



MSE MachLe Bayes Theorem

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Bayes Theorem and the Gaussian Distribution



- Apply Bayesian learning, especially Bayes' theorem and the Bayes classifier
- Explain how a Gaussian Mixture Model (GMM) is trained and evaluated, given the respective equations and the EM algorithm
- Apply GMMs for **pattern recognition tasks** on audio data

Based on material by

- Stuart Russell, UC Berkeley
- T. Stadelmann, R. Ewerth & B. Freisleben, U Marburg



I. Probability Theory

(a short repetition)

 $p(X, Y) = p(Y|X) \cdot p(X)$ $= p(X|Y) \cdot p(Y)$

Educational Objectives



- you have repeated the basic rules of probability theory.
- you know the difference between a joint and a conditional probability distribution.
- you know how to apply **Bayes Theorem** to calculate the posterior probability distribution for simple discrete examples.
- You can name the prior probability distribution, the likelihood function, the evidence, and you know how to marginalize over a joint probability distribution.
- you know the basic properties of a multivariate Gaussian probability distribution. You can plot a 2D Gaussian probability distribution given the mean vector μ and the covariance matrix Σ
- you can estimate the parameters of a multivariate Gaussian distribution from data points using a kernel density estimation method.

Basic Probability Theory (recap)



Probability and random variable:

p(x = x): the probability of variable x being in state x.

 $p(x = \mathbf{x}) = \begin{cases} 1 & \text{we are certain } x \text{ is in state } \mathbf{x} \\ 0 & \text{we are certain } x \text{ is not in state } \mathbf{x} \end{cases}$

Values between 0 and 1 represent the degree of certainty of state occupancy.

Domain: dom()

dom() denotes the states *x* can take. For example:

 $dom(coin) = \{heads, tails\}.$

When summing over a variable x, the interpretation is that all states of x are included

$$\sum_{x} f(x) \equiv \sum_{\mathbf{s} \in \operatorname{dom}(x)} f(x = \mathbf{s}).$$

Basic Rules of Probability



Sum Rule:

$$p(X) = \sum_{Y} p(X,Y) \qquad \quad p(Y) = \sum_{X} p(X,Y) \qquad \qquad \text{Marginal}$$

Product Rule:

$$p(X,Y) = p(Y|X) \cdot p(X) = p(X|Y) \cdot p(Y)$$
 Conditional

Bayes Theorem:

$$p(Y|X) = \frac{p(X|Y) \cdot p(Y)}{p(X)} = \frac{p(X|Y) \cdot p(Y)}{\sum_{y \in Y} p(X,y)} = \frac{p(X|Y) \cdot p(Y)}{\sum_{y} p(X|y) \cdot p(y)}$$
Bayes Rule

Probability Tables – Joint Probability

- Two colored boxes (X=r, X=b) with apples (Y=a) and oranges (Y=o)
- We may ask: What is the overall probability that the selection procedure will pick an apple? p(Y = a) = ?
- Or: "given that we have chosen an orange, what is the probability that the box we chose was the blue one?".

p(X = b|Y = o) =?

Using the concept of the joint probability (density), the marginal probability and the sum and product rule, we can answer all those questions. We define:

$$p(X,Y) = p(X = x_i, Y = y_i) = \frac{n_{ij}}{N}$$







If we count the frequencies, we get the following table. In total, there are 12 fruits, 8 are in a red box, 4 in a blue box. We have 5 apples and 7 oranges in total.

$n_{ij}(X,Y)$	Y = a	Y = o	n(X)
X = r	2	6	8
X = b	3	1	4
n(Y)	5	7	N = 12

We can convert this into a probability table by normalization:

p(X,Y)	Y = a	Y = o	p(X)
X = r	$\frac{2}{12}$	$\frac{6}{12}$	$\frac{8}{12}$
X = b	$\frac{3}{12}$	$\frac{1}{12}$	$\frac{4}{12}$
p(Y)	$\frac{5}{12}$	$\frac{7}{12}$	1

Conditional Probabilities

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- This table is the joint probability of this problem, the colums at the borders are the marginals. Now we can easily calculate the conditional probabilities using the joint and the marginals.

$$p(Y = a | X = r) = \frac{p(Y = a, X = r)}{p(X = r)} = \frac{\frac{2}{12}}{\frac{8}{12}} = \frac{1}{4}$$

$$p(Y = o | X = r) = \frac{p(Y = o, X = r)}{p(X = r)} = \frac{\frac{6}{12}}{\frac{8}{12}} = \frac{3}{4}$$

$$p(Y = a | X = b) = \frac{p(Y = a, X = b)}{p(X = b)} = \frac{\frac{3}{12}}{\frac{4}{12}} = \frac{3}{4}$$

$$p(Y = o | X = b) = \frac{p(Y = o, X = b)}{p(X = b)} = \frac{\frac{1}{12}}{\frac{4}{12}} = \frac{1}{4}$$

Bayes Theorem

Using Bayes Theorem, we can calculate the probability to draw an apple (5 from 12) resp. Orange (7 from 12):

$$p(Y = a) = p(Y = a | X = r) \cdot p(X = r) + p(Y = a) | X = b) \cdot p(X = b)$$
$$= \frac{1}{4} \cdot \frac{8}{12} + \frac{3}{4} \cdot \frac{4}{12} = \frac{5}{12}$$

The conditionals are not symmetric:

$$p(Y = a | X = r) = \frac{p(Y = a, X = r)}{p(X = r)} = \frac{\frac{2}{12}}{\frac{8}{12}} = \frac{1}{4}$$

$$p(X = r | Y = a) = \frac{p(Y = a, X = r)}{p(Y = a)} = \frac{\frac{2}{12}}{\frac{5}{12}} = \frac{2}{5}$$

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Bayes Theorem



We can test Bayes rule:

$$\frac{1}{4} = p(Y = a | X = r) = \frac{p(X = r | Y = a) \cdot p(Y = a)}{p(X = r)} = \frac{\frac{2}{5} \cdot \frac{5}{12}}{\frac{8}{12}}$$

