Expectation Maximization and Gaussian Mixture Model

Lecture 12

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Multi Dimensional Probabilistic Distribution









 $\Pr(x) = \int_{-\infty}^{x} p(x) dx, \quad PDF = p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)_3$

With C++ or Python, How to Generate Gaussian Distribution?

- Rand() returns integer from 0 to RAND_MAX(32767)
 Rand() is NOT Gaussian(Normal) distribution
- Remind the video



```
r \sim N(0,1)
*Marsaglia polar method
double u,v,r;
while(1)
{
    u=2*rand()/((double)RAND MAX)-1;
    v=2*rand()/((double)RAND MAX)-1;
    r=u*u+v*v:
    if (r=0 || r>1)
                         continue:
    break;
}
    = sqrt(-2*loq(r)/r);
r
r
    = u*r;
```

N(0,1) returns Gaussian Distribution



1000 samples

randn(1,1000) generates 1000 samples

Question:

How we generate x with mean and standard deviation?

 $x \sim N(0,1)$ $x' \sim N(\mu, \sigma^2)?$

Gaussian Generation $x' \sim N(\mu, \sigma^2)$

• Mean value: μ is a offset from 0

$$x \sim N(0,1) \implies x' \sim N(0,1) + \mu = N(\mu,1)$$

Standard deviation

$$x \sim N(0,1) \quad \Longrightarrow \quad x' \sim \sigma N(0,1) = N(0,\sigma^2)$$



$$z \sim N(0,1) \qquad z = \frac{x - \mu}{\sigma} \sim N(0,1)$$
$$x \sim \sigma N(0,1) + \mu = N(\mu, \sigma^2)$$

- We learn it at high school, TT.
- Z is called "Normal Distribution" $PDF(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}z^2\right)$
- X is normalized with mean and standard deviation $p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$

Probability in 2D Space

• How to generate 2D Gaussian Distribution?

- Easy. A= randn(1000,2) and plot(A(:,1),A(:,2),'.')



1 DIM
$$Z_1 \sim N(0,1)$$

2 DIM $Z_2 = \begin{pmatrix} x \\ y \end{pmatrix} \sim N\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \sigma^2 \end{pmatrix}$

$$\mu = \begin{pmatrix} x_{mean} \\ y_{mean} \end{pmatrix} \qquad \sigma = ?$$



-10 [⊾] -10

-5

0

5

10

Quiz 1

$$z' = \begin{pmatrix} 2 & \sqrt{3} \\ \sqrt{3} & 1.5 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \qquad \text{Ho}$$

How it will distribute?

Hint :
$$Det \begin{pmatrix} 2 & \sqrt{3} \\ \sqrt{3} & 1.5 \end{pmatrix} = 3 - 3 = 0$$



Quiz 2 Why PDF is Over One?

• What is PDF?

$$\Pr(x) = \int_{-\infty}^{x} p(x) dx, \text{ PDF} = p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

• PDF is not a Probability. p(0) may be over 1.

$$p(x) = p(0)\Big|_{\substack{\sigma=0.1\\\mu=0}} = \frac{1}{0.1\sqrt{2\pi}} \exp\left(-\frac{1}{2}(0)^2\right) \approx 3.99$$

 Gaussian function is NOT a Probabilistic function But is a Probabilistic Density Function

Cumulative Distribution Function(CDF) is the integration of PDF

• Think Probability Exactly

PDF=
$$g(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

$$CDF = \int_{-\infty}^{\infty} g(x)dx = \Pr(x) = \operatorname{Prob}(x)$$



$$\therefore \int_{-\infty}^{\infty} g(x) dx = 1$$

- d(CDF)/dx = PDF
- p(x) in PDF is NOT a probability

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Probabilistic Density Function in n-dim. Space

• 1Dim

$$\Pr(x) = \int_{-\infty}^{x} g(x) dx, \text{ PDF} = g(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^{2}\right) x \sim N(\mu, \sigma^{2})$$

N-Dim

 $\Sigma =$

$$g(\hat{x}) = \left((2\pi)^N Det(\Sigma) \right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \left(x - \mu \right)^T \Sigma^{-1} \left(x - \mu \right) \right) \quad \hat{x} \sim N(\hat{\mu}, \Sigma)$$

• Look, Sigma matrix

0.5

$$\Sigma = \begin{pmatrix} 2 & 0 \\ 0 & 1.5 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \dots & 0.5 \\ 0.5 & \dots \end{pmatrix} \qquad \begin{array}{c} \text{Important for} \\ \text{Map} \\ \text{matching} \end{array}$$

Scale factor for principal axis

Rotation

Two types of Probability

- A Priori Probability
 - When you use probability, you use a prior probability

Pr(A) = 0.6

- Posterior Probability (Conditional probability)
 - Bayesian probability
 - Prob. Of A on condition that B occurs,

Pr(A | B) = 0.6

• A prior and Posterior probability are very different.

Conditional Probability

- What is Pr(A|B)?
 - Probability of A under the Probability of B
 - Or Probability of A within the given B





Posterior Prob.

- When events A and B occur,
- P(A): Probability of A occurrence
- P(B): Probability of B occurrence.
- P(A^B): Probability of Both A and B occurrence
- Definition:

$$\therefore \mathbf{P}(A \mid B) = \frac{P(\mathbf{A}^{\wedge} \mathbf{B})}{P(B)}$$

 $P(A | B)P(B) = P(A^B) = P(B | A)P(A)$ $\therefore P(A | B) = \frac{P(B | A)P(A)}{P(B)}$

Engineering Notation

$$P(w \mid x) = \frac{P(x \mid w)P(w)}{P(x)}$$

$$Posterior = \frac{likelihood \times prior}{Evidence}$$

In engineering, likelihood is one of the popular solution.

Prob. Of Event X between w1 and w2



Prior Prob. : $p(w_1), p(w_2)$ p(x) = ? p(x) = + $= p(x, w_1) + p(x, w_2)$ $= p(x | w_1) p(w_1) + p(x | w_2) p(w_2)$

- p(x)= Probability of event x's occurrence
- Posterior probability must be required for Classification

$$p(w_1 \mid x) = \frac{p(x \mid w_1) p(w_1)}{p(x)} = \frac{p(x \mid w_1) p(w_1)}{\sum_i p(x_i \mid w_i) p(w_i)}$$



2 Concept of Clustering



What is a Clustering?

- Grouping similar objects and labeling a Group
 - Labeling a Class
- Grouping a set of Objects which are more similar to each other than to those in other groups





Clustering Method Important Tools for Intelligent Robotics

• Pattern recognition requires Class definition



2 classes

• How many classes here?



• There are only two lumps \rightarrow Two clusters.

Famous Clustering method

- 1. K-Means Clustering method
 - Geometry based method
 - Simple and low computational burdens.
 - Shortcoming: Initial guess determines the final result

- 2. Expectation Maximization method
 - Probabilistic method
 - Very popular for **fitting Mixture Distribution**
 - Back bone of Gaussian Mixture Model (GMM)



K-Means Clustering

- Find Mean value (Centroid) for each cluster
- Algorithm
- 1. Assume there are K clusters.
- 2. Guess each centroid of cluster.
- 3. Find k points to closest centroid
- 4. Recompute the centroid of each cluster.



ex/ml/l12kmean.py



def gendata(): a=randn(100,2)*10 a[:,1] = a[:,1] + 50 a[:,2] = a[:,2] + 50 b=randn(50,2)*5 b[:,1] = b[:,1] +70 b[:,2] = b[:,2] +60 Blue ~ $N(\mu,\sigma^2) = N([50,50], \begin{bmatrix} 10^2 & 0\\ 0 & 10^2 \end{bmatrix})$ Red ~ $N(\mu,\sigma^2) = N([70,60], \begin{bmatrix} 5^2 & 0\\ 0 & 5^2 \end{bmatrix})$

- Two groups with Blue and Red
- It looks easy to find two groups

Real Problem is to find Two Groups



- It is NOT easy.
- By iteration, we find two groups from initial guesses.

112 kmean.test($\mu_{1x}, \mu_{1y}, \mu_{2x}, \mu_{2y}$, *iteration*)



 \sim

I2kmean.test with Different Guesses



• The Results are strongly affected by Initial Guesses

Centroid of Cluster What is it?

- In k means cluster,
 - Centroid approaches mean value of the test distribution.
 - But, it is not on the Exact mean value.
 - Why?
- Think the role of K mean cluster.
 - K closest points are Not whole data. Just Sample.

 \rightarrow In each turn, K mean clustering method find the centroid of K closest points.

- If Initial centroid is biased, centroid is sometimes biased.

• If we guess wrong number of centroid, how it works?

Wrong Number of Groups



kmean.test3(50,50,70,70,60,30,20)

kmean.test3(40,80,70,30,50,50,20)

• Thus, what is the Answer? \rightarrow No answer in General.₂₉

3 Expectation Maximization



Robotics

Introduction to Expectation Maximization

- Let's think EM in a simple way.
- We have random variable, X
- Maybe, X has two groups.
- How we separate X with two groups, probabilistically?





EM has two Steps

- Clusters are represented by Probability Distribution
 - K-means Clustering is a set of data around centroids.
 - But, clusters in EM are the Probabilistic Distribution
- Assumption:
 - Data are the Mixture of Gaussian Distributions
 - Blue, Red, and Green points are mixed with Gaussian distribution



$$g(\hat{x}) = \left((2\pi)^d Det(\Sigma) \right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \left(x - \mu \right)^T \Sigma^{-1} \left(x - \mu \right) \right)$$
$$p(\hat{x}_{Blue} \mid C_{Blue}), p(\hat{x}_{Red} \mid C_{Red}), p(\hat{x}_{Green} \mid C_{Green})$$
$$\hat{x} = \left\{ \hat{x}_{Blue}, \hat{x}_{Red}, \hat{x}_{Green} \right\}$$



Repeat E-M

rearrange class

Expectation

Maximization

Probabilistic Density Function has mean and variance

- **0. Data is given** $\hat{x} = \{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4, \hat{x}_5, \hat{x}_6, \hat{x}_7, \hat{x}_8, \hat{x}_9\}$
- 1. Guess groups $\hat{x} = \{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4, \hat{x}_5, \hat{x}_6, \hat{x}_7, \hat{x}_8, \hat{x}_9\}$ Expectation
- 2. maximum PDF is wrong in some data

 $\hat{x} = \{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4, \hat{x}_5, \hat{x}_6, \hat{x}_7, \hat{x}_8, \hat{x}_9\}$

• 3. Find mean and variance for each group Maximization

$$\hat{\mu}_{1} = mean(\hat{x}_{1}, \hat{x}_{2}) \qquad s_{1} = std(\hat{x}_{1}, \hat{x}_{2}) \hat{\mu}_{2} = mean(\hat{x}_{3}, \hat{x}_{4}, \hat{x}_{5}, \hat{x}_{6}, \hat{x}_{7}) \qquad s_{2} = std(\hat{x}_{3}, \hat{x}_{4}, \hat{x}_{5}, \hat{x}_{6}, \hat{x}_{7}) \hat{\mu}_{3} = mean(\hat{x}_{8}, \hat{x}_{9}) \qquad s_{3} = std(\hat{x}_{8}, \hat{x}_{9})$$

Fix

 $\hat{x} = \{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4, \hat{x}_5, \hat{x}_6, \hat{x}_7, \hat{x}_8, \hat{x}_9\}$

Expectation and Maximization Step 1. Expectation

Density function, p(x|c) for each cluster, C

$$p(\hat{x} | C) = \left((2\pi)^d Det(\Sigma) \right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \left(x - \mu \right)^T \Sigma^{-1} \left(x - \mu \right) \right)$$

Density function, P(x) for clustering model, M = {C₀, C₁,...,C_k}
 W is the fraction of the Cluster C in the entire data

$$\hat{x} = \{\hat{x}_{1}, \hat{x}_{2}, \hat{x}_{3}, \hat{x}_{4}, \hat{x}_{5}, \hat{x}_{6}, \hat{x}_{7}, \hat{x}_{8}, \hat{x}_{9}\} \longrightarrow W_{Blue} = W_{Red} = W_{Green} = \frac{1}{3}$$

$$P(x) = \sum_{i}^{k} W_{i} p(x \mid C_{i})$$

• Assign points to Clusters

$$P(C_i | x) = W_i \frac{p(x | C_i)}{P(x)} = \frac{W_i p(x | C_i)}{\sum_{i=1}^{k} W_i p(x | C_i)}$$

Expectation and Maximization Step 2: Maximization

• Recompute Model $M' = \{C_0, C_1, ..., C_k\}$

$$W_i = \frac{1}{n} \sum_{x} P(C_i \mid x)$$

$$\mu_i = \frac{\sum_{x} x P(C_i \mid x)}{\sum_{x} P(C_i \mid x)}$$

$$\Sigma_i = \frac{\sum_{x} (x - \mu_i)^2 P(C_i \mid x)}{\sum_{x} P(C_i \mid x)}$$

EM in 1 Dim.



- Assume that there are 2 groups
- Guess x with Blue and Red groups



- Use same initial guess
- It is very Robust

 $\hat{\mu}_1 = 3, \hat{\mu}_2 = 5$ $\sigma_1 = \sigma_2 = 1$ $W_1 = W_2 = 0.5$

But, EM is designed Carefully

- EM looks simple.
- E-M or M-E shows very different result
- 1. Expectation with given parameters
 - Initial Guess of mean, variance, and fraction factor, W are first used.
 - At the first step, Do not calculate mean, variance, and so on
- 2. Maximization with p(c|x), and not with p(x|c)
 - E and M looks similar. It causes confusion
- 3. If M(calculate parameters) works first, EM often fails.

Example) ex/ml/l12em1.py Generate Blue and Red



Example) ex/ml/l12em1.py Initial Guess

```
def em():
    # step 0: guess model
    n = size(c,1)
    x = array(n,2)
    x[:,1] = c
    x[:,2] = randint(2,n,1)
    W = array(1,2)
    mb = 3
    sb =1
    mr = 5
    sr =1
    W[1,1] =0.5
    W[1,2] =0.5
```

pointlabel0.201.3010.113.3011.51

- Matrix X has two column
 - 1st column is random data
 - 2nd column, label 0 is blue and label 1 is red
- Mb=mean of blue
- Sb= standard deviation of blue
- Mr = mean of red
- Sr =standard deviation of red
- W[1,1] = W1
- W[1,2] = W2

Example) ex/ml/l12em1.py Expectation



- P(x|C) is the p.d.f. of x with respect to a Cluster
- P(C|x) means a new Cluster, C is determined by p(x) comparison

Example) ex/ml/l12em1.py Maximization





- Above two points are regarded as Blue one in the right picture.
 - Because, EM is based on a probabilistic distribution.

Why We Learn EM and GMM? Imitation Learning is Not Doing Memorized Motion

- 1990's: Encoder Recording and Replay
- After 2005: Trajectories are considered as the set of Stochastic Process







Gaussian Mixture Model

Extend k-means Clustering into a Probabilistic framework • as like EM method



Left signal is the mixture of Two Different Gaussian Goal of GMM is to find Multiple Gaussian Distributions

Modeling of GMM

• Assume that the *j* th point of the vector x belongs to the *i* th Cluster.

$$p(x) = \sum_{i} \pi_{i} p(x \mid \mu_{i}, \Sigma_{i}) \qquad \sum_{i} \pi_{i} = 1$$

• Gaussian PDF of the *i* th cluster is defined as,

$$G_i(x) = f(x, \mu_i, \sum_i) = \left((2\pi)^N Det(\Sigma)\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$$

x: the input vector

- μ_i : the mean value of the *i*th cluster
- \sum_{i} : the covariance(variance) of the *i*th cluster

Example i for Cluster and j for input, x



• π is the prior probability.

$$\pi_i = \Pr(x \in C_i)$$

Probability of the *i*th point belongs to the *i*th cluster

$$W_i^j = \frac{\pi_i G_i(x)}{\sum_{k=1} \pi_k G_k(x)}$$



Expectation Procedure: Probability of the *j*th point belongs to the *i*th cluster

$$W_i^{j} = \frac{\pi_i G_i(x)}{\sum_{k=1}^{j} \pi_k G_k(x)} \qquad \qquad W_i^{j} = \frac{\pi_1 G_1(x_j)}{\pi_1 G_1(x_j) + \pi_2 G_2(x_j)}$$

$$x = \begin{bmatrix} 1\\ 1.1\\ 10\\ 10.1 \end{bmatrix} \quad W_1^{j=1} = \frac{\pi_1 G_1(x_1 = 1)}{\pi_1 G_1(x_1 = 1) + \pi_2 G_2(x_1 = 1)} \qquad W_2^{j=1} = \frac{\pi_2 G_2(x_1 = 1)}{\pi_1 G_1(x_1 = 1) + \pi_2 G_2(x_1 = 1)} \\ W_1^{j=2} = \frac{\pi_1 G_1(x_2 = 1.1)}{\pi_1 G_1(x_2 = 1.1) + \pi_2 G_2(x_2 = 1.1)} \qquad W_2^{j=2} = \frac{\pi_2 G_2(x_2 = 1.1)}{\pi_1 G_1(x_2 = 1.1) + \pi_2 G_2(x_2 = 1.1)} \\ W_1^{j=3} = \frac{\pi_1 G_1(10)}{\pi_1 G_1(10) + \pi_2 G_2(10)} \qquad W_2^{j=3} = \frac{\pi_2 G_2(10)}{\pi_1 G_1(10) + \pi_2 G_2(10)} \\ W_1^{j=4} = \frac{\pi_1 G_1(10.1)}{\pi_1 G_1(10.1) + \pi_2 G_2(10.1)} \qquad W_2^{j=4} = \frac{\pi_2 G_2(10.1)}{\pi_1 G_1(10.1) + \pi_2 G_2(10.1)} \\ \end{bmatrix}$$

Maximization

• What is the objective function?

$$p(x) = \sum_{i} \pi_{i} p(x_{i}; \mu_{i}, \Sigma_{i}) \longrightarrow Best \ \mu_{i}, \Sigma_{i} \ for \ Cluster \ i$$
$$p(x_{i}) \rightarrow p\left(x_{i}^{j}, w_{i}^{j}\right) = p\left(x_{i}^{j} \mid w_{i}^{j}\right) p\left(w_{i}^{j}\right)$$

• Log likelihood

$$L(\pi, \mu, \Sigma) = \log \prod_{j} p(x^{j}; \pi, \mu, \Sigma)$$

= $\sum_{j} \log p(x^{j}; \pi, \mu, \Sigma) = \sum_{j} \log p(x^{j} | \mathbf{w}^{j}; \mu, \Sigma) p(\mathbf{w}^{j}; \pi)$

Maximization of Log likelihood

$x = \{x^1, x^2, ..., x^N\}^T$



Example of gmm1

• Edit ex/ml/gmm1



```
def gmm(x,k):
    N =size(x,1)
    # Guess initial model
   m=array(1,k)
    s=array(1,k)
    p=array(1,k)
    W=zeros(N,k)
    for i in range(1,k+1):
        m[i]= x[randint(N)+1]
        s[i]= sqrt(cov(x))
        p[i] = 1./k
    # Do EM
    for it in range(0,100):
        pdf=zeros(N,k)
        # Expectation
        for i in range(1,k+1):
            pdf[:,i] = normpdf(x,m[i],s[i])*p[i]
        sump = sum(pdf, 2)
        for i in range(1,k+1):
            W[:,i]=pdf[:,i].div(sump)
        # Maximization
        p
            = mean(W)
        for i in range(1,k+1):
            m[:,i] = wmean(x,W[:,i])
                    = x - m[:, i]
            Xm
            xm
                    = xm.mul(xm)
                    = wmean(xm,W[:,i])
            v
            s[:,i] = sqrt(v)
        m.Print()
        # draw
        figure(2)
        # original data
        graph(1)
        plotgf(1,3)
        graph(2)
        plotgf(5,1)
        # GMM result
        for i in range(1,k+1):
            graph(2+i)
            plotgf(m[i],s[i],'r')
        loop.pause()
```

Ref:

Maximum Likelihood Estimation(MLE)

- Estimating parameters of a probability distribution
 - by maximizing a likelihood function

$$L(\theta; X) = p(X \mid \theta) = \int p(X, Z \mid \theta) dZ$$

Z: unobserved or latent data

