Cinnamon AI Bootcamp

Anomaly detection using Guassian Mixture Model

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Expectation

In one dimension, given an observation x_i from k^{th} cluster (parameterized by μ and σ). The probability of seeing x_i
$\mathcal{N}(x_i|\mu_k, \sigma_k^2) = \frac{1}{\sqrt{2\pi\sigma_k^2}} exp(-\frac{(x_i-\mu_k)^2}{2\sigma_k^2})$
for each $k = 1, 2, 3, 4, \dots K$

- Without observing the data, the probability of x_i is from the k^{th} cluster
  $p(z_i = k) = \phi_k$
  $(\text{the probability of a random point is drawn from } k^{th} \text{ distribution})$
  This can be interpreted as the "weight" for k-th guassian distribution in the mixture of models, also known as the prior.
- The probability of observing an x_i in the data is the weighted sum (corresponding with ϕ_k for each clusters) of all the K distribution function at the given point x
  $p(x_i) = \sum_{k=1}^{K} \mathcal{N}(x_i|\mu_k, \sigma_k^2)\phi_k$
- Therefore, given an observation x_i, the likelihood of x_i (posterior) belong to k^{th} cluster can be calculated:
  $b_{ik} = p(\mu_k, \sigma_k^2|x_i) = \frac{\mathcal{N}(x_i|\mu_k,\sigma_k^2)p(z_i=k)}{p(x_i)} = \frac{\mathcal{N}(x_i|\mu_k,\sigma_k^2)\phi_k}{\sum_{k=1}^{K}\mathcal{N}(x_i|\mu_k,\sigma_k^2)\phi_k} (\text{proven})$

For multivariate guassian model, the normal can be calculated:
$\mathcal{N}(x_i|\mu_k, \Sigma) = \frac{1}{(2\pi)^{d/2}}|\Sigma|^{-1/2} exp[-\frac{1}{2}(x_i - \mu_k)^T\Sigma^{-1}(x_i - \mu_k)]$

Whereas, Σ is a $d \times d$ covariance matrix that satifies:

- positive semi-definite
- symmetric along diagonal

Maximization

For each step, we update the parameters (in a multivariate style) as follow:
$m_k = \sum_i b_{ik}$
$(\text{sum of all likelihood allocated to cluster k})$

$\hat{\phi}_k = \frac{m_k}{m}$
$(\text{fraction of total likelihood})$

$\hat{\mu}_k = \frac{1}{m_k}\sum_i b_{ik}x_i$
$(\text{Weighted mean of assigned data})$

$\hat{\Sigma}_k = \frac{1}{m_k}\sum_i b_{ik}(x_i - \hat{\mu}_k)^T(x_i - \hat{\mu}_k)$
$(\text{Weighted covariance of assigned data})$

Each step **strictly** (theoretically) increases the log-likelihood of our model
$logp(X) = \sum_i log\left[\sum_c \pi_c \mathcal{N}(x_i; \mu_c, \Sigma_c)\right]$

Anomaly detection

For anomaly detection, we can then first calculate the probability of x_i to be drawn from our mixture of Gaussian (with trained params):
$p(x_i) = \sum_{k=1}^{K} \mathcal{N}(x_i|\mu_k, \sigma_k^2)\phi_k$
If $p(x_i) < \lambda$ (which is the threshold we specify in advance) then we will consider x_i to be abnormal

To perform anomaly detection, we can consider the anomaly detection as a classification problem, then we can use classification techniques and metrics to work with it. This time, we want to choose threshold that maximizes the Fscore of the classification task:
$\lambda = \underset{\lambda}{argmax}(Fscore)$

My heuristics of finding a reasonable threshold goes like this:

```
# Init bestFScore and bestThresh to be 0
bestFScore ← 0
bestThresh ← 0

for every thresh in range from 0 to 1

    # Get prediction of model based with thresh
    y_predict ← model.predict(X,thresh)

    # calculate f score based on true score
    currentFScore ← calcFScore(y_true,y_predict)

    if FScore > bestFScore
        bestFSCore ← currentFScore
        bestThresh ← thresh
```

The precision of this method will mostly based on how small we quantize this threshold range - the step of every thresh iteration.

