Machine Intelligence II - Team MensaNord

Sheet 11

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

In [16]:
```
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

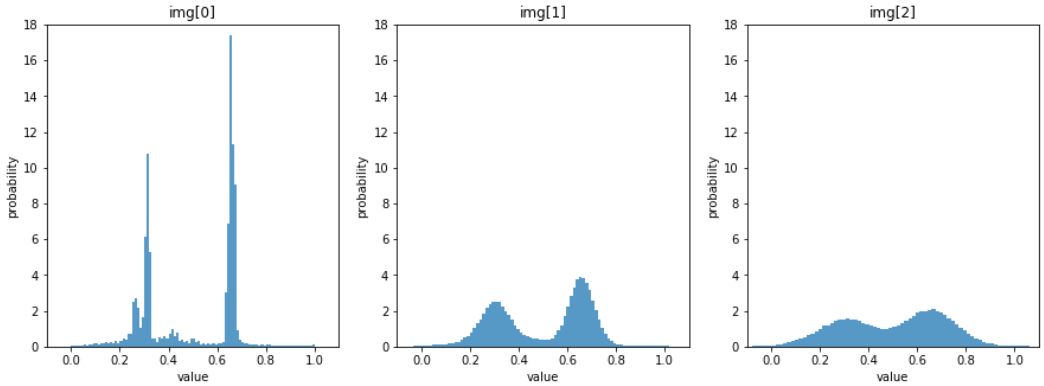
- Load the data into a vector and normalize it such that the values are between 0 and 1.
- Create two new datasets by adding Gaussian noise with zero mean and standard deviation σ N ∈ {0.05, 0.1}.

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])
```

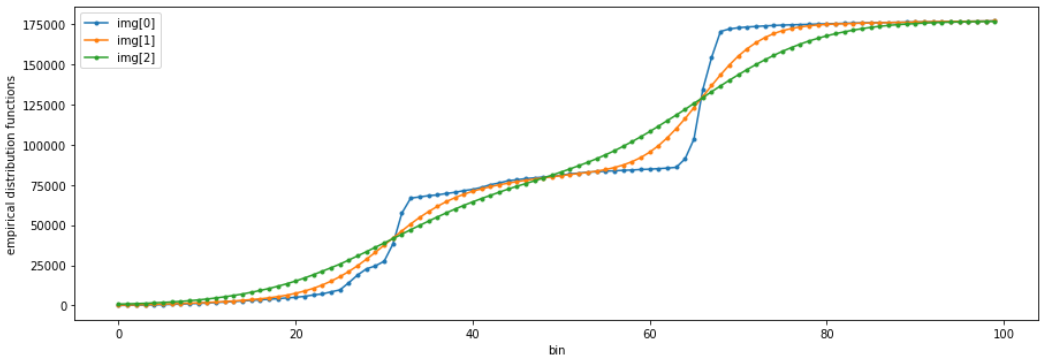
```
$img_orig
shape:          (177500,)
values:         from  0  to  255

$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])
```

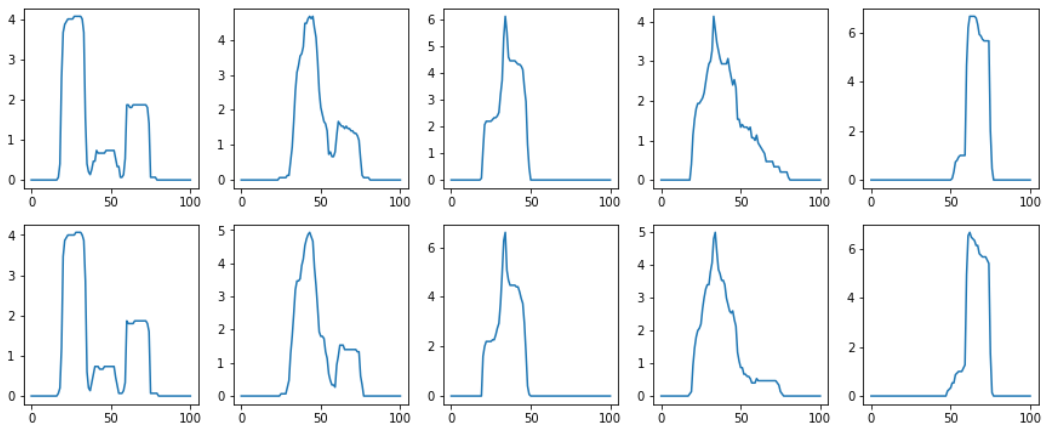
$$P(\underline{x}) = \frac{1}{h^n}\frac{1}{p}\Sigma_{\alpha=1}^{p} H\left(\frac{\underline{x}-\underline{x}^{(\alpha)}}{h}\right)$$

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.

