MSPR 5: Probabilities

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This lecture is based on presentations made in my course 'Advanced Topics in in Music Technology' at Music Technology Group, Universitat Pompeu Fabra between 2007-2011, Barcelona, especially the ones by Stefan Kersten and Srikanth Cherla, closely following

Andrew Moore's machine learning tutorial lectures: Gaussians, Gaussian Mixture Models, http://www.autonlab.org/tutorials/

Christopher Bishop: Pattern Recognition and Machine Learning:
 Chapter 1 (Introduction) 1.2.3 (The Gaussian Distribution) p. 24 27, 2.3 (The Gaussian Distribution) p. 78, 84 bottom - 85 top.

Outline

1 The Gaussian distribution

2 Multi-variate Gaussian Distributions

Applications of Probability Density Estimation

- Of few customers we know the income. Do we have more customers with income around 300 000 DKK or 1 000 000 DKK?
- Estimation of crime rates in different areas before buying a house there
- Updating information in computer vision (on-line object tracking) as new data becomes available



Stormrisks in the US (Image)

http://www.pmarshwx.com/blog/2011/02/03/ aotw-storm-prediction-center-moderate-high-risks/ http://www.cs.utah.edu/~lifeifei/papers/kernelsigmod13.pdf

Random Variables

- Random variable Part of the world whose exact value is uncertain
- Boolean variables {true, false}, e.g. Crown Prince Frederik will win the next KMD Ironman Copenhagen
- Discrete variables take a value from a countable domain, e.g. this piece's genre is one of {jazz, hiphop, country}
- Continuous variables take a value from a continuous domain, e.g. this piece's tempo is close to 94.5 bpm

 From the Kolmogorov's axioms it follows (a simple foundation of probability theory)

$$0 \le P(A) \le 1$$

 $P(\text{true}) = 1$
 $P(\text{false}) = 0$
 $P(A \lor B) = P(A) + P(B) - P(A \land B)$

- The *joint distribution* denotes the probabilities of all combinations of two or more random variables
- Conditional probability

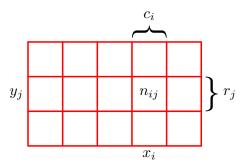
$$P(Y|X) = \frac{P(Y,X)}{P(X)}$$

Multivariate Gaussians

■ Sum rule

$$P(X) = \sum_{Y} P(X, Y)$$

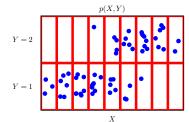
Marginalization over the variable Y given the joint probability P(X, Y)

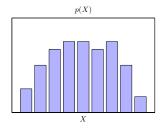


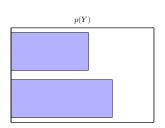
■ Product rule

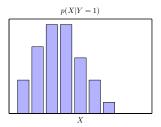
$$P(X, Y) = P(Y|X)P(X)$$

Q: Calculate joint, marginal, and conditional probabilites from a co-occurrence table.









For the Iris data set, the histogram as an estimate for the conditional Probability of petal width under the condition that we have iris species virginica:

P(feat='petal width' — species='virginica'):

```
Petal Width (Iris): Marginal and Conditional Probability

Marg. Pob.: P(test-petal width)

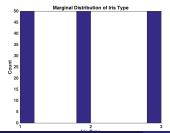
Cond Prob.: P(test-petal width) | apacies-virginica)
```

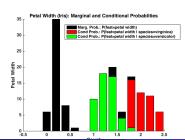
```
adata = textscan(fid, '%f%f%f%f%s', 'delimiter',',');
X=[adata{1} adata{2} adata{3} adata{4}];
idx_virginica=find(strcmp(species, 'Iris-virginica')==1);
idx_versicolor=find(strcmp(species, 'Iris-versicolor')==1);
[hvir bvir]=hist(X(idx_virginica,4),(0:0.2: 2.5));
[hmarg bmarg]=hist(X(:,4),(0:0.2: 2.5));
bar(bmarg,hmarg,'k'); hold on; bar(bvir,hvir,'r');
```

Class Assignment

- For the Iris data set, the histogram as an estimate for the conditional Probability of petal width under the condition that we have iris species versicolor:

 P(petal width | species='versicolor').
- By a histogram, give the marginal probability of the iris type.





Q: Derive Bayes rule from the sum and the product rule.

Bayes' rule is derived from the product rule:

$$P(X, Y) = P(Y, X)$$

$$P(X|Y)P(Y) = P(Y|X)P(X)$$

■ Bayes' rule then becomes

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

■ Bayes rule can be stated as

posterior \propto likelihood \times prior

Independence

- We say that *X* is independent of *Y*, if knowing *Y* doesn't influence our degree of belief in *X*
- P(X|Y) = P(X)

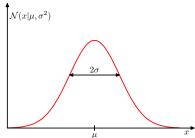
Multivariate Gaussians

Normal distribution of a single variable x (univariate)

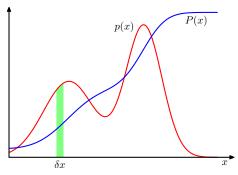
$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{-\frac{(x-\mu)^2}{2\sigma^2}\}$$

- *Mean* μ and *Variance* σ^2
- Desirable properties for a PDF

Positive
$$\mathcal{N}(x|\mu,\sigma^2) > 0$$



Normalized
$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx = 1$$



The probability of x is given by probability distribution p(x).

The probability of $x \in (-\infty, z)$ is given by the cumulative distribution function (CDF) P(x) Matlab y = cdf(pd,x) Consider a probability in the range δx E.g. that a normally distributed random variable falls within $\pm \sigma$:

Result: Probability: 0.6827

Class Assignment

Use the cumulative distribution function in Matlab to calculate what the probability is that a normally distributed random variable falls farther away than 2σ from the mean μ . How does this value relate to the significance level α of a statistical test?

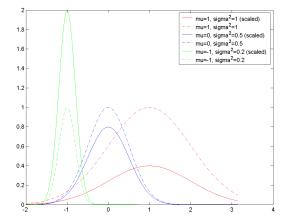
Use the cumulative distribution function in Matlab to calculate what the probability is that a normally distributed random variable falls farther away than 2 σ from the mean μ . How does this value relate to the significance level α of a statistical test?

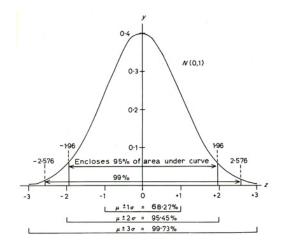
```
mu = 0; sigma = 2; pd = makedist('Normal', mu, sigma); x = [-2*sigma\ 2*sigma\ ]; y = cdf(pd,x) y(1) + 1-y(2) % or 2*y(1)
```

Result: 0.0455

Significance level $\alpha=0.05$ gives an upper limit of the probability that, when rejecting the Nullhypothesis it may still be true.

Examples of Gaussians with Different Means / Variances





Data: I observations of just one feature (1-D, just a number=scalar):

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_I \end{bmatrix}$$
. Fit a 1-dimensional Gaussian to the data histogram by finding

the right estimates \bar{x} for mean μ and s^2 for σ^2 :

$$\mathcal{N}(x|\bar{x},s^2) = \frac{1}{\sqrt{2\pi s^2}} e^{\frac{(x-\bar{x})^2}{2s^2}} \text{ (Matlab: n = pdf('norm', x, xm, sqrt(s2));)}$$
$$\bar{x} = \frac{1}{I} \sum_{i=1}^{I} x_i \text{ (sample mean, Matlab: mean(x))}$$

$$s^2 = \frac{1}{I-1} \sum_{i=1}^{I} (x_i - \bar{x})^2$$
 (sample variance, Matlab: var(x))

Class Assignment

Load the data gauss.mat and fit a Gaussian to the data AO_{-} tr How good is the fit? Use Matlab functions [h p]=hist(x), bar(p,h,'b'). Plot the pdf in the same plot. Normalize the height of the histogram bars h by dividing it with the distance b(2) - b(1) between two bar positions and the number of components in the data vector of that class.

Solution

```
M0=mean(A0_tr); S0=var(A0_tr);
tr_no= size(A0_tr,1);
x=-10:0.1:10;
h=figure; n0=pdf('norm',x,M0,sqrt(S0));
[h0 p0]=hist(A0_tr);
bar(p0,h0/size(A0_tr,1)/(p0(2)-p0(1)),'b'); hold on; plot(x, n0,'b')
% Plot gaussians
```

■ Covariance between feature j (j-th data matrix column) and k (k-th data matrix column):

$$cov(\mathbf{X}_{[:,j]},\mathbf{X}_{[:,k]}) = \frac{1}{I-1} \sum_{i=1}^{I} (x_{ij} - \bar{\mathbf{X}}_{[:,j]})(x_{ik} - \bar{\mathbf{X}}_{[:,k]})$$

■ $J \times J$ covariance matrix:

$$\boldsymbol{\Sigma} = \begin{bmatrix} \operatorname{var}(\boldsymbol{\mathsf{X}}_{[:,1]}) & \operatorname{cov}(\boldsymbol{\mathsf{X}}_{[:,1]}, \boldsymbol{\mathsf{X}}_{[:,2]}) & \dots & \operatorname{cov}(\boldsymbol{\mathsf{X}}_{[:,1]}, \boldsymbol{\mathsf{X}}_{[:,J]}) \\ \operatorname{cov}(\boldsymbol{\mathsf{X}}_{[:,2]}, \boldsymbol{\mathsf{X}}_{[:,1]}) & \operatorname{var}(\boldsymbol{\mathsf{X}}_{[:,2]}) & \dots & \operatorname{cov}(\boldsymbol{\mathsf{X}}_{[:,2]}, \boldsymbol{\mathsf{X}}_{[:,J]}) \\ \vdots & \vdots & \ddots & \vdots \\ \operatorname{cov}(\boldsymbol{\mathsf{X}}_{[:,J]}, \boldsymbol{\mathsf{X}}_{[:,1]}) & \operatorname{cov}(\boldsymbol{\mathsf{X}}_{[:,J]}, \boldsymbol{\mathsf{X}}_{[:,2]}) & \dots & \operatorname{var}(\boldsymbol{\mathsf{X}}_{[:,J]}) \end{bmatrix}$$

The diagonal elements are the variances of each features $1, \dots, J$ Matrix is symmetric

Covariance

I Sample covariance Matrix **C** of all features (columns of centirized data matrix \mathbf{X}_c):

$$\mathbf{C} = \frac{1}{I - 1} \mathbf{X}_c^T \mathbf{X}_c$$

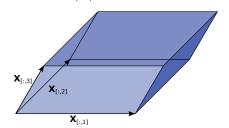
2 Matlab: C=Xc'*Xc/(I-1) or C=cov(X)

Determinant

$$\mathbf{X} := \left(\begin{array}{ccc} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{array}\right)$$

The determinant det assigns a number to square matrix

$$X : c = det(X)$$
, Matlab: $c = det(X)$.



The volumn V of the object (parallepiped) that is sided by the parallelograms defined by the column vectors
X[:,1], X[:,2], X[:,3] of the matrix

X is the absolut value of the determinant of X: Y = |dot(X)|

$$V=|det(\mathbf{X})|$$
.

If det(X) ≠ 0, X is invertible, for det(X) = 0, X is not invertible.

Determinant

Class Assignment

Calculate the determinant of the following matrices and invert them if possible and show that you found the inverse. What was the definition of invertibility for a matrix?

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, A_2 = \begin{bmatrix} 1 & 2 \\ -1 & -2 \end{bmatrix}, A_3 = \begin{bmatrix} 1 & -0.5 \\ -0.5 & 1 \end{bmatrix}$$

```
A1=[1 0; 0 1]; A2=[1 2; -1 -2]; A3=[1 -0.5; -0.5 1];

det(A1); A1=inv(A1); A1*A11 % det(A1)=1

det(A2); inv(A2) % det(A1)=0 (A2 NOT INVERTIBLE!)

det(A3); A3I=inv(A3); A3*A31 % det(A1)=0.75
```

Multi-variate Gaussians

 The multivariate Gaussian distribution for a J-dimensional variable x is given by

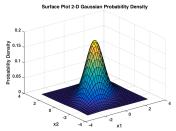
$$\mathcal{N}(\mathbf{x}|\mu, \mathbf{\Sigma}) = rac{1}{2\pi^{J/2}\det\mathbf{\Sigma}^{1/2}}e^{-rac{1}{2}(\mathbf{x}-\mu)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)}$$

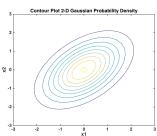
- Defining parameters: μ and Σ
- Mean and Covariance
 - Mean (vector) = μ (J dimensional)
 - Covariance (matrix) = Σ ($J \times J$)
 - \blacksquare det Σ denotes the determinant of Σ

Example Multivariate Gaussian

```
0.5
x_1/x_2 axis
correlated
```

 $\Sigma_1 =$





```
mu = [0 \ 0]; Sigma1 = [1 \ .5; .5 \ 1];
 |x_1| = -3:.2:3; \quad |x_2| = -3:.2:3; \quad |x_1| = |x_2| = |x_2| = |x_1| = |x_2| = |x_2| = |x_1| = |x_2| = |x_2| = |x_1| = |x_1| = |x_2| = |x_1| = |x_2| = |x_1| 
                 F = mvnpdf([X1(:) X2(:)], mu, Sigma1);
_{4}|F = reshape(F, length(x2), length(x1));
                    surf(x1,x2,F);
 6 figure; contour(X1, X2, F)
```

Class Assignment

For the following covariance matrices predict the shape of the normal distribution using that covariance matrix and then plot the distribution as a verification:

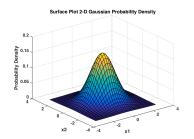
$$oldsymbol{\Sigma}_2 = oldsymbol{\mathsf{I}} = egin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ oldsymbol{\Sigma}_5 = egin{bmatrix} 1 & -0.5 \\ -0.5 & 2 \end{bmatrix} \qquad oldsymbol{\Sigma}_3 = egin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix}$$

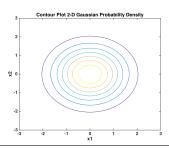
$$\pmb{\Sigma}_3 = \begin{bmatrix} 1 & -0.8 \\ -0.8 & 1 \end{bmatrix}$$

$$\mathbf{\Sigma}_4 = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

$$\Sigma_2 = I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

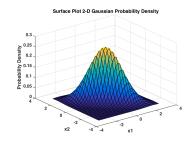
 x_1/x_2 -axis
uncorrelated

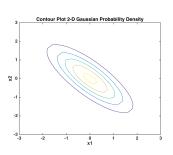




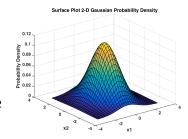
```
mu = [0 0]; Sigma2 = [1 0; 0 1];
x1 = -3:.2:3; x2 = -3:.2:3; [X1,X2] = meshgrid(x1,x2);
F = mvnpdf([X1(:) X2(:)],mu,Sigma1);
F = reshape(F,length(x2),length(x1));
surf(x1,x2,F);
figure; contour(X1,X2,F)
```

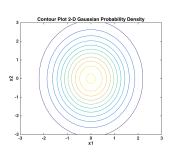
$$egin{aligned} oldsymbol{\Sigma}_3 = \ 1 & -0.8 \ -0.8 & 1 \ x_1/x_2 ext{-axis} \ ext{negatively} \ ext{correlated} \end{aligned}$$



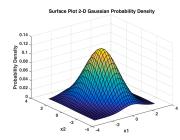


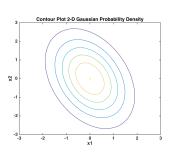
$$\mathbf{\Sigma}_4 = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$
 x_1/x_2 -axis
uncorrelated,
stretched in x_2
direction





$$oldsymbol{\Sigma}_5 = \left[egin{array}{ccc} 1 & -0.5 \ -0.5 & 2 \end{array}
ight] \ x_1/x_2 ext{-axis} \ ext{negatively} \ ext{correlated} \ ext{stretched in } x_2 \ ext{direction} \end{array}$$





Fitting a Gaussian to Multdimensional Data

Data: I observations of J features:

$$\mathbf{X} := \left(\begin{array}{cccccc} x_{11} & x_{12} & \cdots & x_{1j} & \cdots & x_{1J} \\ x_{21} & x_{22} & \cdots & x_{2j} & \cdots & x_{2J} \\ x_{31} & x_{32} & \cdots & x_{3j} & \cdots & x_{3J} \\ \vdots & \vdots & \cdots & \vdots & \cdots & \vdots \\ x_{i1} & x_{i2} & \cdots & x_{ij} & \cdots & x_{iJ} \\ & & \cdots & & \cdots & \\ x_{l1} & x_{l2} & \cdots & x_{lj} & \cdots & x_{lJ} \end{array} \right)$$

Fit a *J*-dimensional Gaussian to the data by finding the right estimates for the mean vector μ for covariance matrix σ : $\mathcal{N}(\mathbf{x}|\mu, \mathbf{\Sigma})$

$$= \frac{1}{2\pi^{J/2}|\boldsymbol{\Sigma}|^{1/2}}e^{-\frac{1}{2}(\mathbf{x}-\mu)^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\mu)}$$

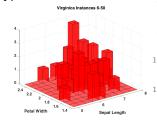
Sample mean vector $\bar{\mathbf{x}}$ estimates true mean vector μ (Matlab: mean(X)):

$$\bar{\mathbf{x}} = \frac{1}{I} \underbrace{(1, 1 \dots, 1)}_{I \times I} \mathbf{X}$$

Sample covariance matrix \mathbf{C} estimates true covariance matrix $\mathbf{\Sigma}$ (Matlab: cov(X))

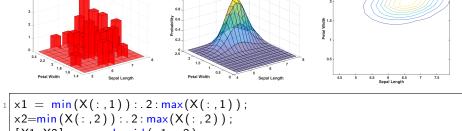
$$C = \frac{1}{I - 1} \mathbf{X}' \mathbf{X}$$

3-D Histogram of components 'Sepal Length' and 'Petal Width' only for the Virginica Iris type



```
fid = fopen([data_path 'iris.data']);
adata = textscan(fid, '%f%f%f%f%s',
    delimiter',',');
fclose (fid);
X=[adata{1} adata{4}];
species=adata {5}:
idx_virginica=find(...
  strcmp(species, 'Iris - virginica')==1);
idx_virginica_tr=idx_virginica(6:50);
mean_virginica=...
  mean(X(idx_virginica_tr ,:));
sig_virginica=cov(X(idx_virginica_tr,:))
hist3(X(idx_virginica_tr ,:),...
  'FaceAlpha',.65, 'FaceColor', 'red');
```

Fitting Gaussian with Full Cov. Matrix to 3-D Histogram



```
x1 = min(X(:,1)):.2:max(X(:,1));
x2=min(X(:,2)):.2:max(X(:,2));

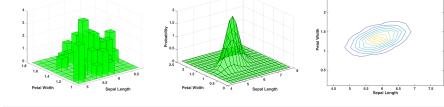
[X1,X2] = meshgrid(x1,x2);
F_virginica = ...
mvnpdf([X1(:) X2(:)], mean_virginica, sig_virginica);
F_virginica = reshape(F_virginica, length(x2), length(x1));
surf(x1,x2,F_virginica, 'FaceAlpha',.5);
contour(X1,X2,F_virginica);
```

Virginica Instances 6-50

Class Assignment

Plot 3-D histogram for instances 5-50 of features 'Sepal Length' and 'Petal Width' the versicolor iris species. Fit a 2-D Gaussian to the histogram and do a surface and contour plot it.

Plot 3-D histogram for instances 5-50 of features 'Sepal Length' and 'Petal Width' the versicolor iris species. Fit a 2-D Gaussian to the histogram and do a surface and contour plot it.



```
...
hist3(X(idx_versicolor_tr ,:), 'FaceAlpha', .65, 'FaceColor','
green');
surf(x1,x2,F_versicolor, 'FaceAlpha', .5, 'FaceColor', 'green');
```

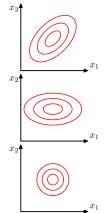
Parameters to Estimate

- In its most general form, the multi-variate Gaussian of *J* dimensions has
 - J(J+1)/2 parameters for the covariance matrix
 - J parameters for the mean vector.
- $lue{}$ The number of parameters increases quadratically with J and hence poses a problem both in parameter estimation and matrix inversion.

Reduction of Parmeters to be Estimated

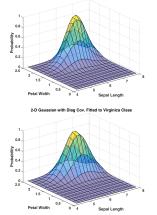
There are two ways of simplifying this problem

- Assume diagonal covariance matrix $(2 \times J)$ parameters.
- Assume equal covariance $\Sigma = \sigma^2 \mathbf{I}$ ((J+1) parameters).

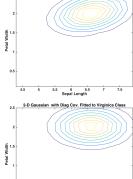


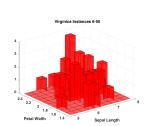
However, these simplifications also limit the modeling capability of the Gaussian

Fit of the Virginica Iris Class with a Gaussian with Diagonal Covariance Matrix



2-D Gaussian Fitted to 2 Features in Virginica Class





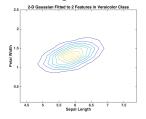
Class Assignment

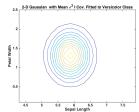
Outline

Fit a Gaussian with covariance matrix of type $\sigma=\sigma^2\mathbf{I}$ to 3-D histogram of features 'Sepal Length' and 'Petal Width' of the versicolor class considering instance 6-50. For σ^2 take the average of the variances for 'Sepal Length' and 'Petal Width' .

Multivariate Gaussians

Fit a Gaussian with covariance matrix of type $\sigma = \sigma^2 \mathbf{I}$ to 3-D histogram of features 'Sepal Length' and 'Petal Width' of the versicolor class considering instance 6-50.



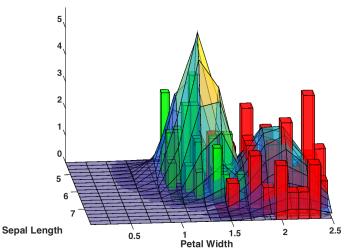


sig_versicolor=mean(diag(sig_versicolor))*diag(ones(2,1));

Gaussian Fit for Predicting the Iris Type Based on Sepal Length and Petal Width only

- We had fitted two Gaussians $\mathcal{N}(\mathbf{x}|\mu_{\textit{virg}}, \mathbf{\Sigma}_{\textit{virg}})\mathcal{N}(\mathbf{x}|\mu_{\textit{vers}}, \mathbf{\Sigma}_{\textit{vers}})$ to the points 6-50 of Virginica and Versicolor Iris data ('Sepal Length' and 'Petal Width').
- The first 5 points of Virginica and Versicolor iris data ('Sepal Length' and 'Petal Width') have not been used for the fitting.
- Let us use the fitted Gaussians, to determine whether these points belong to Virginica or Versicolor according to the rule: If for a point \mathbf{x} $\mathcal{N}(\mathbf{x}|\mu_{\textit{virg}}, \mathbf{\Sigma}_{\textit{virg}}) > \mathcal{N}(\mathbf{x}|\mu_{\textit{vers}}, \mathbf{\Sigma}_{\textit{vers}})$ we predict its class to be Virginica, otherwise Versicolor.
- let us count the wrong predictions.

Classification Versicolor (Green) vs. Virginica (Red)



```
sig_virginica=cov(X(idx_virginica_tr ,:));
 sig_versicolor=cov(X(idx_versicolor_tr ,:));
3 idx_virginica_tst=idx_virginica(1:5);
 idx_versicolor_tst=idx_versicolor(1:5);
5 F_versicolor_tst = mvnpdf(X([idx_virginica_tst;
     idx_versicolor_tst],:),...
       mean_versicolor, sig_versicolor);
7 F_virginica_tst = mvnpdf(X([idx_virginica_tst;
     idx_versicolor_tst],:),...
       mean_virginica , sig_virginica );
9 [F_virginica_tst'; F_versicolor_tst']
 %ans =
0.11 \% 0.18 0.43 0.69 0.66 0.69 0.03 0.16 0.09 0.02 0.15
 \% 0.00 0.00 0.00 0.10 0.00 0.08 0.98 0.19 1.30 0.80
```

Perfect Prediction!

Class Assignment

Outline

- Fit two Gaussians $\mathcal{N}(\mathbf{x}|\mu_{virg}, \mathbf{\Sigma}_{virg})\mathcal{N}(\mathbf{x}|\mu_{vers}, \mathbf{\Sigma}_{vers})$ using a covariance matrix of type $\sigma^2\mathbf{I}$ with σ^2 being the mean variance for 'Sepal Length' and 'Petal Width'. Use to the features 'Sepal Length' and 'Petal Width' of instances 6-50 of the Virginica and Versicolor Iris data.
- Use the fitted Gaussians, to determine whether these points belong to Virginica or Versicolor according to the rule: If for a point \mathbf{x} $\mathcal{N}(\mathbf{x}|\mu_{\text{Virg}}, \mathbf{\Sigma}_{\text{Virg}}) > \mathcal{N}(\mathbf{x}|\mu_{\text{Vers}}, \mathbf{\Sigma}_{\text{Vers}})$ we predict its class to be Virginica, otherwise Versicolor.
- Count the wrong predictions for the first 5 points of Virginica and Versicolor iris data.

Solution

```
sig_virginica=mean(diag(sig_virginica))*diag(ones(2,1));
sig_versicolor=mean(diag(sig_versicolor))*diag(ones(2,1));
F_versicolor_tst = mvnpdf(X([idx_virginica_tst;
    idx_versicolor_tst],:), mean_versicolor, sig_versicolor);
F_virginica_tst = mvnpdf(X([idx_virginica_tst;
    idx_versicolor_tst],:), mean_virginica, sig_virginica);
[F_virginica_tst'; F_versicolor_tst']
```

```
ans =
0.33 0.17 0.39 0.48 0.58 0.22 0.34 0.31 0.02 0.36
0.00 0.32 0.00 0.25 0.02 0.01 0.38 0.02 0.69 0.25
```

4 Errors!