References

[1] Machine Learning TV - Guassian Mixture Model for Clustering

[2] Geeksforgeeks - Guassian Mixture Model

[3] Alexander Ihler - Gaussian Mixture Models and EM

[4] Siraj Raval - Gaussian Mixture Models

[5] https://stats.stackexchange.com/questions/91045/can-a-multivariate-distribution-with-a-singular-covariance-matrix-have-a-density

[6] https://math.stackexchange.com/questions/503476/multivariate-gaussian-density-from-singular-covariance

Implementation

Import libraries

```
import numpy as np
from scipy.stats import multivariate_normal
%matplotlib notebook
import matplotlib.pyplot as plt
import matplotlib.animation as animation
from sklearn.metrics import f1_score
from sklearn.model_selection import train_test_split
import time
```

```
class GaussianMixtureModel:

    # Notation
    # dim: dimension of the data
    # cov: covariance matrix
    # n_clusters: number of clusters
    # N: normal distribution
    # m: number of data points
    # k: k-th cluster
    # i: i-th sample

    def __init__(self,n_clusters=5):

        # Number of clusters that the model converge into
        self.n_clusters = n_clusters

        # Vectorization of different guassian distribution
        # Each line is a distribution parameterized by mu and sigma
        self.gaussians = {}

        # init mu, shape = (K x dim)
        self.gaussians['mu'] = None

        # init cov matrix, shape = (K x dim x dim)
        self.gaussians['cov'] = None

        # init prior (sum to 1), shape = (1,K)
        self.gaussians['prior'] = None

        # dimension of data
        self.dim = None

        # matrix of likelihood of data point to each cluster, shape (m,K)
        self.likelihood = None

        # matrix of normal prob of each data point, shape (m,K)
        self.normal_matrix = None

        # abnormal threshold
        self.abnormal_threshold = None

        # save history
        self.history = {}
        self.history['log_likelihood'] = []
```

```
    def createCov(self):
        # Create a random covaraince matrix that positive definite

        while True:
            A = np.random.normal(size=(self.dim,1))
            B= A*A.T
            # Make sure the matrix is invertible and positive definite
            if np.isfinite(np.linalg.cond(B)) and np.linalg.det(B)>0:
                break
            else:
                continue
        return B


    def normal(self,X,k):
        # Given the list of observation X is from a cluster, what's the
likelihood of seeing X.
        # Return shape: (m,1)
        # Get dimension of data
        dim = X.shape[1]

        # retrieve mu and covariance matrix from cluster k
        mu_k = self.gaussians['mu'][k]
        cov_k = self.gaussians['cov'][k]

        var = multivariate_normal(mean=mu_k, cov=cov_k,allow_singular=True)
        result = np.expand_dims(var.pdf(X),1)
        return  result




    def proba(self,X):
        # The probability of observing x_i in the data.
        # Return shape: (m,1)

        # Get number of data
        m = X.shape[0]

        # Retrieve prior
        prior = self.gaussians['prior']

        # Get dimension of data
        dim = X.shape[1]

        # initialize array of size (m,k), each line represents normal(x_i,k) for
each cluster k
        normal_matrix = np.empty((m,0))

        # for each cluster, append the N result to the right of the matrix
        for k in range(self.n_clusters):
            normal_k = self.normal(X,k)
            normal_matrix = np.hstack((normal_matrix,normal_k))
        self.normal_matrix = normal_matrix

        # times with prior for each cluster then sum for each line
```

```
        proba = np.sum(normal_matrix*prior,axis=1)
        return np.expand_dims(proba,1)

    def step(self,X):

        # Get number of data
