Intelligent Systems: Reasoning and Recognition

James L. Crowley

ENSIMAG 2 / MoSIG M1 Second Semester 2011/2012

Lesson 16 6 april 2012

Multivariate Normal Density Functions

Notation 2

Bayesian Classification (Reminder) 3

The Normal (Gaussian) Density Function 4

The Univariate Normal Density Function 4

The Multivariate Normal Density Function 4

The Mahalanobis Distance 6

Linear Transforms of the Normal Multivariate Density 7

Linear Algebraic Form for Moment Calculation 8

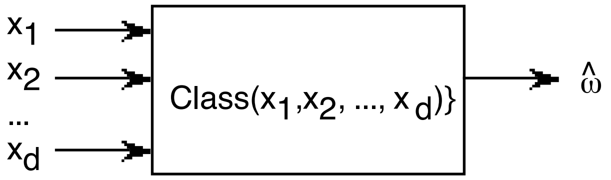
Sources Bibliographiques :
"Pattern Recognition and Machine Learning", C. M. Bishop, Springer Verlag, 2006.
"Pattern Recognition and Scene Analysis", R. E. Duda and P. E. Hart, Wiley, 1973.

Notation

x	a variable
X	a random variable (unpredictable value)
N	The number of possible values for X (Can be infinite).
$\vec{x}$	A vector of D variables.
$\vec{X}$	A vector of D random variables.
D	The number of dimensions for the vector $\vec{x}$ or $\vec{X}$
E	An observation. An event.
C_k	The class k
k	Class index
K	Total number of classes
ω_k	The statement (assertion) that $E \in C_k$
$p(\omega_k) = p(E \in C_k)$	Probability that the observation E is a member of the class k. Note that $p(\omega_k)$ is lower case.
M_k	Number of examples for the class k. (think M = Mass)
M	Total number of examples. $M = \sum_{k=1}^{K} M_k$
$\{X_m^k\}$	A set of M_k examples for the class k. $\{X_m\} = \bigcup_{k=1,K} \{X_m^k\}$
$P(X)$	Probability density function for X
$P(\vec{X})$	Probability density function for $\vec{X}$
$P(\vec{X} \mid \omega_k)$	Probability density for $\vec{X}$ the class k. $\omega_k = E \in C_k$.
h(n)	A histogram of random values for the feature n.
$h_k(n)$	A histogram of random values for the feature n for the class k. $h(x) = \sum_{k=1}^{K} h_k(x)$
Q	Number of cells in $h(n)$. $Q = N^D$

Bayesian Classification (Reminder)

Our problem is to build a box that maps a set of features $\vec{X}$ from an Observation, E into a class C_k from a set of K possible Classes.



Let ω_k be the proposition that the event belongs to class k: $\omega_k = E \in C_k$

ω_k Proposition that event E $\in$ the class k

In order to minimize the number of mistakes, we will maximize the probability that $\omega_k \equiv E \in C_k$

$$\hat{\omega}_k = \arg-\max_k\left\{\Pr(\omega_k \mid \vec{X})\right\}$$

We will call on two tools for this:

1) Baye's Rule :

$$p(\omega_k \mid \vec{X}) = \frac{P(\vec{X} \mid \omega_k)p(\omega_k)}{P(\vec{X})}$$

2) Normal Density Functions

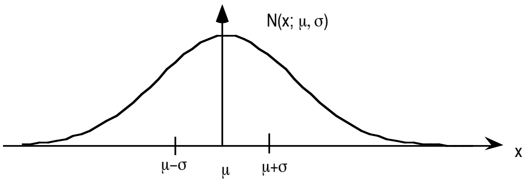
$$P(\vec{X} \mid \omega_k) = \frac{1}{(2\pi)^{\frac{D}{2}} \det(\Sigma_k)^{\frac{1}{2}}} e^{-\frac{1}{2}(\vec{X}-\vec{\mu}_k)^T \Sigma_k^{-1} (\vec{X}-\vec{\mu}_k)}$$

This week we concentrate on Normal Density Functions.

The Normal (Gaussian) Density Function

The Univariate Normal Density Function

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



The parameters of $\mathcal{N}(x;\, \mu,\, \sigma)$ are the first and second moments.

The Multivariate Normal Density Function

$$p(\vec{X}) = \mathcal{N}(\vec{X} \mid \vec{\mu},\, \Sigma) = \frac{1}{(2\pi)^{\frac{D}{2}} \det(\Sigma)^{\frac{1}{2}}} e^{-\frac{1}{2}(\vec{X}-\vec{\mu})^T \Sigma^{-1} (\vec{X}-\vec{\mu})}$$

In most practical cases, an observation is described by D features.
In this case a training set $\{\vec{X}_m\}$ an be used to calculate an average feature $\vec{\mu}$

$$\vec{\mu} = E\{\vec{X}\} = \frac{1}{M}\sum_{m=1}^{M} \vec{X} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \ldots \\ \mu_D \end{pmatrix} = \begin{pmatrix} E\{X_1\} \\ E\{X_2\} \\ \ldots \\ E\{X_D\} \end{pmatrix}$$

For D dimensions, the second moment is a co-variance matrix composed of D^2 terms:

$$\sigma^2_{ij} = E\{(X_i - \mu_i)(X_j - \mu_j)\} = \frac{1}{M}\sum_{m=1}^{M}(X_{im} - \mu_i)(X_{jm} - \mu_j)$$

This is often written

$$\Sigma = E\{(\vec{X} - E\{\vec{X}\})(\vec{X} - E\{\vec{X}\})^T\}$$

and gives

$$\Sigma = \begin{pmatrix} \sigma_{11}^2 & \sigma_{12}^2 & ... & \sigma_{1D}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & ... & \sigma_{2D}^2 \\ ... & ... & ... & ... \\ \sigma_{D1}^2 & \sigma_{D2}^2 & ... & \sigma_{DD}^2 \end{pmatrix}$$

The term $(2\pi)^{\frac{D}{2}}$ $\det(\mathbf{\Sigma})^{\frac{1}{2}}$ is a normalization factor.

$$\int\int ...\int e^{-\frac{1}{2}(\vec{X}-\vec{\mu})^T\,\Sigma^{-1}(\vec{X}-\vec{\mu})} dx_1 dx_2 ... dx_D = (2\pi)^{\frac{D}{2}} \det(\Sigma\ )^{\frac{1}{2}}$$

The determinant, $\det(\mathbf{\Sigma})$ is an operation that gives the volume of $\mathbf{\Sigma}$.

for D=2 $\det\begin{pmatrix} a & b \\ c & d \end{pmatrix} = a\cdot b – c\cdot d$

for D=3

$$\det\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = a\cdot\det\begin{pmatrix} e & f \\ h & i \end{pmatrix} + b\cdot\det\begin{pmatrix} f & d \\ i & g \end{pmatrix} + c\cdot\det\begin{pmatrix} d & e \\ g & h \end{pmatrix}$$

$$= a(ei-fh)+ b(fg-id)+ c(dh-eg)$$

for D > 3 this continues recursively.

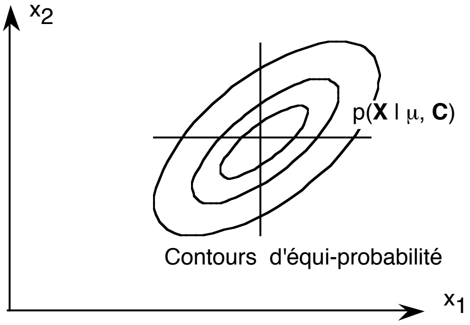
The Mahalanobis Distance

The exponent is positive and quadratic (2nd order). This value is known as the "Distance of Mahalanobis".

$$d(\vec{X};\vec{\mu},\Sigma)^2 = -\frac{1}{2}(\vec{X}-\vec{\mu})^T\,\Sigma^{-1}(\vec{X}-\vec{\mu})$$

This is a distance normalized by the covariance. In this case, the covariance is said to provide the distance metric. This is very useful when the components of X have different units.

The result can be visualized by looking at the equi-probably contours.



If x_i and x_j are statistically independent, then $\sigma_{ij}^2 = 0$
For positive values of σ_{ij}^2, x_i and x_j vary together.
For negative values of σ_{ij}^2, x_i and x_j vary in opposite directions.

For example, consider features x_1 = height *(m)* and x_2 = weight *(kg)*

In most people height and weight vary together and so σ_{12}^2 would be positive

Linear Transforms of the Normal Multivariate Density

The Normal (Gaussian) function is a defined only by its moments.
It is thus invariant to transformations of its moments, that is affine transformations.
The affine transformations include rotation, translation, scale changes and other linear transformations.

For example consider a cosine vector $\vec{R}$, such that $\|\vec{R}\| = 1$

$$\vec{R} = \begin{pmatrix} \cos(\alpha_1) \\ \cos(\alpha_2) \\ \ldots \\ \cos(\alpha_D) \end{pmatrix}$$

A vector $\vec{X}$ may be projected into a space $\vec{Y}$ by

$$\vec{Y} = \vec{R}^T \vec{X}$$

The Normal (Gaussian) function is defined only by its moments.
It is thus invariant to affine transformations of its moments.
The affine transformations include all linear transformations such as rotation, translation, scale changes and sheer.

For a projection onto a 1D vector Y, R is D x 1 : $\vec{Y} = \vec{R}^T \vec{X}$

$$\mu_y = \vec{R}^T \vec{\mu}_x, \qquad \sigma_y^2 = \vec{R}^T \boldsymbol{\Sigma}_x \vec{R}$$

Note that for the Covariance, projection requires pre- and post- multiplication by $\vec{R}$.
We can demonstrate this with a linear algebraic expression of the moments.

Linear Algebraic Form for Moment Calculation

Calculation of the mean and covariance are often expressed using linear algebra. Such expressions are widely used in machine learning.

As before, assume a set of M training examples $\{X_m\}$

Recall $\vec{\mu} = E\{\vec{X}\} = \frac{1}{M}\sum_{m=1}^{M}\vec{X} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \ldots \\ \mu_D \end{pmatrix} = \begin{pmatrix} E\{X_1\} \\ E\{X_2\} \\ \ldots \\ E\{X_D\} \end{pmatrix}$

We can compose a matrix with M columns and D rows from $\{X_m\}$.

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1M} \\ x_{21} & x_{22} & \cdots & x_{2M} \\ \ldots & \ldots & & \ldots \\ x_{D1} & x_{D2} & \cdots & x_{DM} \end{pmatrix}$$

Let us define the unity vector : $\vec{u} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$

Then $\vec{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \ldots \\ \mu_D \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1M} \\ x_{21} & x_{22} & \cdots & x_{2M} \\ \ldots & \ldots & & \ldots \\ x_{D1} & x_{D2} & \cdots & x_{DM} \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = X \cdot \vec{u}$

Let us define $\vec{V}_m = \vec{X}_m - E\{\vec{X}_m\} = \vec{X}_m - \vec{\mu}_m$.

We can compose a matrix with M columns and D rows from $\{V_m\}$.

$$V = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1M} \\ v_{21} & v_{22} & \cdots & v_{2M} \\ \ldots & \ldots & & \ldots \\ v_{D1} & v_{D2} & \cdots & v_{DM} \end{pmatrix}$$

From this: $\Sigma_x = E\{\vec{V}\vec{V}^T\}$ can be computed as a vector product.

$\Sigma_x \equiv V\ V^T$ is a D x D matrix that captures the "co-variance" of the elements of i,j of the vector X in $\{X_m\}$

This can be seen as

$$\Sigma_X = \mathbf{V}\mathbf{V}^T = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Note that we can also write $\Sigma_M = V^T V$ of size M x M.

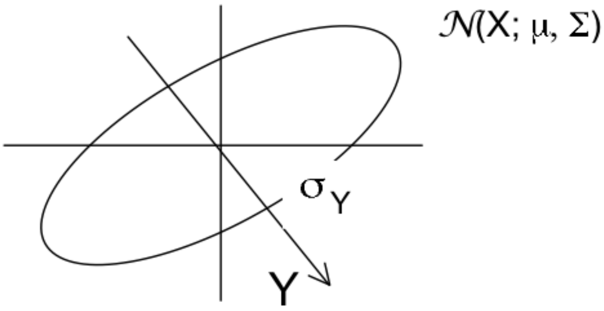
We can use this to show that projection of a covariance requires pre and post multiplication:

Note que $(\vec{R}^T V)^T = (V^T \vec{R})$

Thus
$$\begin{aligned} \Sigma_y &= (\vec{R}^T V)(\vec{R}^T V)^T \\ \Sigma_y &= (\vec{R}^T V)(V^T \vec{R}) \\ \Sigma_y &= \vec{R}^T (V V^T)\vec{R} \\ \Sigma_y &= \vec{R}^T \Sigma_X \vec{R} \end{aligned}$$

Thus projection of a covariance requires pre and post multiplication by $\vec{R}$.
In the case of projection to a 1D vector Y:

$$\sigma_y^2 = \vec{R}^T \Sigma_X \vec{R}$$


$\mathcal{N}(X; \mu, \Sigma)$
σ_Y
Y