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

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
```

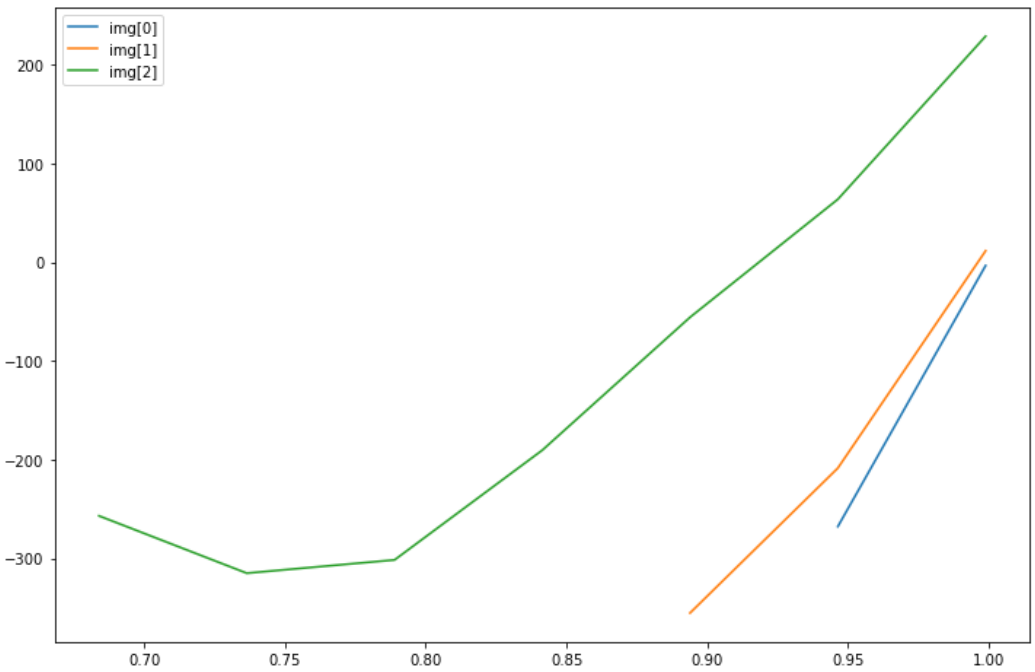
2) Repeat this procedure (without plotting) for a sequence of kernel widths h to get the mean log likelihood (averaged over the different samples) resulting for each value of h.

(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)

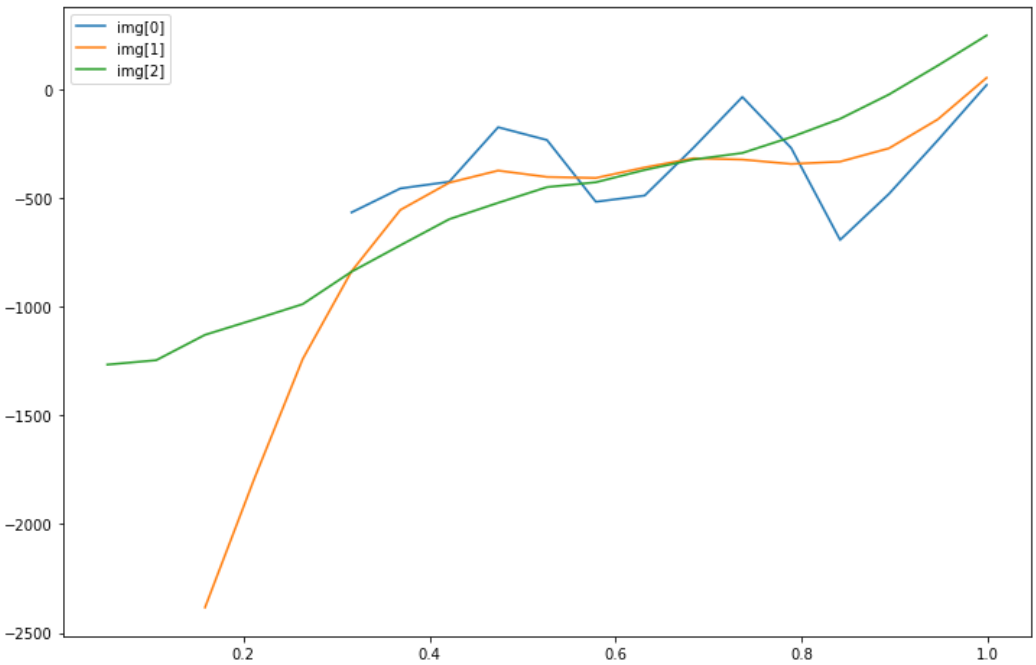
the result is -log(0)=inf (not defined)

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)
```