        m = X.shape[0]

        # Get dimension of data
        dim = X.shape[1]

        p = self.proba(X)
        # Matrix of likelihood. Shape of (m,k)
        likelihood = np.empty((m,0))

        # EXPECTATION
        for k in range(self.n_clusters):
            # retrieve mu, prior and covariance matrix
            mu_k = self.gaussians['mu'][k]
            cov_k = self.gaussians['cov'][k]
            prior_k = self.gaussians['prior'][0][k]


            # compute normal N(x|mu,Sigma)

            N_k = self.normal(X,k)
            # compute likehood at k-th
            lh_k = N_k*prior_k/p
            # likelihood, append to the right
            likelihood = np.hstack((likelihood,lh_k))


        self.likelihood = likelihood

        # MAXIMIZATION

        # Sum of all likelihood allocated to cluster k. Shape (1,k)
        m_k = np.sum(likelihood,axis=0)
        # Update prior and expand dim to (1,K)
        self.gaussians['prior'] = np.expand_dims(m_k/m,axis=0)

        # Update mean
        for k in range(self.n_clusters):
            # likelihood at k-th. shape (m,1)
            lh_k = np.expand_dims(likelihood[:,k],1)
            self.gaussians['mu'][k] = 1/m_k[k]*np.sum(X*lh_k,axis=0)

        # Update cov
        for k in range(self.n_clusters):

            # retrieve mu_k
            mu_k = self.gaussians['mu'][k]
            cov = np.zeros((dim,dim))

            for i in range(m):

                diff = np.expand_dims((X[i]-mu_k),0)
                cov += likelihood[i][k]*(diff.T.dot(diff))/m_k[k]
```

```
            cov_k=cov


            self.gaussians['cov'][k] = cov_k



    def log_likelihood(self,X):

        m = X.shape[0]

        # Retrieve prior
        prior = self.gaussians['prior']

        normal_matrix = np.empty((m,0))

        # for each cluster, append the N result to the right of the matrix
        for k in range(self.n_clusters):
            normal_k = self.normal(X,k)
            normal_matrix = np.hstack((normal_matrix,normal_k))

        return np.log((normal_matrix*prior).sum(axis=1)).sum()

    def fit(self,X, max_iters=15):

        m = X.shape[0]

        # Get dim of data
        self.dim = X.shape[1]

        # init mu, shape = (K x dim)
        mulist=[]
        for k in range(self.n_clusters):
            random_mu = X[np.random.randint(low=0,high=len(X))]
            mulist.append(random_mu)
        self.gaussians['mu'] = np.array(mulist)

        # init covariance matrixes based on different sample of data, shape = (K
x dim x dim)
        # Make sure every k-th covariance has det > 0
        self.gaussians['cov'] = np.array([self.createCov() for i in
range(self.n_clusters)])


        # init prior (sum to 1), shape = (1,K)

 self.gaussians['prior']=np.random.dirichlet(np.ones(self.n_clusters),size=1)


        for i in range(max_iters):
            print("step ",i,end=' ')
            # EM
            self.step(X)

            # calculate log likelihood
            log_lh = self.log_likelihood(X)
```

```
            self.history['log_likelihood'].append(log_lh)
            print("log likelihood: ",log_lh)

    def fit_anomaly(self,X,y):

        # Get the probabilities of X, shape (m,1)
        proba = self.proba(X)

        best_thresh = 0
        best_f1_score = 0
        for thresh in np.arange(0.0, 1.0, 0.01):
            y_pred = (proba < thresh)*1
            current_f1_score = f1_score(y,y_pred)
            if current_f1_score > best_f1_score:
                best_thresh = thresh
                best_f1_score = current_f1_score
        self.abnormal_thresh = best_thresh

    def predict_anomaly(self,X):
        return ((self.proba(X) < self.abnormal_thresh)*1)[:,0]

    def predict(self,X):
        return self.likelihood.argmax(axis=1)
```

Load data

```
from scipy.io import loadmat
data = loadmat('cardio.mat')
X = data['X']
Y = data['y'][:,0]
X_pos = X[Y==1]
X_neg = X[Y==0]
```

Fit the model

```
# If get an error..please kindly run again, it works like magic
max_iters = 25
model = GaussianMixtureModel(n_clusters=3)
model.fit(X_neg,max_iters=max_iters)
```

```
step  0 log likelihood:  -29648.09566980788
step  1 log likelihood:  -27017.829010462443
step  2 log likelihood:  -20763.011394036635
step  3 log likelihood:  -20411.81808227092
step  4 log likelihood:  -16254.972129542499
step  5 log likelihood:  -18808.83768816995
step  6 log likelihood:  -18222.167533118132
step  7 log likelihood:  -19019.31283192718
step  8 log likelihood:  -16693.097569541373
step  9 log likelihood:  -15754.080540565357
step  10 log likelihood:  -17165.63427113998
step  11 log likelihood:  -18144.603903942956
```

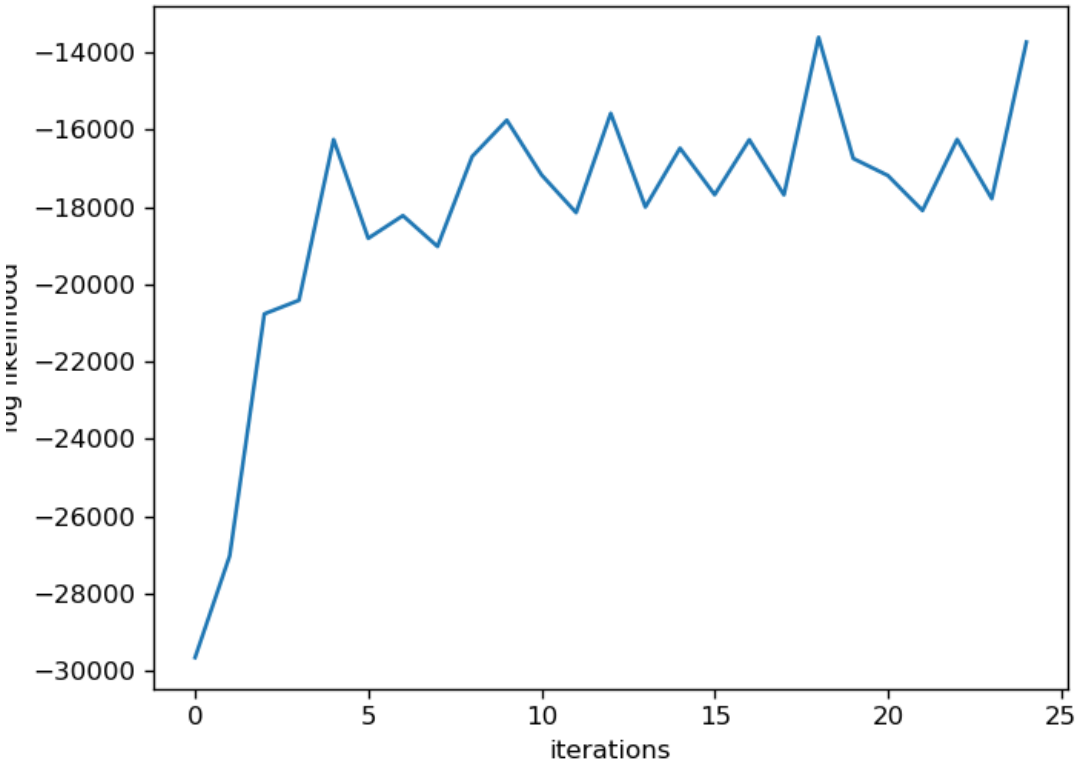
```
step  12 log likelihood:  -15576.866400905454
step  13 log likelihood:  -17999.78642934142
step  14 log likelihood:  -16478.429327816782
step  15 log likelihood:  -17680.948988829023
step  16 log likelihood:  -16259.88385697005
step  17 log likelihood:  -17685.400630068107
step  18 log likelihood:  -13612.120217283362
step  19 log likelihood:  -16744.341883208228
step  20 log likelihood:  -17184.802608799924
step  21 log likelihood:  -18089.517709427233
step  22 log likelihood:  -16251.41448306101
step  23 log likelihood:  -17784.196754483743
step  24 log likelihood:  -13736.053543139955
```

```
model.predict(X_neg)
```

```
array([2, 2, 2, ..., 1, 1, 1])
```

```
import matplotlib.pyplot as plt
plt.plot(range(0,max_iters),model.history['log_likelihood'])
plt.xlabel("iterations")
plt.ylabel("log likelihood")
```

```
<IPython.core.display.Javascript object>
```




```
Text(0, 0.5, 'log likelihood')
```

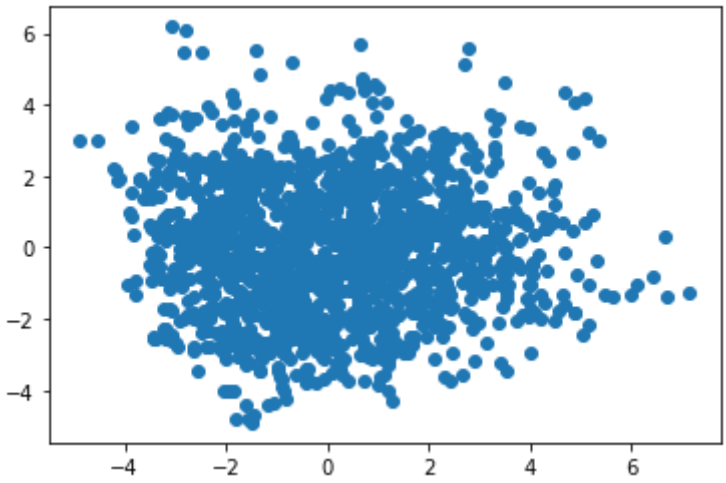
Theoretically speaking, the log likelihood should strictly increase every EM steps. But this fluctuates a lot. Proof for covariance exploding while compute GMM: https://stackoverflow.com/questions/41216856/gmm-loglikelihood-isnt-monotonic

Test on 2D Data

```
from sklearn.decomposition import PCA
# We use PCA to chop down component for visualization
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_neg)
```

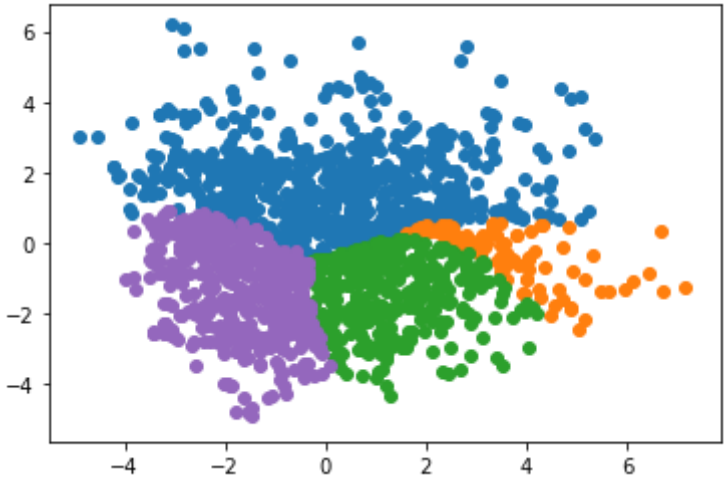
```
%matplotlib inline
plt.scatter(X_pca[:,0],X_pca[:,1])
```

```
<matplotlib.collections.PathCollection at 0x7fa6964a8a90>
```



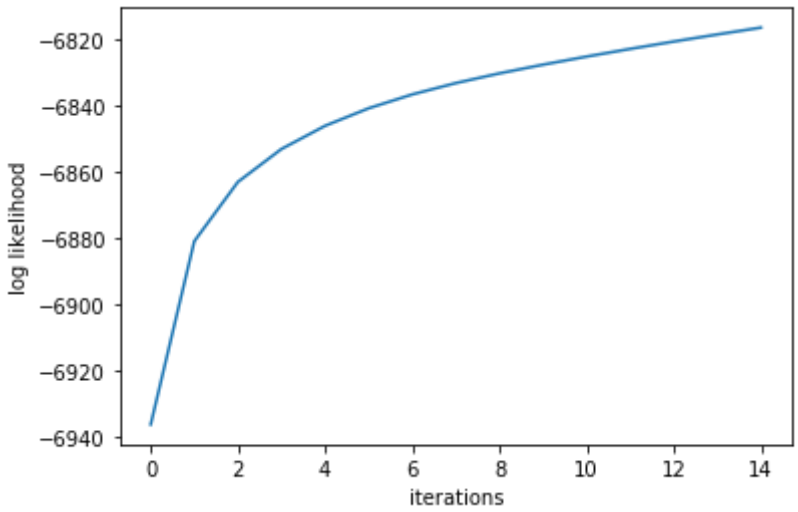

```
# color
n_clusters=5
GMM = GaussianMixtureModel(n_clusters=n_clusters)
GMM.fit(X_pca)
pred = GMM.predict(X_pca)
for i in range(n_clusters):
    plt.scatter(X_pca[pred==i][:,0],X_pca[pred==i][:,1])
```

```
step   0 log likelihood:  -6936.498042841801
step   1 log likelihood:  -6881.033094855808
step   2 log likelihood:  -6863.089359218
step   3 log likelihood:  -6853.1139641404225
step   4 log likelihood:  -6846.103005940182
step   5 log likelihood:  -6840.786948358567
step   6 log likelihood:  -6836.593528419803
step   7 log likelihood:  -6833.16042820256
step   8 log likelihood:  -6830.221247496595
step   9 log likelihood:  -6827.586635106269
step   10 log likelihood:  -6825.138137541355
step   11 log likelihood:  -6822.813001653121
step   12 log likelihood:  -6820.5832604964835
step   13 log likelihood:  -6818.437720031083
step   14 log likelihood:  -6816.3710552946595
```



```
import matplotlib.pyplot as plt
plt.plot(range(0,max_iters),GMM.history['log_likelihood'])
plt.xlabel("iterations")
plt.ylabel("log likelihood")
```

```
Text(0, 0.5, 'log likelihood')
```



This time, with low dimensional data, we can see the smooth curve without fluctuation.

Another 2D data

```
# We generate a dummy data
test_data = np.vstack([np.random.multivariate_normal([0,0],np.identity(2), size=
(500,)),
                       np.random.multivariate_normal([-1,3],np.array([[2, 1],
                                                                      [1, 1]]),
size=(500,))])
```

See how the algo converge..with animation

- **See "EM-coverge.gif"**

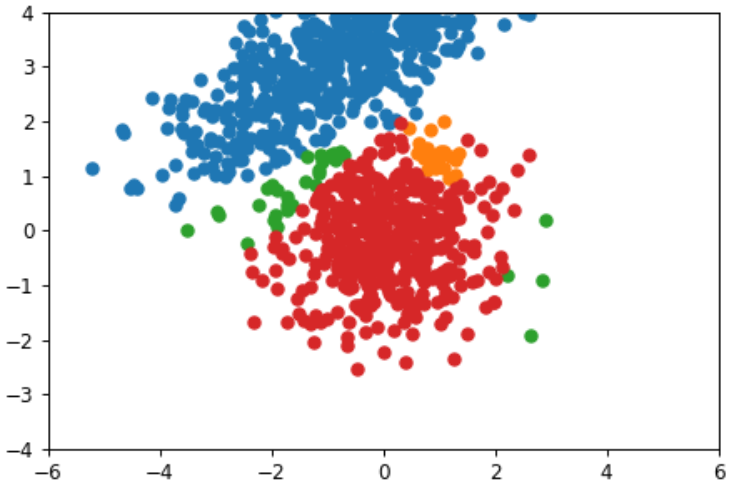
Animation

```
n_clusters=4
GMM = GaussianMixtureModel(n_clusters=n_clusters)
GMM.fit(test_data,max_iters=1)

pred = GMM.predict(test_data)
def update(curr):
    if curr==0:
        time.sleep(1)
```

```
    # check if animation is at the last frame, and if so, stop the animation a
    plt.cla()
    plt.axis([-6,6,-4,4])
    GMM.step(test_data)
    pred = GMM.predict(test_data)
    if curr == 50:
        a.event_source.stop()
    for i in range(n_clusters):
        plt.scatter(test_data[pred==i][:,0],test_data[pred==i][:,1])


fig = plt.figure()
a = animation.FuncAnimation(fig, update, interval=300)
```

```
step  0 log likelihood:  -3597.0089883804017
```

```
<IPython.core.display.Javascript object>
```



Anomaly Detection

```
from scipy.io import loadmat
data = loadmat('cardio.mat')
X = data['X']
y = data['y'][:,0]
X_neg = X[y==0]

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
random_state=42)
X_train_pos = X_train[y_train==1]
X_train_neg = X_train[y_train==0]
```

```
max_iters = 15
n_clusters = 50
model = GaussianMixtureModel(n_clusters=n_clusters)
model.fit(X_neg,max_iters=max_iters)
model.fit_anomaly(X_train,y_train)
y_pred = model.predict_anomaly(X_test)
print("f_score",f1_score(y_test,y_pred))
```

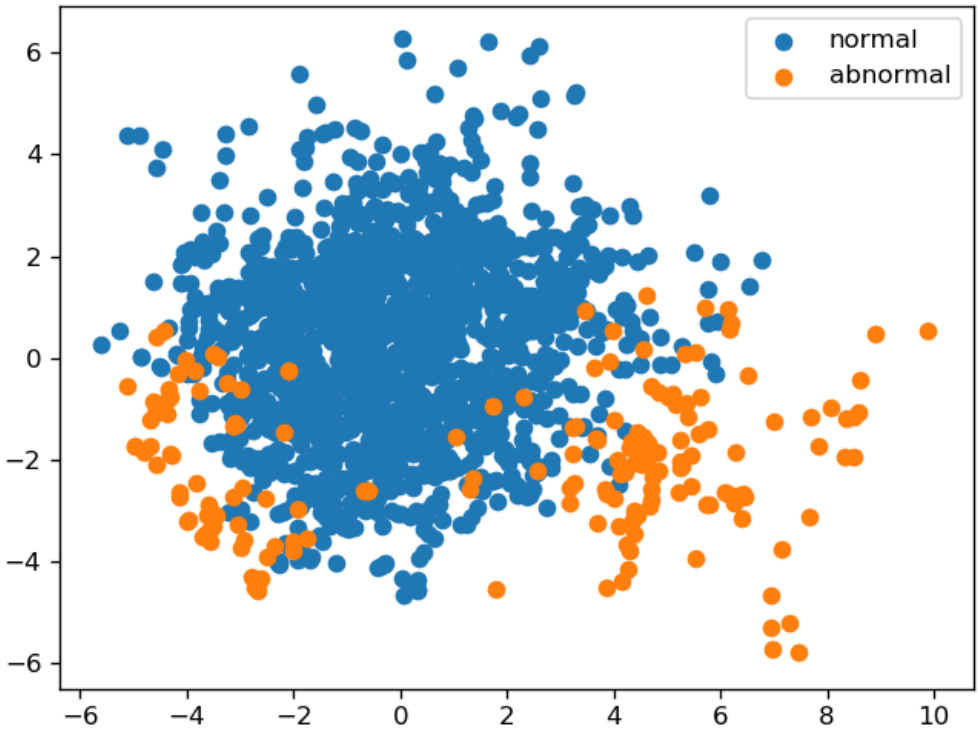
```
step  0 log likelihood:  -29868.031893025778
step  1 log likelihood:  -25992.91774279897
step  2 log likelihood:  -12006.193659331431
step  3 log likelihood:  -11539.055401766866
step  4 log likelihood:  1868.388206985157
step  5 log likelihood:  -2675.832581853343
step  6 log likelihood:  -1883.259437267283
step  7 log likelihood:  -1321.4469390036493
step  8 log likelihood:  -1095.7346028413508
step  9 log likelihood:  1419.0057023779998
step  10 log likelihood:  390.158272769224
step  11 log likelihood:  2504.339117670591
step  12 log likelihood:  607.6431981096216
step  13 log likelihood:  -1108.3172664638541
step  14 log likelihood:  4360.656247917903
f_score 0.6073298429319371
```

Visualization

For the sake of visualization, we'll transfer our data to a lower dimensional space using PCA with n_components = 2 (2D)

```
from sklearn.decomposition import PCA
# We use PCA to chop down component for visualization
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X)
plt.figure()
plt.scatter(X_pca[y==0][:,0],X_pca[y==0][:,1])
plt.scatter(X_pca[y==1][:,0],X_pca[y==1][:,1])
plt.gca().legend(['normal','abnormal'])
```

```
<IPython.core.display.Javascript object>
```




```
<matplotlib.legend.Legend at 0x7f95ba308dd0>
```

Looks like a lot of abnormal points are very close to normal one, which makes this a hard problem

```
X_pca_train, X_pca_test, y_pca_train, y_pca_test = train_test_split(X_pca, y,
test_size=0.3, random_state=42)
X_pca_neg = X_pca[y==0]
max_iters = 20
n_clusters = 10
model = GaussianMixtureModel(n_clusters=n_clusters)
model.fit(X_pca_neg,max_iters=max_iters)
model.fit_anomaly(X_train,y_train)
print("f_score",f1_score(model.predict_anomaly(X_test),y_test))
```

```
step  0 log likelihood:  -6799.681463511612
step  1 log likelihood:  -6780.82062910768
step  2 log likelihood:  -6772.3958123271295
step  3 log likelihood:  -6767.136885233344
step  4 log likelihood:  -6763.18008116076
step  5 log likelihood:  -6759.795269089522
step  6 log likelihood:  -6756.624989256733
step  7 log likelihood:  -6753.475115096862
step  8 log likelihood:  -6750.240268912708
step  9 log likelihood:  -6746.875841882809
```

```
step  10 log likelihood:  -6743.387674776432
step  11 log likelihood:  -6739.827672285434
step  12 log likelihood:  -6736.287476629035
step  13 log likelihood:  -6732.882884812425
step  14 log likelihood:  -6729.727817547063
step  15 log likelihood:  -6726.906743456097
step  16 log likelihood:  -6724.4586743077125
step  17 log likelihood:  -6722.378712136084
step  18 log likelihood:  -6720.631871325933
step  19 log likelihood:  -6719.169276134922
f_score 0.5471698113207547
```

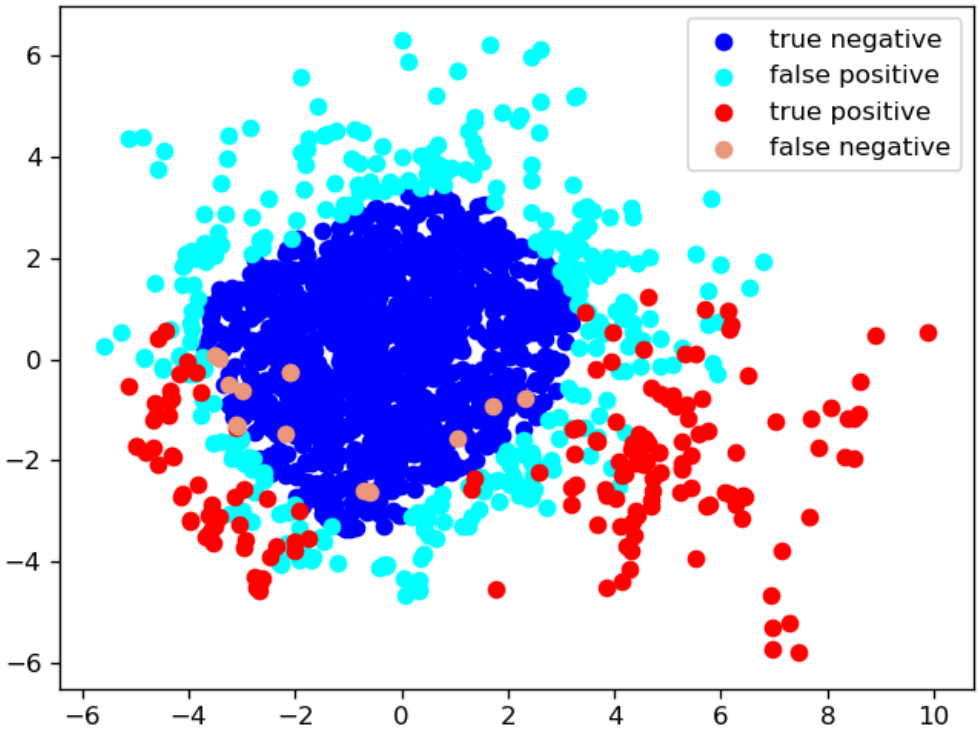
```
/home/phat-ngu/.conda/envs/tf2/lib/python3.7/site-
packages/sklearn/metrics/classification.py:1437: UndefinedMetricWarning: F-score
is ill-defined and being set to 0.0 due to no predicted samples.
  'precision', 'predicted', average, warn_for)
```

```
y_pred = model.predict_anomaly(X_pca)
X_true_pos = X_pca[np.logical_and((y_pred==1),(y==1))]
X_true_neg =  X_pca[np.logical_and((y_pred==0),(y==0))]
X_false_pos =  X_pca[np.logical_and((y_pred==1),(y!=1))]
X_false_neg =   X_pca[np.logical_and((y_pred==0),(y!=0))]
```

Visualize the classification result

```
plt.figure()

plt.scatter(X_true_neg[:,0],X_true_neg[:,1],color="blue")
plt.scatter(X_false_pos[:,0],X_false_pos[:,1],color="cyan")
plt.scatter(X_true_pos[:,0],X_true_pos[:,1],color="red")
plt.scatter(X_false_neg[:,0],X_false_neg[:,1],color='darksalmon')
plt.gca().legend(['true negative','false positive','true positive','false
negative'])
```

```
<IPython.core.display.Javascript object>
```




```
<matplotlib.legend.Legend at 0x7f95ba28d950>
```