Gaussian Mixture Models (GMM)

A GMM is a probability density distribution composed of multiple Gaussians (components). An observation $\mathbf{x}$ is generated by the kth of K components according to some probability π_k. Hence the density of $\mathbf{x}$ is given by:

$$f_{\mathbf{X}|\Theta}(\mathbf{x}|\Theta) = \sum_{k=1}^{K} \pi_k g_k(\mathbf{x}|\theta_k)$$

where $g_k(\mathbf{x}|\theta_k)$ is a Gaussian distribution with parameters $\theta_k = (\mu, \mathbf{\Sigma})_k$, and all parameters are in $\Theta = ((\pi, \mu, \mathbf{\Sigma})_k : k \in \{1, K\})$.

Illustration

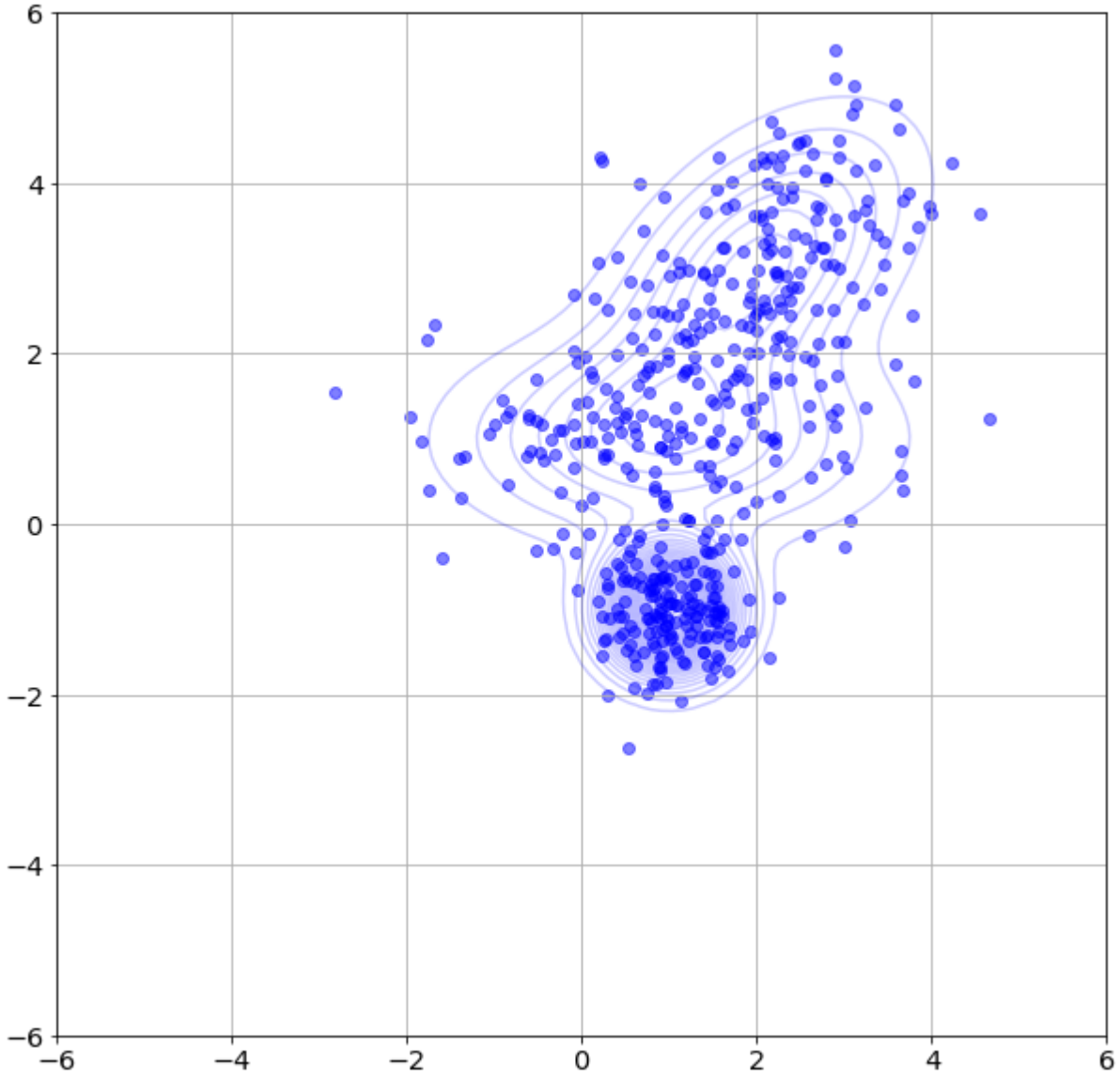
A recipe for generating a dataset:

- Observations $\mathbf{x} \in \mathbb{R}^2$.
- Most of the time we make an observation, it is generated by one multivariate Gaussian
- The rest of the time it is generated by another multivariate Gaussian
- Define π_1, π_2 in proportion to frequency
- Define parameters of each multivariate Gaussian
- Sample!

In [14]:

```
import numpy as np
N = 500
pi = [0.33,0.33,0.34]
K = len(pi)
param_muA1 = [2,3]; param_muA2 = [1,1]; param_muA3 = [1,-1];
param_CA1 = np.array([[1,0.5],[0.5,1]]); param_CA2 = np.array([[2,0],
[0,0.5]])
param_CA3 = np.array([[1,0],[0,1]])/5

from sklearn import mixture
import scipy

GMMA = mixture.GaussianMixture(K)
GMMA.fit(np.random.uniform(size=[N,2])) # this is just to instantiate the
object in R2
GMMA.weights_ = pi
GMMA.means_ = np.array([param_muA1, param_muA2,param_muA3])
GMMA.covariances_ = np.array([param_CA1, param_CA2,param_CA3])
ZA = GMMA.sample(N)
```

```
xx, yy = np.meshgrid(np.linspace(-6,6,100), np.linspace(-6,6,100))
points = np.stack((xx, yy), axis=-1)
pdfA1_true = scipy.stats.multivariate_normal.pdf(points, param_muA1,
param_CA1)
pdfA2_true = scipy.stats.multivariate_normal.pdf(points, param_muA2,
param_CA2)
pdfA3_true = scipy.stats.multivariate_normal.pdf(points, param_muA3,
param_CA3)

import matplotlib.pyplot as plt
# The following makes the plot look nice
params = {'legend.fontsize': 'x-large','figure.figsize': (10, 10),
         'axes.labelsize': 'x-large','axes.titlesize':'x-large',
         'xtick.labelsize':'x-large','ytick.labelsize':'x-large'}
plt.rcParams.update(params)

fig = plt.figure(); ax = fig.add_subplot(111)
ax.scatter(ZA[0][:,0],ZA[0][:,1],alpha=0.5,c='blue')
ax.contour(xx, yy,
GMMA.weights_[0]*pdfA1_true+GMMA.weights_[1]*pdfA2_true+GMMA.weights_[2]*pdfA

           levels=40, colors='blue', alpha=0.2)
plt.grid()
plt.show()
```



Illustration

Now we want to fit a GMM to a given dataset:

- Select number of components K.
- Run expectation maximization (EM) on the dataset.
- Results are not deterministic, so run several times with random initializations.
- Possibility of failure, e.g., K too large.

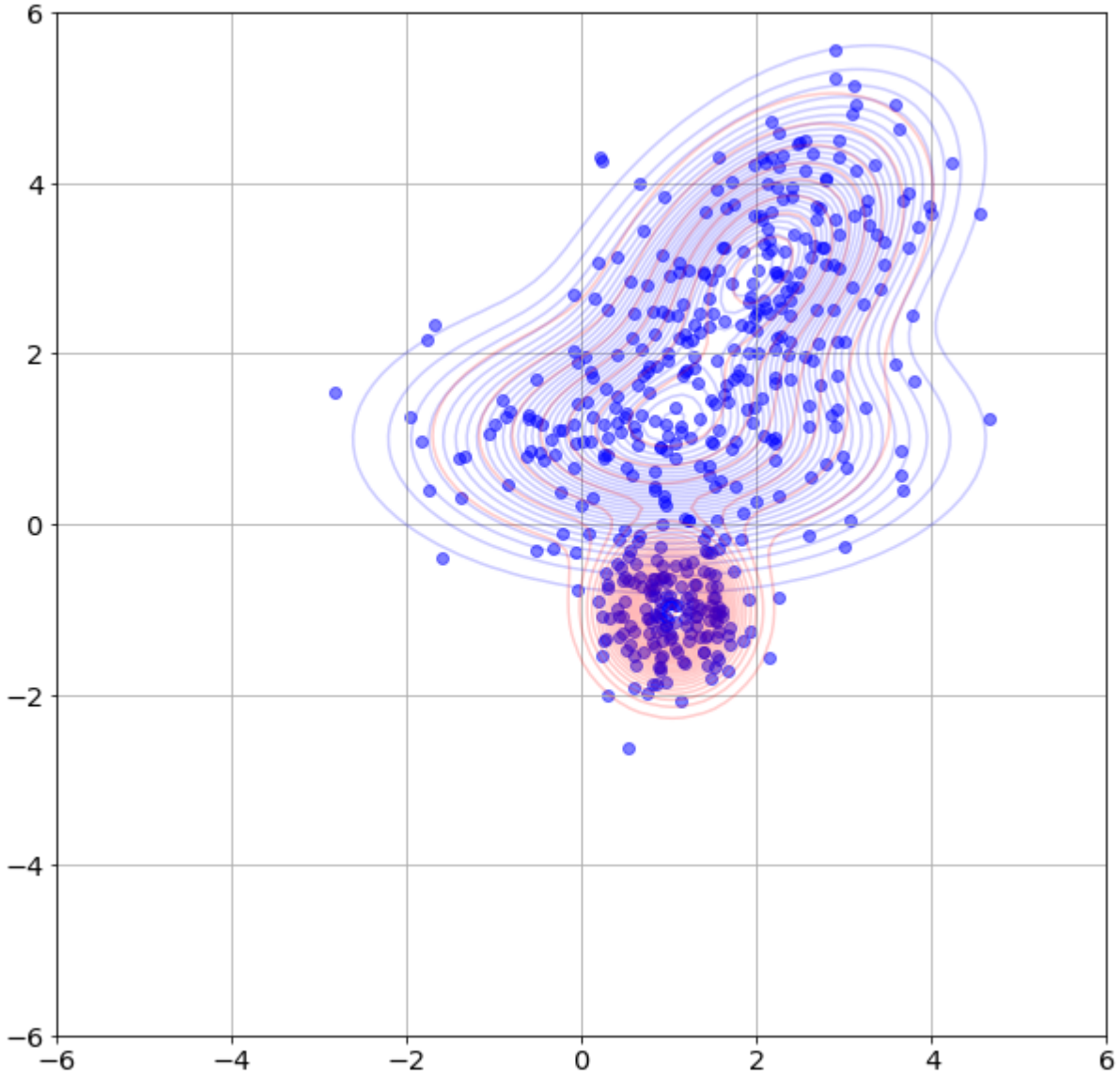
See sklearn.mixture

In [15]:

```
K = 3
GMMA_hat = mixture.GaussianMixture(K,covariance_type='full',verbose=1,

n_init=5,init_params='kmeans',warm_start=True)
GMMA_hat.fit(ZA[0])
print('Mixture weights:',GMMA_hat.weights_,'True:',pi)
```

```
fig = plt.figure(); ax = fig.add_subplot(111)
ax.scatter(ZA[0][:,0],ZA[0][:,1],alpha=0.5,c='blue')
xx, yy = np.meshgrid(np.linspace(-6,6,100), np.linspace(-6,6,100))
points = np.stack((xx, yy), axis=-1)
ax.contour(xx, yy, GMMA.weights_[0]*pdfA1_true+GMMA.weights_[1]*pdfA2_true,
           levels=40, colors='blue', alpha=0.2)
pdf_hat = []

for kk in range(K):
    if len(GMMA_hat.covariances_.shape) == 2:
        pdf_hat.append(GMMA_hat.weights_[kk]*
                       scipy.stats.multivariate_normal.pdf(points,
GMMA_hat.means_[kk], GMMA_hat.covariances_[0]))
    else:
        pdf_hat.append(GMMA_hat.weights_[kk]*
                       scipy.stats.multivariate_normal.pdf(points,
GMMA_hat.means_[kk], GMMA_hat.covariances_[kk]))
sumpdf_hat = np.array(pdf_hat).sum(axis=0)
ax.contour(xx, yy, sumpdf_hat,
           levels=40, colors='red', alpha=0.2)
plt.grid(); plt.show()
```

```
Initialization 0
Initialization converged: True
Initialization 1
Initialization converged: True
Initialization 2
Initialization converged: True
Initialization 3
  Iteration 10
Initialization converged: True
Initialization 4
Initialization converged: True
Mixture weights: [0.34740544 0.3402191  0.31237547] True: [0.33, 0.33, 0.34]
```



How do we judge model fit? How do we choose K?

A GMM allows us to compute a density for each point in the dataset.

We can compute the negative log likelihood of the training set given Θ.

$$L_{\mathcal{D}}(\Theta) = -\log P[\mathcal{D}|\Theta] = -\log \prod_{n=1}^{N} f_{\mathbf{X}|\mathbf{\Theta}}(\mathbf{x}_n|\Theta) \tag{1}$$

$$= -\sum_{n=1}^{N} \log f_{\mathbf{X}|\mathbf{\Theta}}(\mathbf{x}_n|\Theta) \tag{2}$$

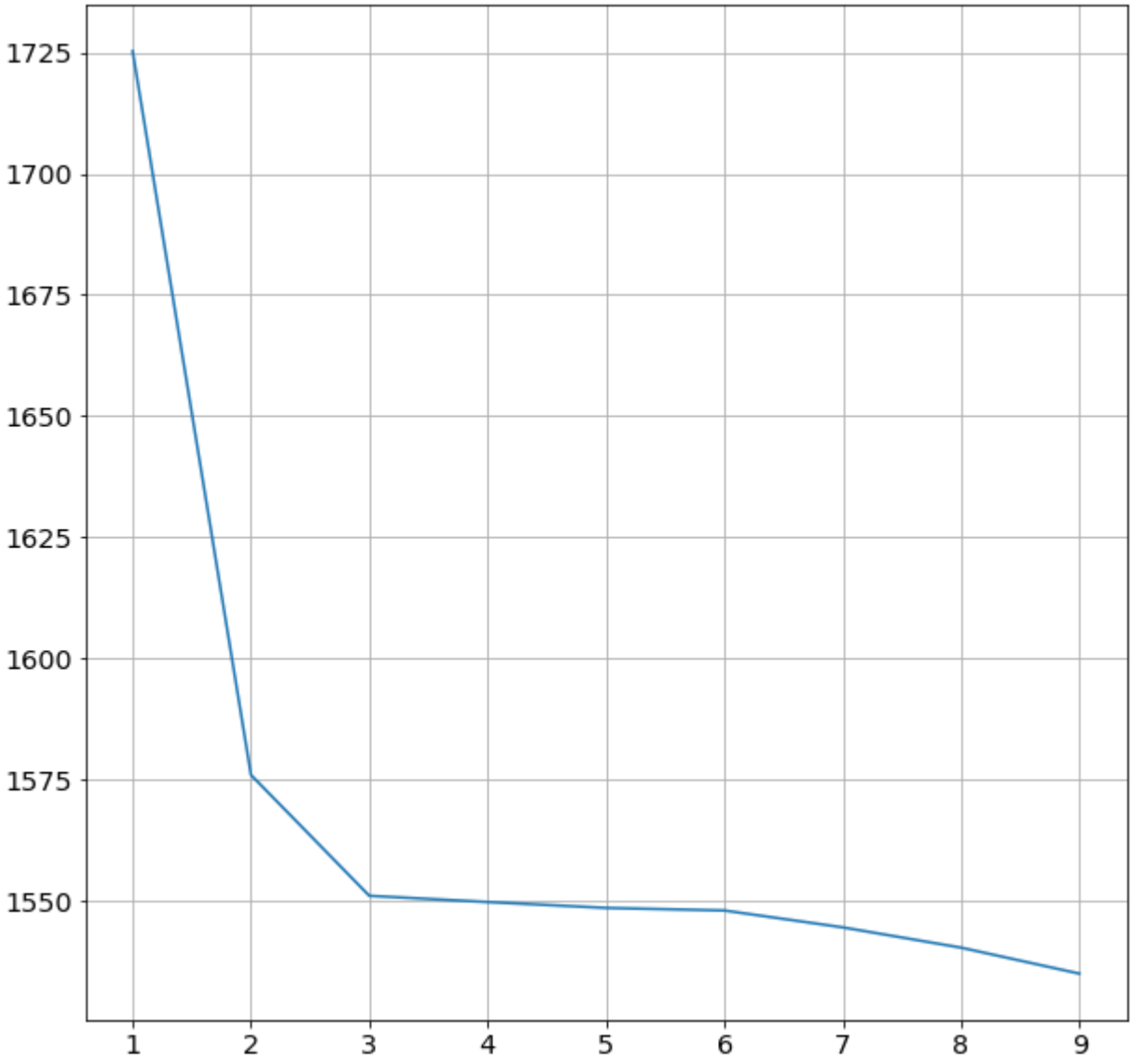
assuming all observations are iid.

If our model is quite far from our data, we expect this value to be large.

Thus, we can compute $L_{\mathcal{D}}(\Theta)$ for several K and select the order based on this.

In [16]:
```
llvals = []
```

```
KK = range(1,10)
for kk in KK:
    GMMA_hat = mixture.GaussianMixture(kk,covariance_type='full',verbose=0,

n_init=5,init_params='kmeans',warm_start=False)
    GMMA_hat.fit(ZA[0])
    llvals.append(-np.sum(GMMA_hat.score_samples(ZA[0])))

fig = plt.figure(); ax = fig.add_subplot(111)
plt.plot(KK,llvals,label='LL')
plt.grid(); plt.draw()
```



How do we judge model fit? How do we choose K?

Another measure is the Akaike information criterion (AIC), which considers the number of model parameters M:

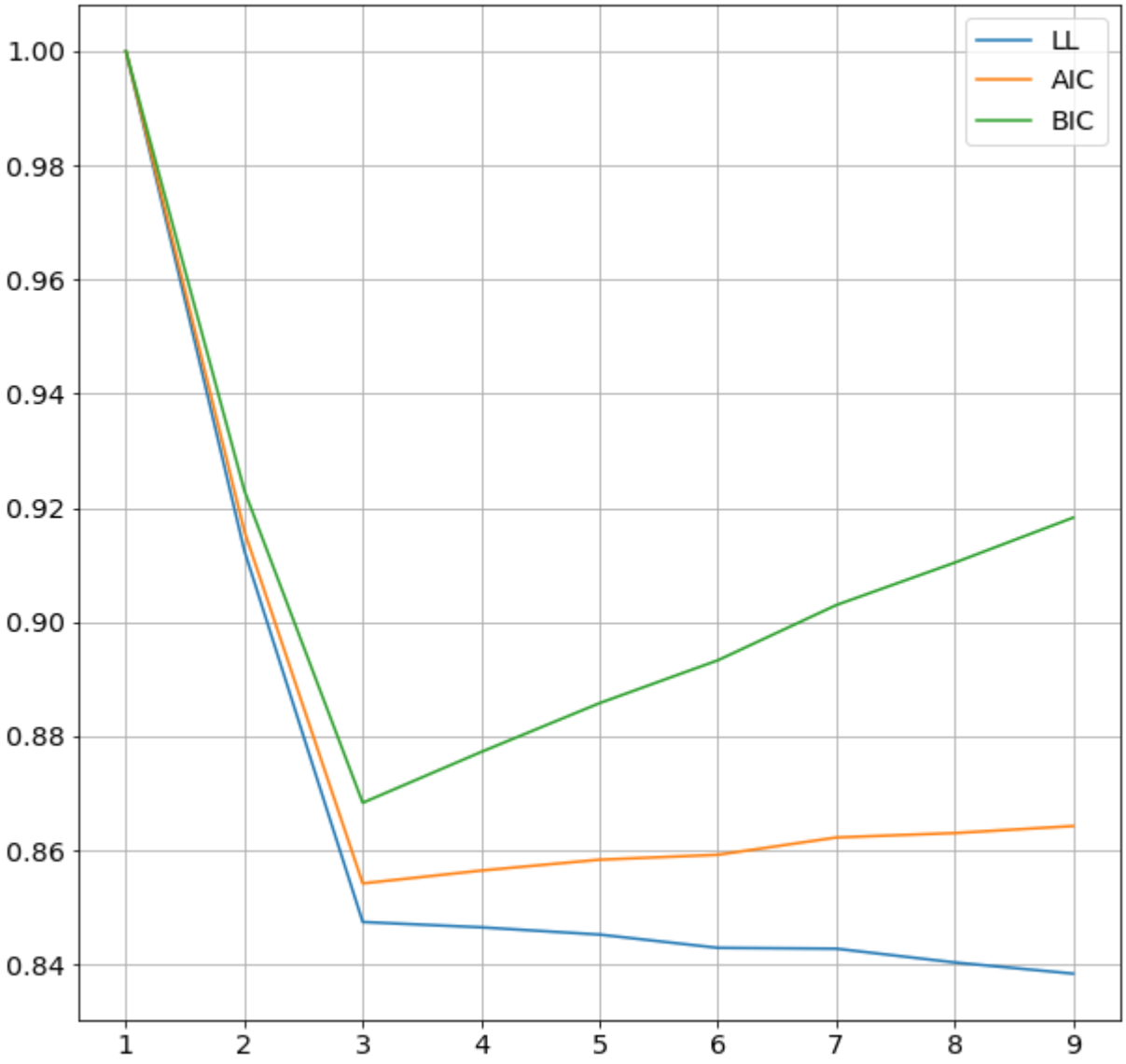
$$AIC(M) = 2M - 2\log\prod_{n=1}^{N} f_{\mathbf{X}|\Theta}(\mathbf{x}_n|\Theta)$$

Yet another measure is the Bayes information criterion (BIC), which also considers the number of observations N:

$$BIC(M) = M\log(N) - 2\log\prod_{n=1}^{N} f_{\mathbf{X}|\theta_i}(\mathbf{x}_n|\theta_i)$$

In [7]:

```
llvals = []
aic = []
bic = []
KK = range(1,10)
for kk in KK:
    GMMA_hat = mixture.GaussianMixture(kk,covariance_type='full',verbose=0,

n_init=5,init_params='kmeans',warm_start=False)
    GMMA_hat.fit(ZA[0])
    llvals.append(-np.sum(GMMA_hat.score_samples(ZA[0])))
    aic.append(GMMA_hat.aic(ZA[0]))
    bic.append(GMMA_hat.bic(ZA[0]))



fig = plt.figure(); ax = fig.add_subplot(111)
plt.plot(KK,llvals/np.max(llvals),label='LL')
plt.plot(KK,aic/np.max(aic),label='AIC')
plt.plot(KK,bic/np.max(bic),label='BIC')
plt.legend()
plt.grid(); plt.draw()
```


LL
AIC
BIC
1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
0.84
1
2
3
4
5
6
7
8
9