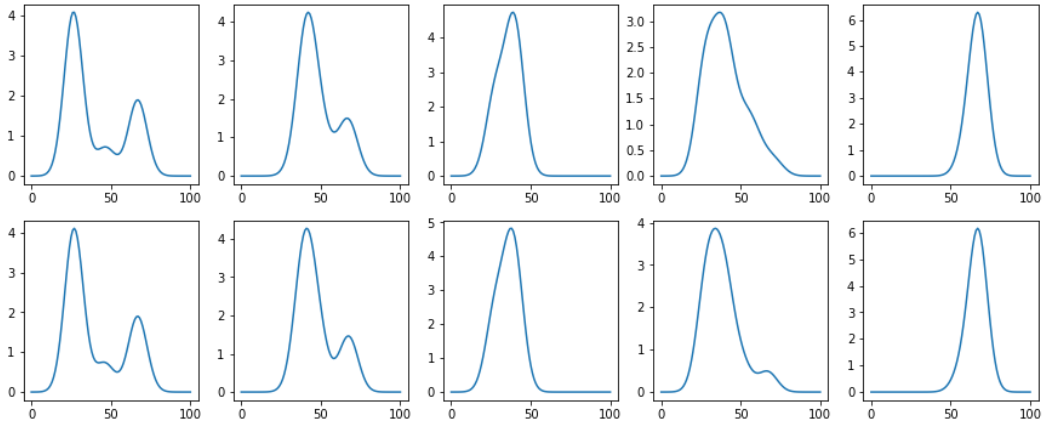
```
calc data[0]
.

/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.

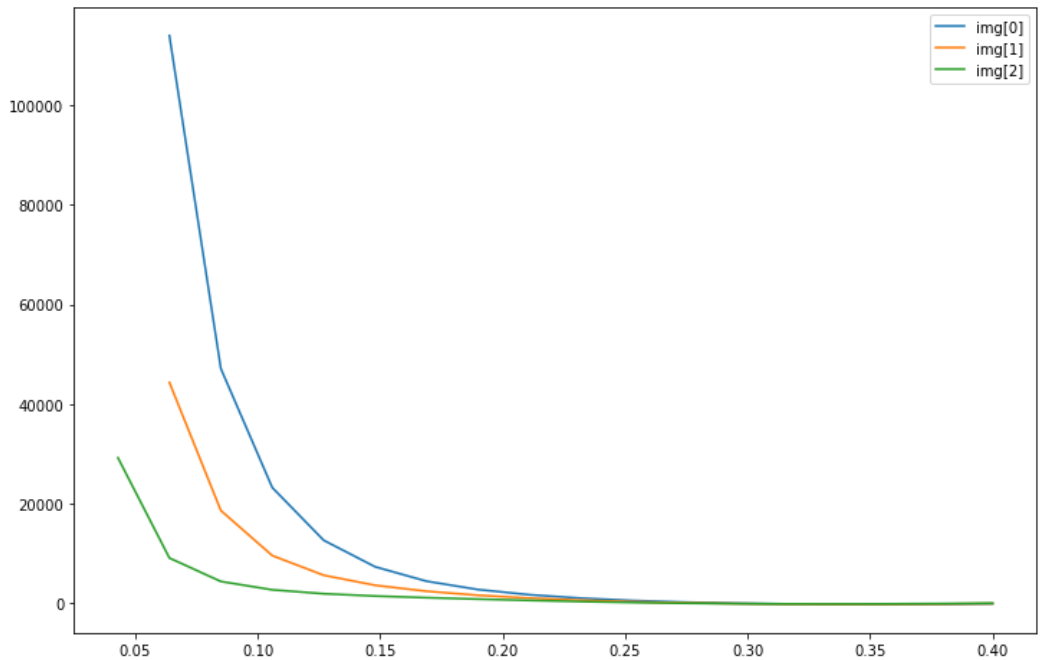
In [12]:
```
def Gaussian(x,h):
    """
    gaussian kernel function
    """

    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])
```



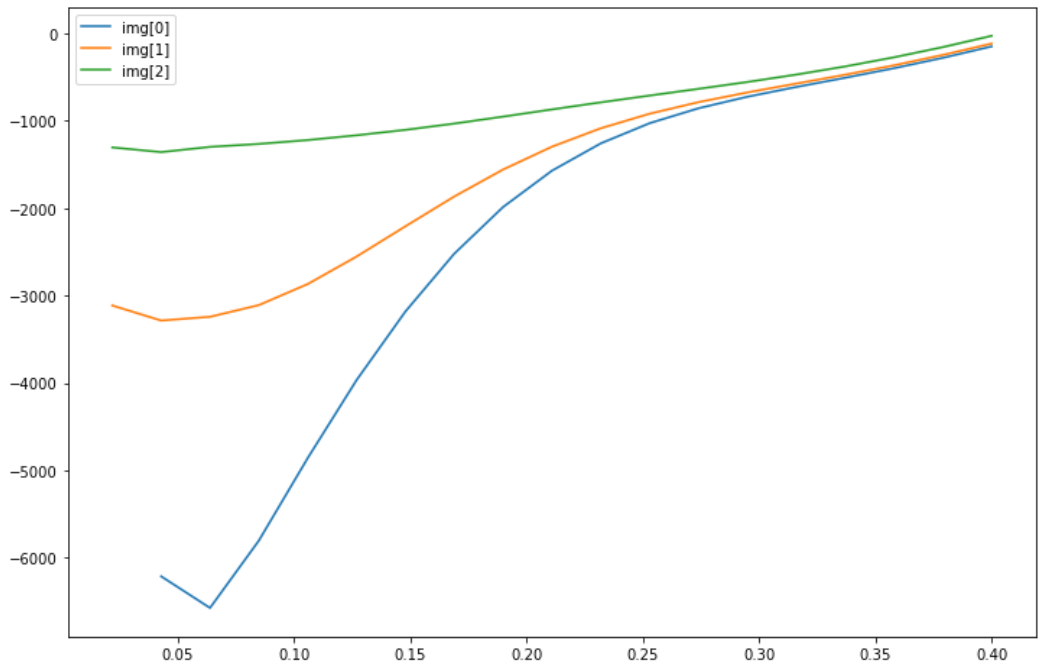
In [13]:
```
hs = np.linspace(0.001, 0.4, 20)
plot_negLL(kernel=Gaussian)
```

```
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]
..................
```



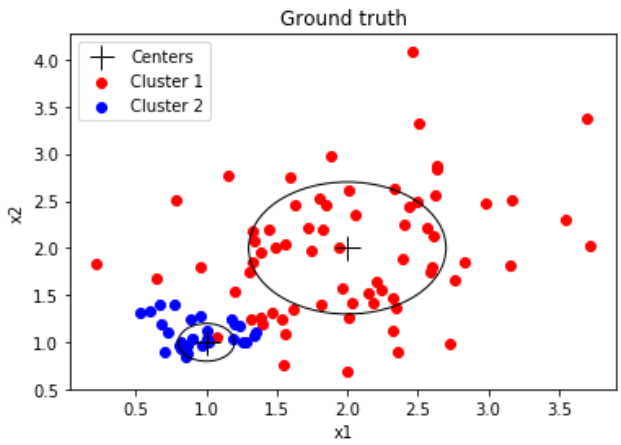
Exercise 2

1.1 Create dataset

In [17]:
```
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 [18]:
```
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[18]: <matplotlib.text.Text at 0x7f1ea7ddc2b0>



1.2 Run Expectation-Maximization algorithm

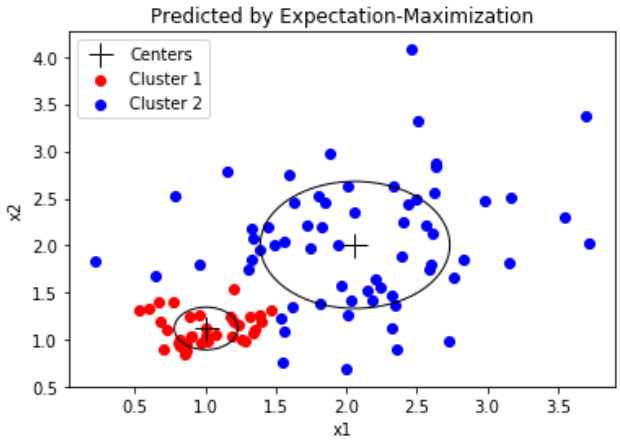
See slide 18 of the lecture for an outline of the algorithm.

In [19]:
```
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: [[ 1.53518244  1.92693386]
 [ 1.49432597  1.95412241]]
Initial variances: [ 1.20752752  1.40122925]


Step 1
--------------------------------------------------
Distances of X[0] to proposed centers: 1.07545424393 1.11929886145
Likelihoods of X[0]: [ 0.08164578  0.07263752]
Assignment probabilities of X[0]: [ 0.52919388  0.47080612]

Distance of centers: 0.280723619496
Distance of variances: 0.65552846138
Distance of priors: 0.0234334427061
Distance of centers: 0.321569568555
Distance of variances: 0.805770461625
Distance of priors: 0.0234334427061
Maximum distance: 0.805770461625

New centers: [[ 1.68565079  1.68994225]
 [ 1.69703919  1.70449401]]
New variances: [ 0.55199906  0.59545879]
New priors: [ 0.52343344  0.47656656]
==================================================

Step 2
--------------------------------------------------
Distances of X[0] to proposed centers: 0.925878542461 0.912824005713
Likelihoods of X[0]: [ 0.13263358  0.13277191]
Assignment probabilities of X[0]: [ 0.52317341  0.47682659]

Distance of centers: 0.0192030419474
Distance of variances: 0.0473781660305
Distance of priors: 0.00150350251231
Distance of centers: 0.0212764995336
Distance of variances: 0.0431780185607
Distance of priors: 0.00150350251231
Maximum distance: 0.0473781660305

New centers: [[ 1.67119465  1.67730196]
 [ 1.71304903  1.71850737]]
New variances: [ 0.50462089  0.55228077]
New priors: [ 0.52493695  0.47506305]
==================================================

Step 3
--------------------------------------------------
Distances of X[0] to proposed centers: 0.941885882031 0.895414167829
Likelihoods of X[0]: [ 0.13094807  0.13945031]
Assignment probabilities of X[0]: [ 0.50922972  0.49077028]

Distance of centers: 0.034645355738
Distance of variances: 0.0156526663467
Distance of priors: 8.38670160043e-05
Distance of centers: 0.0383057699216
Distance of variances: 0.0146373996722
Distance of priors: 8.38670160042e-05
Maximum distance: 0.0383057699216

New centers: [[ 1.644676    1.65500708]
 [ 1.74236895  1.74315842]]
New variances: [ 0.48896822  0.56691817]
New priors: [ 0.52502081  0.47497919]
==================================================

Step 4
--------------------------------------------------
Distances of X[0] to proposed centers: 0.971410487325 0.86405440215
```

In [20]:
```
plot_data(X, which_gaussian_em, cluster_centers_em, cluster_stds_em)
plt.title('Predicted by Expectation-Maximization')
```

Out[20]: <matplotlib.text.Text at 0x7f1ea8125b38>

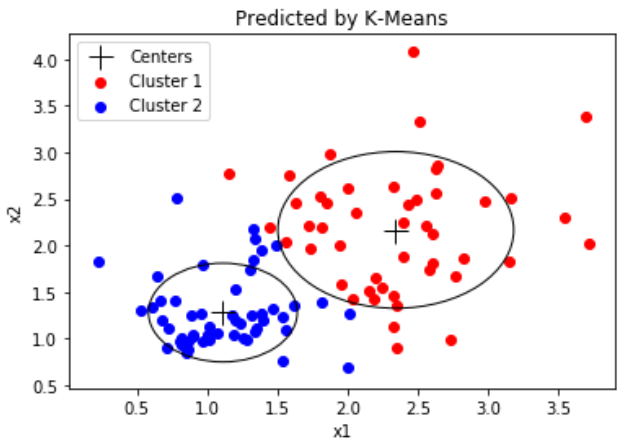


1.3 Run K-means algorithm

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

In [21]:
```
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[21]: <matplotlib.text.Text at 0x7f1ea182ddd8>



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.

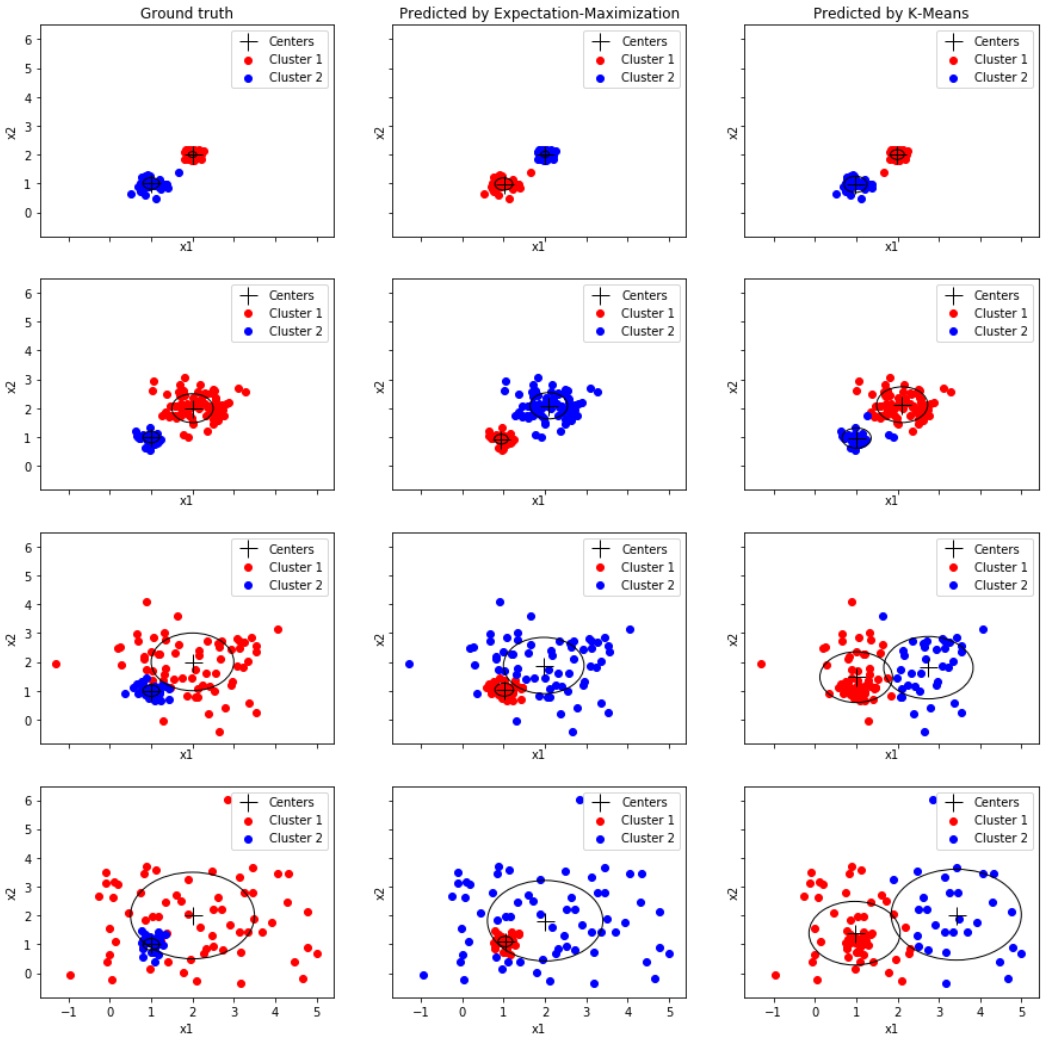
1.4 Initialize EM algorithm with cluster parameters from K-Means

In [22]:
```
_, _, _, 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 27 steps with random initalization
Took 18 steps with initialization from K-means
```

1.5 Repeat analysis for different σ_1 values

In [23]:
```
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 [ ]: