += 1
        if verbose:
            print('Step', step)
            print('-'*50)

        # Store old parameter values to calculate distance later on.
        w_old = w.copy()
        sigma_squared_old = sigma_squared.copy()
        P_prior_old = P_prior.copy()

        if verbose:
            print('Distances of X[0] to proposed centers:', np.linalg.no
rm(X[0] - w[0]), np.linalg.norm(X[0] - w[1]))

        # E-Step: Calculate likelihood for each data point.
        for (alpha, q), _ in np.ndenumerate(P_likelihood):
            P_likelihood[alpha, q] = multivariate_normal.pdf(X[alpha], w
[q], sigma_squared[q])

        if verbose:
            print('Likelihoods of X[0]:', P_likelihood[0])

        # E-Step: Calculate assignment probabilities (posterior) for eac
h data point.
        for (q, alpha), _ in np.ndenumerate(P_posterior):
            P_posterior[q, alpha] = (P_likelihood[alpha, q] * P_prior[q]
) / np.sum([P_likelihood[alpha, r] * P_prior[r] for r in range(M)])
```

```
Initial centers: [[ 1.46659184  1.00840719]
 [ 1.6887331   1.12294994]]
Initial variances: [ 0.5361026   0.70008899]


Step 1
--------------------------------------------------
Distances of X[0] to proposed centers: 1.85350407169 1.61364405175
Likelihoods of X[0]: [ 0.01205145  0.03540212]
Assignment probabilities of X[0]: [ 0.25396298  0.74603702]

Distance of centers: 0.342350730667
Distance of variances: 0.110843800222
Distance of priors: 0.0167596416462
Distance of centers: 0.524949058885
Distance of variances: 0.0296240647638
Distance of priors: 0.0167596416462
Maximum distance: 0.524949058885

New centers: [[ 1.48212253  1.35040546]
 [ 1.77121556  1.64137848]]
New variances: [ 0.4252588   0.67046492]
New priors: [ 0.48324036  0.51675964]
==================================================

Step 2
--------------------------------------------------
Distances of X[0] to proposed centers: 1.62914122605 1.22944655952
Likelihoods of X[0]: [ 0.01651657  0.07689418]
Assignment probabilities of X[0]: [ 0.16726584  0.83273416]

Distance of centers: 0.0786590556623
Distance of variances: 0.109721539659
Distance of priors: 0.0198215038604
Distance of centers: 0.095987506979
Distance of variances: 0.115427169678
Distance of priors: 0.0198215038604
Maximum distance: 0.115427169678

New centers: [[ 1.42750401  1.29380101]
 [ 1.83803828  1.71028659]]
New variances: [ 0.31553726  0.55503775]
New priors: [ 0.50306186  0.49693814]
==================================================

Step 3
--------------------------------------------------
Distances of X[0] to proposed centers: 1.7061377005 1.13732100628
Likelihoods of X[0]: [ 0.00500651  0.08942159]
Assignment probabilities of X[0]: [ 0.05363756  0.94636244]

Distance of centers: 0.128839810635
Distance of variances: 0.07181587876
Distance of priors: 0.00931422469505
Distance of centers: 0.146548054939
Distance of variances: 0.0102699546013
Distance of priors: 0.00931422469505
Maximum distance: 0.146548054939

New centers: [[ 1.33514188  1.20397376]
 [ 1.94293049  1.81262893]]
New variances: [ 0.24372138  0.5447678 ]
New priors: [ 0.51237609  0.48762391]
==================================================

Step 4
--------------------------------------------------
Distances of X[0] to proposed centers: 1.83326132432 0.996785807261
```

In [9]:
```
plot_data(X, which_gaussian_em, cluster_centers_em, cluster_stds_em)
plt.title('Predicted by Expectation-Maximization'
```

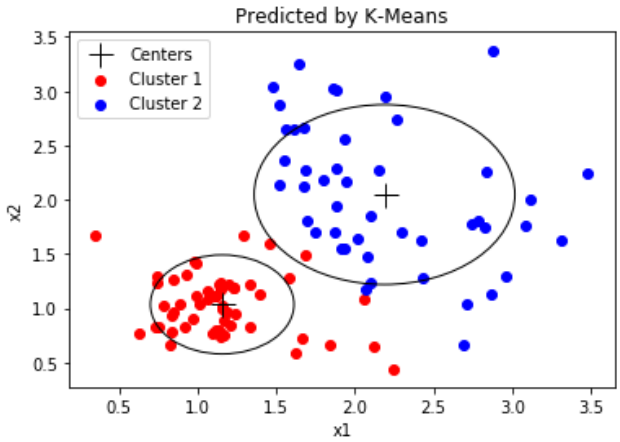
```
  File "<ipython-input-9-623819f06fb1>", line 2
    plt.title('Predicted by Expectation-Maximization'
                                                     ^
SyntaxError: unexpected EOF while parsing
```

1.3 Run K-means algorithm

For simplicity, we use the sklearn version of K-means here. The detailed algorithm was already implemented in a previous exercise.

In [10]:
```
from sklearn.cluster import KMeans

def run_k_means(X):
    km = KMeans(2)
    km.fit(X)
    which_gaussian_km = km.predict(X)
    cluster_stds = np.array([np.sqrt(variance(X[which_gaussian_km == 0])
), np.sqrt(variance(X[which_gaussian_km == 1]))])
    return which_gaussian_km, km.cluster_centers_, cluster_stds

which_gaussian_km, cluster_centers_km, cluster_stds_km = run_k_means(X)

plot_data(X, which_gaussian_km, cluster_centers_km, cluster_stds_km)
plt.title('Predicted by K-Means')
```

Out[10]: <matplotlib.text.Text at 0x7f14dfe64da0>



K-means clusters the data point by establishing a straight separation line. This cannot fully capture the nature of the data, e.g. the points around the lower left Gaussian, which actually belong to the upper right Gaussian.

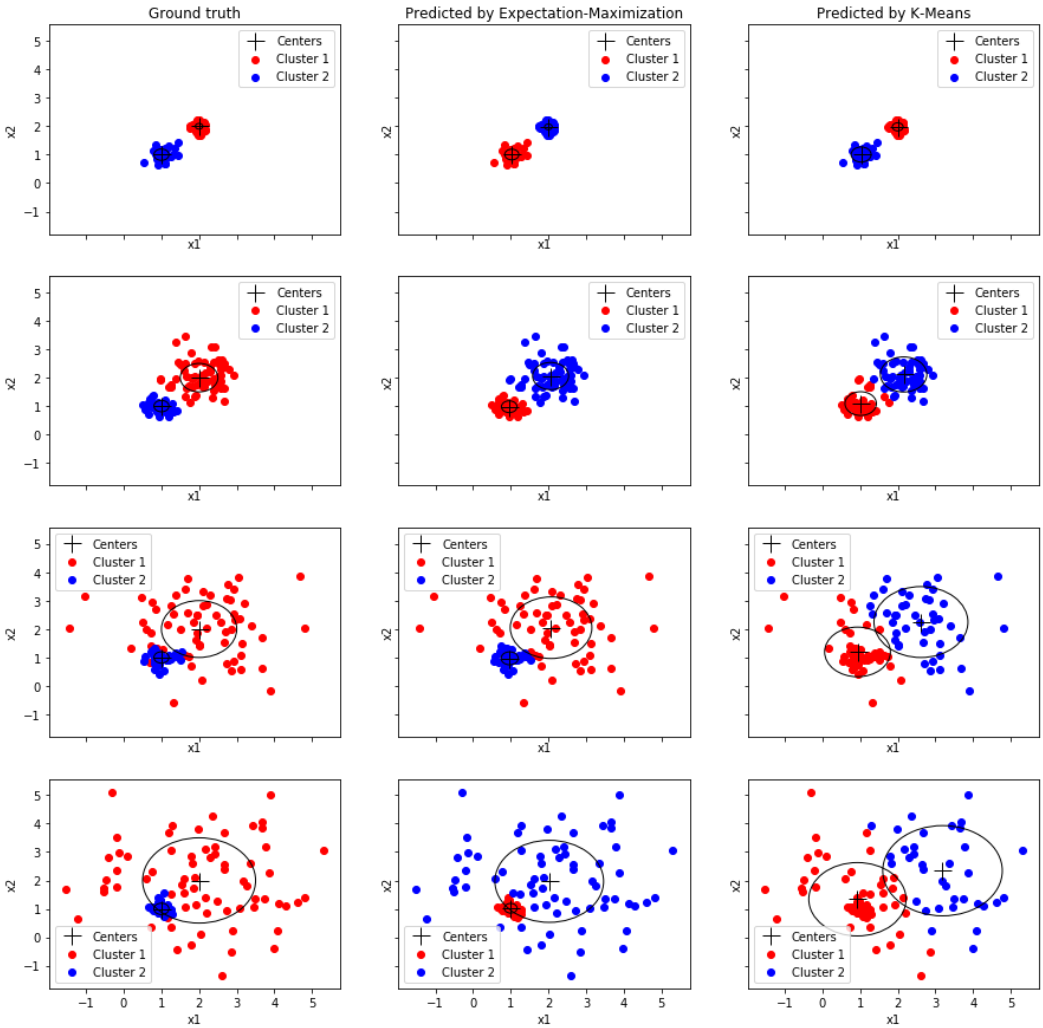
1.4 Initialize EM algorithm with cluster parameters from K-Means

In [11]:
```
_, _, _, num_steps_em_km = run_expectation_maximization(X, cluster_cente
rs_km, cluster_stds_km**2)

print('Took', num_steps_em, 'steps with random initalization')
print('Took', num_steps_em_km, 'steps with initialization from K-means')
```

```
Took 14 steps with random initalization
Took 10 steps with initialization from K-means
```

1.5 Repeat analysis for different σ_1 values

In [12]:
```
sigma1s = [0.1, 0.5, 1, 1.5]
fig, axes = plt.subplots(len(sigma1s), 3, figsize=(15, 15), sharex=True,
sharey=True)

for i, (sigma1, horizontal_axes) in enumerate(zip(sigma1s, axes)):
    X, which_gaussian = create_data(sigma1)

    plt.sca(horizontal_axes[0])
    plot_data(X, which_gaussian, [w1, w2], [sigma1, sigma2])
    if i == 0:
        plt.title('Ground truth')

    which_gaussian_em, cluster_centers_em, cluster_stds_em, num_steps_em
= run_expectation_maximization(X)
    plt.sca(horizontal_axes[1])
    plot_data(X, which_gaussian_em, cluster_centers_em, cluster_stds_em)
    if i == 0:
        plt.title('Predicted by Expectation-Maximization')

    which_gaussian_km, cluster_centers_km, cluster_stds_km = run_k_means
(X)
    plt.sca(horizontal_axes[2])
    plot_data(X, which_gaussian_km, cluster_centers_km, cluster_stds_km)
    if i == 0:
        plt.title('Predicted by K-Means')
```



Each row corresponds to increasing σ_1 (the values are 0.1, 0.5, 1, 1.5).

K-means and Expectation-Maximization show similar results for small σ_1, i.e. if the clusters are clearly separated. With increasing σ_1, the Gaussians overlap more and more, and K-means fails to cluster them correctly.

In [ ]: