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01. Procedure

Procedure

- 1. Train/Test samples generation
- 2. Training: Find mean vectors by K-means clustering
- 3. Training: Choose maximum distance
- 4. Test

Assume

Training data has **no class**(Unsupervised learning)

No information of **how many sample point** are in each class

The number of cluster is 5

We can evaluate prediction of test data is corrected or not

Evaluation

T = # of match that is predicted to the right class.

F = # of match that is predicted to the wrong class.

Accuracy = T / T + F

02. Generate train/test set

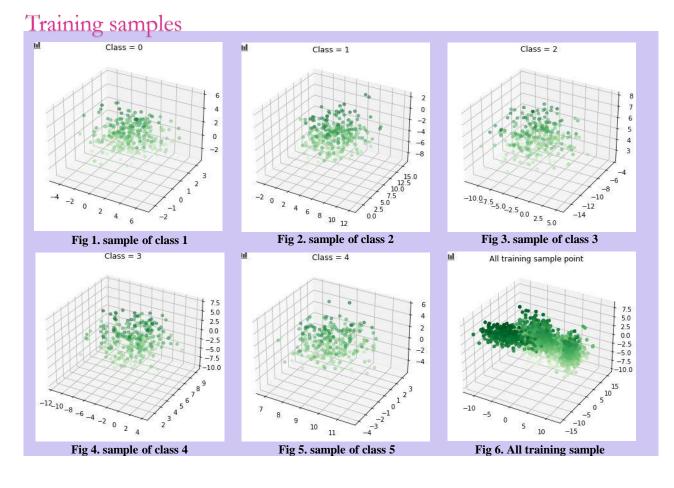
Train/Test samples generation

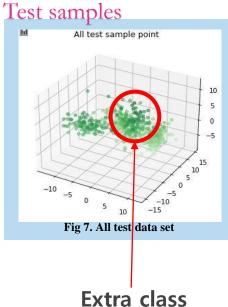
- Train set
- Consisted of 5 classes
- Randomly generate 300 sample points per a class

- Test set
- Consisted of 6 classes which 5 classes are same as train set and 1 class is not same.
- Randomly generate 100 sample points per a class.

Class	X	Y	Z	Class	X	Y	Z
0	N(1,4)	N(1,1)	N(1,2.25)	5	N(5,2.25)	N(-4,6.25)	N(4,12.25)
1	N(5,6.25)	N(7,9)	N(-3,4)		Fig 2. Table o	of extra class for test	
2	N(-4,9)	N(-10,2.25)	N(5,1)				
3	N(-3,7.29)	N(6,2.25)	N(-1,9)				
4	N(9,1)	N(0,2.25)	N(0,4)				
Fig 1. Table of Train set distribution							

02. Generate train/test set





03. Training

Training: Find mean vectors by K-means clustering

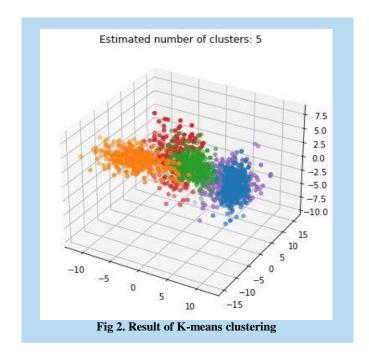
- K-means clustering(K=5)
- I. Choose seed point randomly
- II. Divide all point to a cluster which has **nearest** centroid from the point



- III. Recalculate **centroid** of clusters
- IV. Repeat 2,3 until **converge**

Mean vector	X	Y	Z	
Class 0	1.0602	1.3509	0.9158	
Class 1	5.3074	7.5098	-3.1818	
Class 2	-3.8317	-9.8629	5.0319	
Class 3	-3.5391	6.4290	-1.1532	
Class 4	8.8335	0.1976	-0.3490	

Fig 1. mean vector of cluster by K-means clustering



03. Training

Training: Choose maximum distance

- Maximum likelihood for finding covariance of a cluster
- \checkmark K-means clustering으로부터 나온 **centroid**와 그 **centroid를 포함하는 클러스터에 속하는 모든 점**들에 대한 가능성(likelihood)를 최대화하는 Σ_z 계산

$$Z_i = [x_i, y_i, z_i]_{i=1}^N \in Cluster(k)$$

$$P(Z|\Sigma_z) = \prod_{i=1}^N P(Z_i|\Sigma_z) = \prod_{i=1}^N \frac{1}{\sqrt{2\pi}^3|\Sigma_z|^{\frac{1}{2}}} exp(-\frac{1}{2}(Z_i - u_z)^T \Sigma_z^{-1}(Z_i - u_z))$$
: likelihood

$$\Sigma_z = argmax_{\Sigma_z} P(Z|\Sigma_z) = argmax_{\Sigma_z} \ln P(Z|\Sigma_z)$$



$$\frac{\partial}{\partial \Sigma_z} \ln \prod_{i=1}^N \frac{1}{\sqrt{2\pi}^3 |\Sigma_z|^2} exp(-\frac{1}{2}(Z_i - u_z)^T \Sigma_z^{-1} (Z_i - u_z)) = 0$$
 일 때의 Σ_z 가 K-means 클러스터에 의해 나온 centroid와 해당 클러스터에 속하는 샘플포인트들의 likelihood function을 maximize한다.



$$\Sigma_z = \frac{1}{N} \sum_{i=1}^N (Z_i - u_z)^T \Sigma_z^{-1} (Z_i - u_z)$$
: empirical covariance

✓ Gaussian distribution의 실제 확률 분포를 모를 경우, Covariance matrix를 샘플 데이터를 통해 구한 empirical covariance Σ_z 로 설정하면 maximum likelihood를 얻음

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03. Training

- 2 From covariance matrix, find maximum weighted distance
- ▶ 각 클러스터는 maximum distance를 갖음
- \triangleright 클러스터의 centriod와 test sample point의 Distance의 계산은 euclidean distance가 아닌, 클러스터 covariance matrix의 σ_x , σ_y , σ_z 값에 따라 x, y, z에 weight를 부여하여 계산

 $Distance(k(C_{kx},C_{ky},C_{kz}),P_i(x_i,y_i,z_i)):$ 클러스터 k와 i번째 sample의 거리

Distance
$$(k, P_i) = \frac{|c_{kx} - x_i|^2}{\sigma_x^2} + \frac{|c_{ky} - y_i|^2}{\sigma_y^2} + \frac{|c_{kz} - z_i|^2}{\sigma_z^2}$$

Distance(k, P_i) < c (c:constanct)</p>

타원체의 내부의 점일 경우에만 cluster에 속한 것으로 판정

	σ_{χ}^{2}	σ_y^2	$\sigma_{\!\scriptscriptstyle Z}^{\;\;2}$	C(constant)	# of Correct
Class0	3.6803	2.2208	2.9527	9	545
Class1	4.8532	6.1886	4.2016	10	549
Class2	8.6057	3.8973	1.0286	11	545
Class3	5.4869	2.2065	8.3600	11	343
Class4	1.7645	2.5653	4.1939	12	543

Fig 1. Empirical variance

Fig 2. Choose maximum distance

Compare probability density function with Empirical variance and mean

- ▶ K-means clustering을 통해 클러스터의 **centroid(Empirical mean)**를 찾고, 샘플데이터에 label(class)를 할당(Unsupervised)
- Maximum likelihood 를 통해 각 클러스터의 empirical covariance를 계산하고, 클러스터의 x, y, z의 variance를 이용하여 euclidean distance 가 아닌 weighted distance를 계산

Class	X	Y	Z	
0	N(1,4)	N(1,1)	N(1,2.25)	
1	N(5,6.25)	N(7,9)	N(-3,4)	
2	N(-4,9)	N(-10,2.25)	N(5,1)	
3	N(-3,7.29)	N(6,2.25)	N(-1,9)	
4	N(9,1)	N(0,2.25)	N(0,4)	

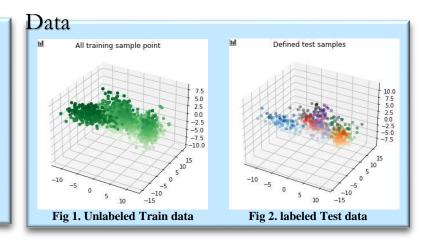
Fig 1. Defined probability density function

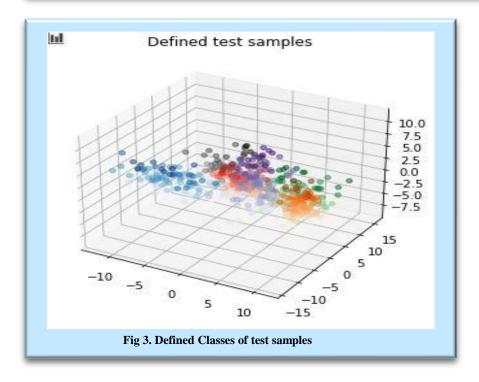
Class	X	Y	Z
0	N(1.0602, 3.6803)	N(1.3509, 2.2208)	N(0.9158, 2.9527)
1	N(5.3074,	N(7.5098,	N(-3.1818
	4.8532)	6.1886)	, 4.2016)
2	N(-3.8317	N(-9.8629	N(5.0319
	, 8.6057)	, 3.8973)	, 1.0286)
3	N(-3.5391	N(6.4290	N(-1.1532
	, 5.4869)	, 2.2065)	, 8.3600)
4	N(8.8335	N(0.1976	N(-0.3490
	, 1.7645)	, 2.5653)	, 4.1939)

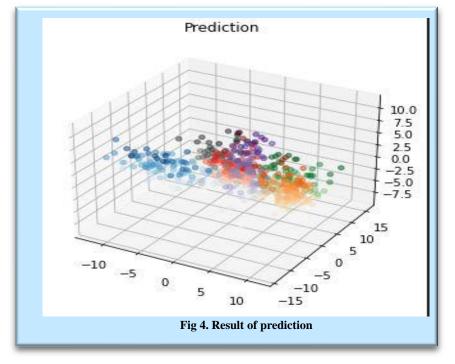
Fig 2. Empirical mean and variance from samples

- Predict Condition
- Condition 1 : find the nearest cluster
 Find nearest centroid of Cluster k
- Condition 2 : check the distance

Distance
$$(k, P_i) = \frac{|c_{kx} - x_i|^2}{\sigma_x^2} + \frac{|c_{ky} - y_i|^2}{\sigma_y^2} + \frac{|c_{kz} - z_i|^2}{\sigma_z^2} < 10$$







Class	# of correct	# of wrong	Accuracy
0	98	2	0.98
1	84	16	0.84
2	98	2	0.98
3	85	15	0.85
4	100	0	1
Extra	84	16	0.84
Total	549	51	0.915

Fig 1. Table of recognizing result

Cluster representation with Maximum distance

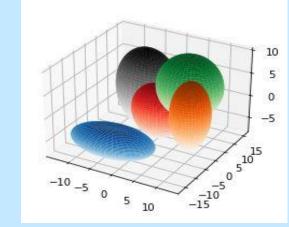


Fig 1. Vector space with maximum distance of each cluster

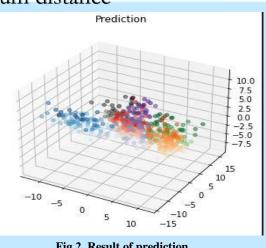
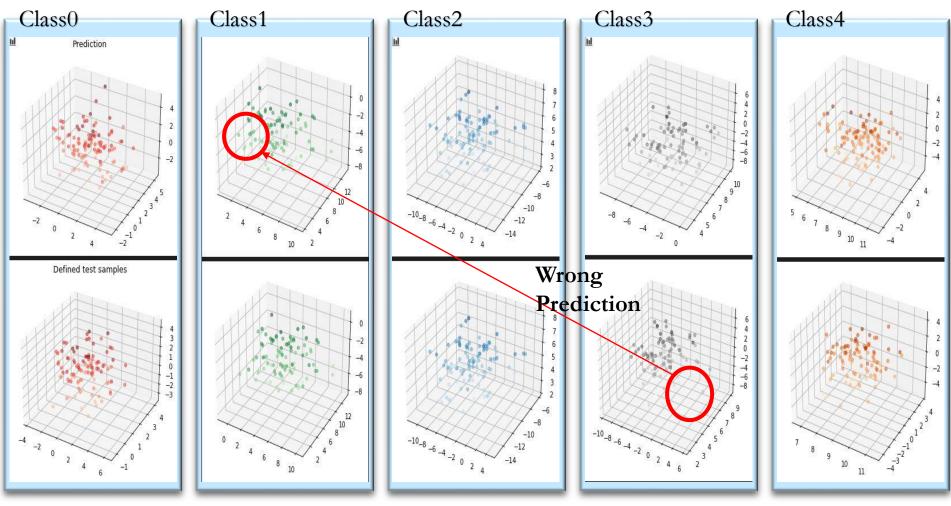


Fig 2. Result of prediction

- Training Sample point를 통 해 구한 covariance matrix 를 이용하여 축이 $\sqrt{10}\sigma_{x}$, $\sqrt{10}\sigma_{y}$, $\sqrt{10}\sigma_{z}$ 길이 의 Recognize boundary 생 성
- 해당 영역 밖의 점은 Figure2의 보라색(Extra class)로 판별



Upper figure : Prediction

Under figure : predefined classes

Conclusion

▶ 두 정규분포의 Mean vector 차이는 작고 Variance가 큰 경우, 잘못된 예측을 하기 쉽다.

Class	X	Y	Z	Class	# of	# of	Accuracy
1	N(5,6.25)	N(7,9)	N(-3,4)	1	correct 84	wrong 16	0.84
3	N(-3,7.29)	N(6,2.25)	N(-1,9)	3	85	15	0.85

▶ Labeling 되어 있지 않는 데이터셋으로 **K-means clustering**과 Maximum likelihood를 활용하여 recognize을 위한 클러스터 영역을 생성할 수 있다.