Inspector Clouseau

 Image: Second system
 Image: Second system

 Image: Second

Inspector Clouseau arrives at the scene of a crime. The Butler (B) and Maid (M) are his main suspects. The inspector has a prior belief of 0.6 that the Butler is the murderer, and a prior belief of 0.2 that the Maid is the murderer. These probabilities are independent in the sense that p(B, M) = p(B)p(M). (It is possible that both the Butler and the Maid murdered the victim or neither). The inspector's *prior* criminal knowledge can be formulated mathematically as follows:

 $\operatorname{dom}(B) = \operatorname{dom}(M) = \{\operatorname{murderer}, \operatorname{not} \operatorname{murderer}\}$

 $\begin{array}{ll} \operatorname{dom}(K) = \{ \text{knife used}, \text{knife not used} \} \\ p(B = \operatorname{murderer}) = 0.6, \qquad p(M = \operatorname{murderer}) = 0.2 \\ p(\text{knife used} | B = \operatorname{not murderer}, \quad M = \operatorname{not murderer}) &= 0.3 \\ p(\text{knife used} | B = \operatorname{not murderer}, \quad M = \operatorname{murderer}) &= 0.2 \\ p(\text{knife used} | B = \operatorname{murderer}, \quad M = \operatorname{not murderer}) &= 0.6 \\ p(\text{knife used} | B = \operatorname{murderer}, \quad M = \operatorname{murderer}) &= 0.1 \end{array}$

The victim lies dead in the room and the inspector quickly finds the murder weapon, a Knife (K). What is the probability that the Butler is the murderer? (Remember that it might be that neither is the murderer).

Inspector Clouseau II



Using b for the two states of B and m for the two states of M,

$$p(B|K) = \sum_{m} p(B, m|K) = \sum_{m} \frac{p(B, m, K)}{p(K)} = \frac{p(B) \sum_{m} p(K|B, m)p(m)}{\sum_{b} p(b) \sum_{m} p(K|b, m)p(m)}$$

Plugging in the values we have

$$p(B = \text{murderer}|\text{knife used}) = \frac{\frac{6}{10} \left(\frac{2}{10} \times \frac{1}{10} + \frac{8}{10} \times \frac{6}{10}\right)}{\frac{6}{10} \left(\frac{2}{10} \times \frac{1}{10} + \frac{8}{10} \times \frac{6}{10}\right) + \frac{4}{10} \left(\frac{2}{10} \times \frac{2}{10} + \frac{8}{10} \times \frac{3}{10}\right)}{\frac{300}{412}} \approx 0.73$$

Hence knowing that the knife was the murder weapon strengthens our belief that the butler did it.

Exercise: compute the probability that the Butler and not the Maid is the murderer.

Joint Probability | Joint Probability Density





Gaussian distribution (1D)



Normal distribution with mean μ and variance σ^2 :

$$p(x) = \mathcal{N}(x|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$
$$\mathbf{E}[x] = \int x \cdot p(x)dx = \mu$$
$$\mathbf{E}[x^2] = \int x^2 \cdot p(x)dx = \mu^2 + \sigma^2$$
$$\mathbf{VAR}[x] = \mathbf{E}[x^2] - \mathbf{E}[x]^2 = \sigma^2$$
Normal Distribution

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Multivariate Gaussian Distribution

Gaussian defined over a vector x of continuous variables in a D-dimensional space with mean vector μ and covariance matrix Σ , where $|\Sigma|$ is the determinant of Σ .

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mu, \mathbf{\Sigma}) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mu)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)\right\}$$

Multivariate Gaussian Distribution

The **quadratic form** in the argument of the exponential is called <u>Mahalanobis</u> <u>distance</u>:

$$\Delta = (\mathbf{x} - \mu)^T \mathbf{\Sigma}^{-1} (\mathbf{x} - \mu)$$

Without loss of generality, we can assume that Σ is **symmetric** with **real** eigenvalues and an orthonormal set of eigenvectors u_i .

A bivariate Gaussian distribution





Multivariate Normal Distribution

```
from scipy.stats import multivariate_normal
import numpy as np import matplotlib.pyplot as plt
```

```
F = multivariate normal(mu, Sigma)
#draw random samples from the multivariate distribution #and try to
reconstruct the gaussian distribution
NSamples=10000
x, y = np.mgrid[-3:3:.1, -3:3:.1]
pos = np.dstack((x, y))
MVGauss = multivariate normal(mu, Sigma)
MVGSamples = MVGauss.rvs(size=NSamples)
XS = MVGSamples[:,0]
YS = MVGSamples[:,1]
fig2 = plt.figure('Using Scikit Learn')
ax2 = fig2.add subplot(111)
ax2.contourf(x, y, F.pdf(pos))
ax2.set xlabel("x")
ax2.set ylabel("y")
```

```
fig3 = plt.figure('Using Scikit Learn to draw random samples')
ax3 = fig3.add_subplot(111) ax3.scatter(XS,YS) ax3.set_xlabel("x")
ax3.set_ylabel("y")
```

2

-2

0.20

0.15

0.10

0.05



Multivariate Gaussian Distribution

Since Σ ist real and symmetric, the eigenvectors λ_i are real and the eigenvectors can be chosen from an orthonormal set, so that:



The quadratic form becomes

 $\Delta^2 = \sum_{i=1}^{D} \frac{y_i^2}{\lambda_i} \qquad \qquad y_j = \mathbf{u_j}^T \left(\mathbf{x} - \mu\right)$

This describes D-dimensional ellipsoids with main axes $\sqrt{\lambda_i}$.

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Probability Distributions

The deterimant is given by the product of the eigenvalues:

$$|\mathbf{\Sigma}|^{1/2} = \prod_{j=1}^D \lambda_j^{1/2}$$

In the orthonormal coordinate of the eigenvectors, the multivariate Gaussian distribution takes the form:

$$p(\mathbf{y}) = p(\mathbf{x}) \cdot |J| = \prod_{j=1}^{D} \frac{1}{(2\pi\lambda_j)^{1/2}} \exp\left\{-\frac{y_j^2}{2\lambda_j}\right\}$$

One can show:

$$\begin{split} \mathbb{E}[\mathbf{x}] &= \boldsymbol{\mu} & \text{Expectation value} \\ \mathbb{E}[\mathbf{x}\mathbf{x}^{T}] &= \boldsymbol{\mu}\boldsymbol{\mu}^{T} + \boldsymbol{\Sigma} & \text{Correlation} \\ &\cos[\mathbf{x}] &= \mathbb{E}[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{T}] = \boldsymbol{\Sigma} & \text{Covariance} \end{split}$$

Conditional Gaussian distributions

we partition x into two disjoint subsets x_a and x_b . Without loss of generality, we can take x_a to form the first *M* components of *x*, with x_b comprising the remaining D - M components:

$$\mathbf{x} = egin{pmatrix} \mathbf{x}_a \ \mathbf{x}_b \end{pmatrix} \quad oldsymbol{\mu} = egin{pmatrix} oldsymbol{\mu}_a \ oldsymbol{\mu}_b \end{pmatrix} \quad oldsymbol{\Sigma} = egin{pmatrix} oldsymbol{\Sigma}_{aa} & oldsymbol{\Sigma}_{ab} \ oldsymbol{\Sigma}_{ba} & oldsymbol{\Sigma}_{bb} \end{pmatrix}$$

In many situations, it will be convenient to work with the inverse of the covariance matrix, the precision matrix:

$${f \Lambda}\equiv {f \Sigma}^{-1}$$

$$oldsymbol{\Lambda} = \left(egin{array}{ccc} oldsymbol{\Lambda}_{aa} & oldsymbol{\Lambda}_{ab} \ oldsymbol{\Lambda}_{ba} & oldsymbol{\Lambda}_{bb} \end{array}
ight)$$

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Conditional Gaussian distributions II



To calculate the conditional $p(x_a|x_b)$, we have a look at the exponent:

$$-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) =$$
$$-\frac{1}{2}(\mathbf{x}_{\mathbf{a}}-\boldsymbol{\mu}_{a})^T\boldsymbol{\Lambda}_{aa}(\mathbf{x}_{\mathbf{a}}-\boldsymbol{\mu}_{a}) -\frac{1}{2}(\mathbf{x}_{\mathbf{a}}-\boldsymbol{\mu}_{a})^T\boldsymbol{\Lambda}_{ab}(\mathbf{x}_{\mathbf{b}}-\boldsymbol{\mu}_{b})$$
$$-\frac{1}{2}(\mathbf{x}_{\mathbf{b}}-\boldsymbol{\mu}_{b})^T\boldsymbol{\Lambda}_{ba}(\mathbf{x}_{\mathbf{a}}-\boldsymbol{\mu}_{a}) -\frac{1}{2}(\mathbf{x}_{\mathbf{b}}-\boldsymbol{\mu}_{b})^T\boldsymbol{\Lambda}_{bb}(\mathbf{x}_{\mathbf{b}}-\boldsymbol{\mu}_{b})$$

- We see that as a function of x_a , this is again a quadratic form, and hence the corresponding conditional distribution $p(x_a|x_b)$, will be Gaussian.
- Because this distribution is completely characterized by its **mean** and its **covariance**, our goal will be to identify expressions for the mean and covariance of $p(x_a|x_b)$, by inspection of the above equation:
- Completing the square:

$$-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) = -\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x} + \mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \text{const}$$

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Conditional Gaussian distributions III

Quadratic term: $-\frac{1}{2}\mathbf{x}_{a}^{T}\mathbf{\Lambda}_{aa}\mathbf{x}_{a}$

The covariance of $p(x_a|x_b)$ is therefore given by: $\Sigma_{a|b} = \Lambda_{aa}^{-1}$

Linear term:

$$\mathbf{x}_{a}^{T}\left\{ \mathbf{\Lambda}_{aa} oldsymbol{\mu}_{a} - oldsymbol{\Lambda}_{ab} (\mathbf{x}_{b} - oldsymbol{\mu}_{b})
ight\} = \mathbf{x}_{a}^{T}\left\{ \mathbf{\Sigma}_{a|b}^{-1} oldsymbol{\mu}_{a|b}
ight\}$$

The term in curly brackets must be equal to: $\Sigma_{a|b}^{-1}\mu_{a|b}$ Therefore we have:

$$\boldsymbol{\mu}_{a|b} = \boldsymbol{\Sigma}_{a|b} \left\{ \boldsymbol{\Lambda}_{aa} \boldsymbol{\mu}_{a} - \boldsymbol{\Lambda}_{ab} (\mathbf{x}_{b} - \boldsymbol{\mu}_{b}) \right\} = \boldsymbol{\mu}_{a} - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_{b} - \boldsymbol{\mu}_{b})$$

$$oldsymbol{\mu}_{a|b} = oldsymbol{\mu}_a - oldsymbol{\Lambda}_{aa}^{-1} oldsymbol{\Lambda}_{ab} (\mathbf{x}_b - oldsymbol{\mu}_b)$$
 $oldsymbol{\Sigma}_{a|b} = oldsymbol{\Lambda}_{aa}^{-1}$

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Summary



Covariance matrix

Precision matrix

$$oldsymbol{\Sigma} = \left(egin{array}{ccc} oldsymbol{\Sigma}_{aa} & oldsymbol{\Sigma}_{ab} \ oldsymbol{\Sigma}_{ba} & oldsymbol{\Sigma}_{bb} \end{array}
ight) \qquad egin{array}{ccc} oldsymbol{\Lambda} = oldsymbol{\Sigma}^{-1} = \left(egin{array}{ccc} oldsymbol{\Lambda}_{aa} & oldsymbol{\Lambda}_{ab} \ oldsymbol{\Lambda}_{ba} & oldsymbol{\Lambda}_{bb} \end{array}
ight)$$

Conditional probability distribution

$$p(\mathbf{x}_{a}|\mathbf{x}_{b}) = \mathcal{N}\left(\mathbf{x}_{a}|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Lambda}_{aa}^{-1}\right)$$
$$\boldsymbol{\mu}_{a|b} = \boldsymbol{\mu}_{a} - \boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab}(\mathbf{x}_{b} - \boldsymbol{\mu}_{b})$$
$$\boldsymbol{\Sigma}_{a|b} = \boldsymbol{\Lambda}_{aa}^{-1}$$

Conditional Probability Distribution of a Gaussian $\mu_{a|b}=\mu_a+\Sigma_{ab}\Sigma_{bb}^{-1}(\mathbf{x}_b-\mu_b)$

$$oldsymbol{\Sigma}_{a|b} = oldsymbol{\Sigma}_{aa} - oldsymbol{\Sigma}_{ab} oldsymbol{\Sigma}_{bb}^{-1} oldsymbol{\Sigma}_{ba}$$

• Marginal probability distribution:

$$p(\mathbf{x}_a) = \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$$

Example: Squirrel on a Tree (Mitchell)

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Joint probability density - marginal - conditional





Figure 2.9 The plot on the left shows the contours of a Gaussian distribution $p(x_a, x_b)$ over two variables, and the plot on the right shows the marginal distribution $p(x_a)$ (blue curve) and the conditional distribution $p(x_a|x_b)$ for $x_b = 0.7$ (red curve).

Belief Networks (Bayesian Networks)

- Definition: A belief network is a directed acyclic graph (DAG) in which each node has associated the conditional probability of the node given its parents.
- The joint distribution is obtained by taking the product of the conditional probabilities:

p(A, B, C, D, E) = p(A)p(B)p(C|A, B)p(D|C)p(E|B, C)



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Example: Burglar Alarm

Sally's burglar Alarm is sounding. Has she been Burgled, or was the alarm triggered by an Earthquake? She turns the car Radio on for news of earthquakes.

General case:
$$p(A, R, E, B) = p(A|R, E, B)p(R, E, B)$$

= $p(A|R, E, B)p(R|E, B)p(E, B)$
= $p(A|R, E, B)p(R|E, B)p(E|B)p(B)$

Assumptions:

- The alarm is not directly influenced by any report on the radio: p(A|R, E, B) = p(A|E, B)
- The radio broadcast is not directly influenced by the burglar variable: p(R|E,B) = p(R|E)
- Burglaries don't directly "cause" earthquakes: p(E|B) = p(E)
- Therefore:

$$p(A, R, E, B) = p(A|E, B) \cdot p(R|E) \cdot p(E) \cdot p(B)$$

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Directed acyclic graph





p(A|B, E)

A larm = 1	Burglar	Earthquake
0.9999	1	1
0.99	1	0
0.99	0	1
0.0001	0	0

p(R|E)

Radio = 1	Earthquake
1	1
0	0

The remaining tables are p(B = 1) = 0.01 and $p(E = 1) = 10^{-6}$

The tables and graphical structure fully specify the distribution.

Inference



Initial evidence: The alarm is sounding A = 1:

$$p(B = 1|A = 1) = \frac{\sum_{E,R} p(B = 1, E, A = 1, R)}{\sum_{B,E,R} p(B, E, A = 1, R)}$$
$$= \frac{\sum_{E,R} p(A = 1|B = 1, E)p(B = 1)p(E)p(R|E)}{\sum_{B,E,R} p(A = 1|B, E)p(B)p(E)p(R|E)} \approx 0.99$$

Additional Evidence: (R = 1), The radio broadcasts an earthquake warning:

A similar calculation gives $p(B = 1 | A = 1, R = 1) \approx 0.01$.

Initially, because the alarm sounds, Sally thinks that she's been burgled. However, this probability drops dramatically when she hears that there has been an earthquake. The earthquake "explains away" to an extent the fact that the alarm is ringing.

Examples of Belief Networks in Machine Learning



- **Prediction** (discriminative): p(class | input)
- **Prediction** (generative): $p(class | input) \propto p(input | class) \cdot p(class)$
- **Time-series:** Markov chains, Hidden Markov Models.
- **Unsupervised learning:** $p(data) = \sum_{latent} p(data|latent) \cdot p(latent)$
- And many more: Personally I find the framework very useful for understanding and rationalising the many different approaches in machine learning and related areas.

Conditional Independence I





denotes that the two sets of variables X and Y are independent of each other given the state of the set of variables Z. This means that

$$p(X, Y \mid Z) = p(X \mid Z) \cdot p(Y \mid Z)$$
$$p(X \mid Y, Z) = p(X \mid Z)$$

for all states of X, Y, Z. In case the conditioning set is empty we may also write

$X \perp \!\!\!\perp Y$

in which case X is (unconditionally) independent of Y.

Conditional Independence II





In (a), (b) and (c), A, B are conditionally independent given C:
(a) p(A, B|C) = p(A,B,C)/p(C) = p(A|C)p(B|C)p(C)/p(C) = p(A|C)p(B|C)
(b) p(A, B|C) = p(A)p(C|A)p(B|C)/p(C) = p(A,C)p(B|C)/p(C) = p(A|C)p(B|C)
(c) p(A, B|C) = p(A|C)p(C|B)p(B)/p(C) = p(A|C)p(B,C)/p(C) = p(A|C)p(B|C)
In (d) the variables A, B are conditionally dependent given C:

 $p(A, B|C) \propto p(C|A, B)p(A)p(B)$

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Conditional Independence III





In (a), (b) and (c), the variables A;B are marginally dependent.

In (d) the variables A, B are **marginally independent**.

$$p(A, B) = \sum_{C} p(A, B, C) = \sum_{C} p(A)p(B)p(C|A, B) = p(A)p(B)$$

Collider

- A collider contains two or more incoming arrows along a chosen path.
- Summary of two previous slides:



If C has more than one incoming link, then $A \perp\!\!\!\perp B$ and $A \not\!\!\perp B \mid C$. In this case C is called collider.



If C has at most one incoming link, then $A \perp B \mid C$ and $A \not\perp B$. In this case C is called non-collider.



Summary

- We can reason with certain or uncertain evidence using repeated application of Bayes' rule.
- A belief network represents a factorisation of a distribution into conditional probabilities of variables dependent on parental variables.
- Belief networks correspond to **directed acyclic graphs (DAG)**.
- Variables are **conditionally independent** $x \perp ||y||z$ if $p(x, y|z) = p(x|z) \cdot p(y|z)$; the absence of a link in a belief network corresponds to a conditional independence statement.
- If in the graph representing the belief network, two variables are independent, then they are independent in any distribution consistent with the belief network structure.
- Belief networks are natural for representing `causal' influences.

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Recap: Probability distributions and PDFs



Terminology: its probability density function (pdf) is one way to describe a distribution.

What does a pdf tell about a set of data?

- Where to expect samples ...with which probability
- Correlation/covariance of dimensions
- ➔ For data coming from some stochastic processes, the pdf tells everything there is to know about the data
- → Allows for sampling data from the underlying distribution

(generative modeling)

An example generative model

 The univariate Gaussian
 A parametric pdf, recoverable from data (Gaussianity given)





II. Bayes' Theorem



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Bayes' theorem One of the cornerstones of modern data analysis

$p(h|X) = \frac{p(X|h) \cdot p(h)}{p(X)}$

with (in a machine learning context with training data X and model h)

- p(X|h) the **likelihood** of the data, given the model \rightarrow called the **evidence** for h
- p(X) the a priori probability of the training data $X \rightarrow$ this normalization factor is **rarely** needed/used
- p(h) is the **a priori** probability of hypothesis $h \rightarrow$ often neglected in practice due to dominance of evidence

Use cases

- Generally: **Convert** between prior and posterior probabilities
- Specific example: Model selection ٠
 - \rightarrow Given competing $h_i \in \mathcal{H}$, one can calculate the likelihood $p(X|h_i)$, then select best $\hat{h} = \max_{h_i} p(h_i | X) \approx \max_{h_i} p(X | h_i)$



Rev. Thomas Bayes, 1701-1761



Bayes Theorem



Prior, Likelihood and Posterior

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- For data D and variable θ , Bayes' rule tells us how to update our prior beliefs about the variable θ in light of the data to a posterior belief:



- The *evidence* is also called the *marginal likelihood*.
- The term *likelihood* is used for the probability that a model generates observed data.

Prior, Likelihood and Posterior



■ if we condition on the model M, we have

$$p(\theta \mid \mathcal{D}, M) = \frac{p(\mathcal{D} \mid \theta, M) \cdot p(\theta \mid M)}{p(\mathcal{D} \mid M)}$$

The MAP assignment: The Most probable A Posteriori (MAP) setting is that which maximises the posterior,

$$\hat{\theta}_{MAP} = \underset{\theta}{\operatorname{argmax}} \{ p(\theta \mid \mathcal{D}, M) \} = \underset{\theta}{\operatorname{argmax}} \{ p(\theta, \mathcal{D} \mid M) \}$$

The Max. Likelihood assignment: when $p(\theta|M) = \text{const}$

$$\hat{\theta}_{\mathrm{ML}} = \underset{\theta}{\operatorname{argmax}} \{ p(\theta | \mathcal{D}, M) \} = \underset{\theta}{\operatorname{argmax}} \{ p(\mathcal{D} | \theta, M) \}$$

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The Bayes optimal classifier Classification's «gold standard»



Theoretically optimal (=most probable) classification

Combine predictions of all hypotheses, weighted by their posterior probabilities: (where y_i is a label from the set Y of classes)

$$P(Y = y_k | X_1, \dots, X_n) = \frac{P(Y = y_k) P(X_1, \dots, X_n | Y = y_k)}{\sum_j P(Y = y_j) P(X_1, \dots, X_n | Y = y_j)}$$
$$= \frac{P(Y = y_k) \prod_i P(X_i | Y = y_k)}{\sum_j P(Y = y_j) \prod_i P(X_i | Y = y_j)}$$

$$Y \longleftarrow \underset{y_k}{\operatorname{argmax}} P(Y = y_k) \prod_i P(X_i | Y = y_k)$$

Naive Bayes Classifier

- No other method using the same \mathcal{H} and X can do better on average
- In particular outperforms simply taking the classification of the MAP hypothesis, enforces the idea of ensemble learning
- Computationally intractable (linear in |ℋ| → see Reader (also on Moodle): <u>http://www.cs.cmu.edu/~tom/mlbook/NBayesLogReg.pdf</u>)

Maximum Likelihood revisited



A quick example of a maximum likelihood estimate

- You flip a coin 10 times and observe the following sequence (H, T, T, H, T, T, T, T, H, T)¶
- What's the MLE of observing 3 heads in 10 trials?
- simple answer:

The frequentist MLE is (# of successes) / (# of trials) or 3/10

Maximum Likelihood Approach: What is the expected probability for head given the observed data? Solving first derivative of binomial distribution :

$$L(\theta \mid X = 3) = {\binom{10}{3}} \cdot \theta^3 \cdot (1 - \theta)^7$$

$$\log\{L(\theta)\} = \log\binom{10}{3} + 3\log\theta + 7\log(1-\theta)$$

$$\frac{\partial \log\{L(\theta)\}}{\partial \theta} = \frac{3}{\theta} - \frac{7}{1-\theta} = 0$$
$$\theta_{ML} = \frac{3}{10}$$

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Maximum Likelihood for a Gaussian

Given a data set $\mathbf{X} = (x_1, x_2, ..., x_n)^T$ in which the observations $\{x_n\}$ are assumed to be drawn independently from a multivariate Gaussian distribution, we can estimate the parameters of the distribution by **maximum likelihood**.

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{N \cdot D}{2} \ln(2\pi) - \frac{N}{2} \ln |\boldsymbol{\Sigma}| - \frac{1}{2} \sum_{n=1}^{N} (x_n - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (x_n - \boldsymbol{\mu})$$

By simple rearrangement, we see that the log likelihood function depends on the data set only through the two quantities (sufficient statistics for a Gaussian)



Derivative with respect to μ and setting it to zero yields the ML estimate for μ

$$\frac{\partial}{\partial \boldsymbol{\mu}} \ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \boldsymbol{\Sigma}^{-1}(x_n - \boldsymbol{\mu}) \Longrightarrow \boldsymbol{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

sample mean

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ML estimate for the covariance is biased



If we evaluate the expectations of the maximum likelihood solutions under the true distribution, we obtain the following results:

$$\mathbb{E}[\mu_{\mathbf{ML}}] = \int \boldsymbol{\mu}_{\mathbf{ML}} \cdot p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \mathbf{dX} = \boldsymbol{\mu}$$
$$\mathbb{E}[\mathbf{x}\mathbf{x}^{\mathbf{T}}] = \boldsymbol{\mu}\boldsymbol{\mu}^{T} + \delta_{mn}\boldsymbol{\Sigma}$$
$$\mathbb{E}[\boldsymbol{\Sigma}_{\mathbf{ML}}] = \frac{N-1}{N}\boldsymbol{\Sigma}$$

We see that the expectation of the maximum likelihood estimate for the mean is equal to the true mean. However, the maximum likelihood estimate for the covariance has an expectation that is less than the true value, and hence it is biased.

$$\tilde{\boldsymbol{\Sigma}} = \frac{1}{N-1} \sum_{n=1}^{N} (x_n - \boldsymbol{\mu}_{\mathrm{ML}}) (x_n - \boldsymbol{\mu}_{\mathrm{ML}})^T$$

Unbiased estimator of the covariance

Bayesian Inference for a Gaussian

The maximum likelihood framework gave point estimates for the parameters μ and Σ . Now we develop a Bayesian treatment by introducing prior distributions over these parameters.

$$p(\mathbf{X}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \frac{1}{(2\pi\sigma^2)^{N/2}} \exp\left\{-\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2\right\}$$

NB: the **likelihood function** $p(\mathbf{X}|\mu)$ is <u>not a probability distribution over μ </u> and is not normalized. if we choose a prior $p(\mu)$ given by a Gaussian, it will be a **conjugate distribution** for this likelihood function because the corresponding posterior will be a product of two exponentials of quadratic functions of μ and hence will also be Gaussian.

$$p(\mu) = \mathcal{N}(\mu|\mu_0, \sigma_0^2)$$
 $p(\mu|\mathbf{X}) \propto p(\mathbf{X}|\mu) \cdot p(\mu)$

In the exercices using completing the square in the exponent, you will be able to show that the posterior distribution is given by:

$$p(\mu|\mathbf{X}) = \mathcal{N}(\mu|\mu_N, \sigma_N^2)$$

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Bayesian Inference for a Gaussian II

The **posterior distribution** is a compromise between the prior mean μ_0 and the maximum likelihood solution μ_{ML} . If the number of observed data points N = 0, then μ_N reduces to the prior mean μ_0 as expected. For $N \to \infty$, the posterior mean μ_N is given by the maximum likelihood solution μ_{ML} .

$$\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \cdot \mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2} \cdot \mu_{\rm ML}$$



$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

the precisions (inverse variance) are additive, so that the precision of the posterior is given by the precision of the prior plus one contribution of the data precision from each of the observed data points.

As we increase the number of observed data points, the precision steadily increases, the posterior gets infinitly peaked around the ML solution.

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III. Gaussian Mixture Models

(& the EM algorithm)



Recap: Probabilistic mixture models

Generative models for unknown, multivariate distributions

Mixture Models

Approximate an arbitrary distribution by a linear combination of a simpler, "well-behaved" distribution

→ Mathematically tractable, compact formulation, allows sampling & inference

The Gaussian Mixture Model (GMM)

- Modeled by a weighted sum of *N* multivariate • **Gaussians** (*N* being sufficiently large)
- Often used because of and "nice" mathematical properties • of Gaussian pdf and central limit theorem (~ data from natural phenomena tend to be Gaussian distributed)
- The Gaussians' **parameters** can be estimated efficiently • using the EM algorithm

Example of a multivariate (2D) Gaussian distribution: samples and contour plot.



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EM (expectation maximization)

The EM algorithm

- Iterative method to learn in the presence of unobserved variables
 - → A typical hidden variable is some sort of group/cluster membership
- Good convergence guarantees (finds local maximum)

A general-purpose, *unsupervised* learning algorithm

Example

- A given dataset is known to be generated by either of 2 Gaussians (with equal probability)
- Only the data is observed
 - → Which Gaussian generated a certain point is unobserved (Z)
 - → The Gaussians' **parameters** θ are unknown
- The means & variances of these Gaussians shall be learned
 - ➔ Needs an estimation of the membership probability of each point tc either Gaussian







The EM algorithm (contd.)

1. Start with a random initial hypothesis Example: **Pretend to know the parameters** μ , σ^2 of the 2 Gaussians E-Step (e.g., pick random values) update variables (e.g., memberships) (e.g., parameters)

2. E-Step: Estimate expected values of unobserved variables, assuming the current hypothesis holds

Example: Compute probabilities p_{ti} that feature vector x_t was produced by Gaussian i

(i.e.,
$$p_{ti} = p(G = i | x_t) = \frac{p(x_t | G = i)p(G = i)}{p(x_t)} \approx p(x_t | G = i) = g_i(x_t, \mu_i, \sigma_i)$$
 with g_i being the

Gaussian pdf

and G the unobserved random variable indicating membership to one of the Gaussians)

- **3.** M-Step: Calculate new Maximum Likelihood (ML) estimate of hypothesis, assuming the expected values from (2) hold **Calculate the** μ_i , σ_i^2 , given the currently assigned membership Example: (i.e., using standard ML estimation: $\mu_i = \frac{1}{T} \sum_{t=1}^T p_{ti} \cdot x_t$, $\sigma_i^2 = \frac{1}{T} \sum_{t=1}^T p_{ti} \cdot (x_t - \mu_i)^2$)
- 4. Repeat with step 2 until convergence Always replacing old estimates with new ones



M-Step

update hypothesis

Example: EM for GMM

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This suggests an **iterative algorithm**, in the case where both Z and θ are unknkown,e.g. for two unknown classes (membership $Z = \{1,2\}$, e.g. male, female) is unknown. Input data is $X = \{x_1, x_2, ..., x_N\}$, weights and heights of N male and female persons.

- 1. First, initialize the model parameters $\theta = \{\mu_k, \sigma_k^2\}$ to some random values, here a Gaussian for each gender k = 1, 2.
- 2. E-Step: Compute the probability of each possible value of $Z = \{1,2\}$, given θ = probability that x_i is member of class z_i

$$z_{ij} = p(Z = j \mid x_i) = \frac{p(x_i \mid Z = j) \cdot p(Z = j)}{\sum_{k=1}^2 p(x_i \mid Z = k)} \approx \frac{p(x = x_i \mid \mu_j)}{\sum_{k=1}^2 p(x = x_i \mid \mu_k)} = \frac{e^{-\frac{1}{2\sigma_j^2}(x_i - \mu_j)}}{\sum_{k=1}^2 e^{-\frac{1}{2\sigma_k^2}(x_i - \mu_k)^2}}$$

3. **M-Step:** Then, use the just-computed values of **Z** to compute a better estimate for the parameters $\theta = \{\mu_n, \sigma^2\}$ $\hat{\mu}_j = \mathbb{E}(\mu_j) = \frac{\sum_{i=1}^N p(Z = j \mid x_i) \cdot x_i}{\sum_{i=1}^N p(Z = j \mid x_i)}$

$$\hat{\mu}_j = \mathbb{E}(\mu_j) = \frac{\sum_{i=1}^N p(Z = j \mid x_i)}{\sum_{i=1}^N p(Z = j \mid x_i)}$$

 $\widehat{\sigma^2}_j = \mathbb{E}(\sigma_j^2) = \frac{1}{N} \sum_{i=1}^N z_{ij} \cdot (x_i - \hat{\mu}_j)^2$



4. Repeat with step 2 until convergence Always replacing old estimates with new ones

General Description: EM Algorithm

Given the statistical model which generates a set *X* of observed data, a set of unobserved latent data *Z* (e.g membership), and a vector of unknown parameters θ , along with a *likelihood function* $L(\theta; X, Z) = p(X, Z|\theta)$ the maximum likelihood estimate (MLE) of the unknown parameters θ is determined by **maximizing** the (log) *marginal likelihood* of the observed data

$$L(\theta; X) = p(X|\theta) = \int_{Z} p(X, Z|\theta) \, dZ \quad \Rightarrow \quad \widehat{\theta}_{ML} = \arg \max_{\theta} \{\log[p(X|\theta)]\}$$

However, the exact calculation of the sum is extremely difficult: The EM algorithm seeks to find the MLE of the marginal likelihood by **iteratively applying these two steps**:

1. Expectation step (E-step)

Calculate the expected value of the log likelihood function, with respect to the conditional distribution of *Z* given *X* under the current estimate of the parameters θ_t

$$Q(\theta | \theta_t) = \mathbb{E}_{Z | X, \theta_t} \left[\log p(X, Z | \theta) \right]$$

2. Maximization step (M-step): Find the parameters that maximize this quantity:

$$\theta_{t+1} = \arg \max_{\theta} Q(\theta | \theta_t)$$

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Motivation: EM for GMM

- If the value of the parameters θ is known, usually the value of the latent variables Z can be found by maximizing the log-likelihood over all possible values of Z, either simply by iterating over Z or using a Viterbi algorithm for hidden Markov models.
- Conversely, if we know the value of the latent variables Z, we can find an estimate of the parameters θ fairly easily, typically by simply grouping the observed data points according to the value of the associated latent variable and averaging the values.

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Applications of the EM algorithm



Applications:

- Unsupervised learning of clusters
- Filling in missing data from a sample set
- Discovering values of latent (i.e. hidden) variables (Z)
- Estimating parameters of HMMs (hidden Markov models)
- Estimating parameters of finite mixtures [mixture models]



3. APPLICATION TO VOICE RECOGNITION

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GMMs as generative models for voice modeling





Reference

• Reynolds, Rose, *«Robust Text-Independent Speaker Identification Using Gaussian Mixture Speaker Models»*, 1995

Key ideas

- Take the estimated probability density function (pdf) p(x|h) of a speaker's D-dim. training vectors x as a model of his voice
- Model the pdf as a weighted sum of M
 D-dimensional Gaussians
 (e.g., M = 32, D = 16)



GMM with 3 mixtures in 1 dimension. Solid line shows GMM density, dashed lines show constituting Gaussian densities.

Speaker Id # Diarization (a.k.a. tracking, clustering): Segment an audio-stream by voice identity

(who spoke when, no prior knowledge of any kind)

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The task of speaker recognition

$(\rightarrow$ see appendix for an introduction to speech processing)

Speaker recognition



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GMM rationale

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Hybrid solution between non-parametric clusters

(vector quantization) and compact smoothing (single Gaussian):

Smooth approximation of arbitrary densities

Implicit clustering into broad phonetic classes



Fig. 3. Comparison of distribution modeling: (a) Histogram of a single cepstral coefficient from a 25 second utterance by a male speaker; (b) maximum likelihood unimodal Gaussian model; (c) GMM and its 10 underlying component densities; (d) histogram of the data assigned to the VQ centroid locations of a 10-element codebook.

GMM comparison with other techniques; from [Reynolds and Rose, 1995].

Mathematical formulation of the GMM

Using diagonal covariance (\rightarrow see appendix for reasons)

Notation

- h: model (GMM) ٠
- w: weight (scalar) ٠
- μ : **mean** vector ٠
- σ^2 : variance vector (the diagonal of the ٠ covariance matrix)
- g_i : **Gaussian pdf** of i^{th} (out of *M*) mixtures •
- x: feature vector •
- *D*: dimensionality of *x*, μ , σ^2 ٠
- p: density/likelihood of a feature • vector given the model





- **Model** consists of: $h = \{w_i, \mu_i, \sigma_i^2\}$
 - \rightarrow subject to i = 1..M and $\sum_{i=1}^{M} w_i = 1$

Condition on weights to sum up to 1

The multimodal Gaussian with diagonal covariance computes as

$$g_{i}(x,\mu_{i},\sigma_{i}^{2}) = \prod_{d=1}^{D} \frac{1}{\sqrt{2\pi\sigma_{id}^{2}}} \cdot e^{-\frac{(x-\mu_{id})^{2}}{2\sigma_{id}^{2}}}$$

duct over the assumedly
t marginals (dimensions) The univariate Gaussian pdf

Model evaluation:

$$p(x|h) = \sum_{i=1}^{M} w_i \cdot g_i(x, \mu_i, \Sigma_i)$$

Formulae

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GMM training via the EM algorithm



 \rightarrow see appendix

to it

Maximum likelihood training

Initialize model $h = \{w_i, \mu_i, \sigma_i^2\}$ using data $X = \{x_1 \dots x_T\}$

 \rightarrow Instead of pure random initialization, find better values via subsequent clustering (e.g., with k-means)

E-Step:

The (properly normalized) probability $p_{ti}(i|x_t,h) = \frac{w_i \cdot g_i(x_t,\mu_i,I_D \cdot \sigma_i^2)}{\sum_{i=1}^M w_i \cdot g_i(x_t,\mu_i,I_D \cdot \sigma_i^2)} \stackrel{\text{of } x_t \text{ being issued by mixture } i}{\sum_{i=1}^M w_i \cdot g_i(x_t,\mu_i,I_D \cdot \sigma_i^2)}$

M-Step:

$$w_{i} = \frac{1}{T} \sum_{t=1}^{T} p_{ti}(i|x_{t}, h)$$
Mixture *i*'s weight is just the mean probability of all training vectors being assigned to it
$$\mu_{i} = \frac{1}{T \cdot w_{i}} \sum_{t=1}^{T} p_{ti}(i|x_{t}, h) \cdot x_{t}$$

$$\sigma_{i}^{2} = \left(\frac{1}{T \cdot w_{i}} \sum_{t=1}^{T} p_{ti}(i|x_{t}, h) \cdot x_{t}^{2}\right) - \mu_{i}^{2}$$

Alternative: Training via maximum a posteriori (MAP) adaptation (i.e. uses a priori knowledge) → see Reynolds, Quatieri, Dunn, «Speaker Verification Using Adapted Gaussian Mixture Models», 2000

Doing speaker identification

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Finding the speaker *s* of a new utterance, given a set of trained speaker models

- Utterance represented by its feature vector sequence $X = \{x_1 ... x_T\}$
- Speakers models given by {*h*₁..*h*_S}



Model comparison via generalized likelihood ration (GLR)

Absolute likelihood values are not meaningful, but their ratios are

→ To decide if given models h_1 , h_2 trained on utterances X_1 , X_2 are actually of the same speaker, threshold GLR **distance measure**:

$$GLR(h_1, h_2) = \log\left(\frac{p(X_1|h_1) \cdot p(X_2|h_2)}{p(X_1 \cup X_2|h_{1\cup 2})}\right)$$

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What GMMs do not capture



Re-synthesizing speech from intermediate stages of the speaker modeling pipeline Original utterance Resynthesized feature vectors (MFCCs) Resynthesized MFCCs from GMM Implication Temporal context isn't modeled by GMMs

More on temporal context modeling:

Friedland, Vinyals, Huang, Müller, *«Prosodic and other Long-Term Features for Speaker Diarization»*, 2009 Stadelmann, Freisleben, *«Unfolding Speaker Clustering Potential – A Biomimetic Approach»*, 2009 Lukic, Vogt, Dürr, Stadelmann, *«Speaker Identification and*

Clustering using Convolutional Neural Networks», 2016

Review

- Understanding uncertain events as random variables gives us a potent arsenal of tools for modeling: E.g., probability density function (pdf) of a random variable tells us everything there is to know about this function
- Thus, estimating the pdf is a rewarding target for (unsupervised) learning
- **Bayes' theorem** is used to turn priors (i.e., prior knowledge) into posteriors (i.e., taking all evidence & priors into account)
- Speaker recognition comes in the flavors of verification, identification or diarization
- The classic approach is **MFCC** features and **GMM** models
- Optimal parameters are best found using **best practices** (→ see appendix)
- EM training iterates between estimating updates values of hidden variables (based on assumed parameters of the sought distribution – E-step), and updating these parameters (based on these new estimates – M-step)

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GMM best practices

- Use log-likelihoods instead of likelihoods
 - → Likelihoods become so small that one ends up with numerical instabilities otherwise
- Use a diagonal covariance matrix
 - → Simpler/faster training, same/better results due to more compact model (with more mixtures)
- Use a variance limit and beware of curse of dimensionality
 - ➔ Prohibit artifacts through underestimation of components
- Use 16-32 mixtures and a minimum of 30s of speech (ML)
- Adapt only means from 512-1024 mixtures per gender (MAP)

Score only with top-scoring mixtures

- Find optimal number of mixtures for data via brute force and BIC
- Compare models via

Score-wise (more precise): Generalized Likelihood Ratio (GLR)

Parameter-wise (faster): Earth Mover's Distance (EMD) or this paper:

Beigi, Maes, Sorensen, *«A distance measure between collections of distributions and its application to speaker recognition»*, 1998

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