

Pattern Recognition and Machine Learning

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Gaussian Probability Density Functions

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Source:

"Pattern Recognition and Machine Learning", C. M. Bishop, Springer Verlag, 2006.

Notation

x	a variable
X	a random variable (unpredictable value)
\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.
k	Class index
K	Total number of classes
ω_k	The statement (assertion) that $E \in T_k$
M_k	Number of examples for the class k . (think $M = \text{Mass}$)
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 .

$$\{X_m\} = \bigcup_{k=1, K} \{X_m^k\}$$

$\{t_m\}$ A set of class labels (indicators) for the samples

$\mu = E\{X_m\}$ The Expected Value, or Average from the M samples.

$\hat{\sigma}^2$ Estimated Variance

$\tilde{\sigma}^2$ True Variance

$$\mathcal{N}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad \text{Gaussian (Normal) Density function.}$$

Expected Values and Moments: ele

The average value is the first moment of the samples

For a numerical feature value for $\{X_m\}$, the "expected value" $E\{X\}$ is defined as the average or the mean:

$$E\{X\} = \frac{1}{M} \sum_{m=1}^M X_m$$

$\mu_x = E\{X\}$ is the first moment (or center of gravity) of the values of $\{X_m\}$.

This can be seen from the histogram $h(x)$.

The mass of the histogram is the zeroth moment, M

$$M = \sum_{n=1}^N h(n)$$

M is also the number of samples used to compute $h(n)$.

The expected value of is the average μ

$$\mu = E\{X_m\} = \frac{1}{M} \sum_{m=1}^M X_m$$

This is also the expected value of n .

$$\mu = \frac{1}{M} \sum_{n=1}^N h(n) \cdot n$$

Thus the center of gravity of the histogram is the expected value of the random variable:

$$\mu = E\{X_m\} = \frac{1}{M} \sum_{m=1}^M X_m = \frac{1}{M} \sum_{n=1}^N h(n) \cdot n$$

The second moment is the expected deviation from the first moment:

$$\sigma^2 = E\{(X - E\{X\})^2\} = \frac{1}{M} \sum_{m=1}^M (X_m - \mu)^2 = \frac{1}{M} \sum_{n=1}^N h(n) \cdot (n - \mu)^2$$

Probability Density Functions

In many cases, the number of possible feature values, N , or the number of features, D , make a histogram based approach infeasible.

In such cases we can replace $h(X)$ with a probability density function (pdf).

A probability density function of a continuous random variable is a function that describes the relative likelihood for this random variable to occur at a given point in the observation space.

Note: Likelihood is not probability.

Definition: "Likelihood" is a relative measure of belief or certainty.

We will use the "likelihood" to determine the parameters for parametric models of probability density functions. To do this, we first need to define probability density functions.

A probability density function, $p(\vec{X})$, is a function of a continuous variable or vector, $\vec{X} \in \mathbb{R}^D$, of random variables such that :

- 1) \vec{X} is a vector of D real valued random variables with values between $[-\infty, \infty]$
- 2) $\int_{-\infty}^{\infty} p(\vec{X}) = 1$

In this case we replace $\frac{1}{M} h(n) \rightarrow p(\vec{X})$

For Bayesian conditional density (where $\omega_k = E \in T_k$)

$$\frac{1}{M_k} h(n | \omega_k) \rightarrow p(\vec{X} | \omega_k)$$

Thus:

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

Note that the ratio of two pdfs gives a probability value!

This equation can be interpreted as

Posterior Probability = Likelihood x prior probability

The probability for a random variable to fall within a given set is given by the integral of its density.

$$p(X \text{ in } [A, B]) = p(X \in [A, B]) = \int_A^B p(x) dx$$

Thus some authors work with Cumulative Distribution functions:

$$P(x) = \int_{x=-\infty}^x p(x) dx$$

Probability Density functions are a primary tool for designing recognition machines.

There is one more tool we need : Gaussian (Normal) density functions:

Expected Values for PDFs

Just as with histograms, the expected value is the first moment of a pdf.

Remember that for a pdf the mass is 1 by definition:

$$S = \int_{-\infty}^{\infty} p(x) dx = 1$$

For the continuous random variable $\{X_m\}$ and the pdf $P(X)$.

$$E\{X\} = \frac{1}{M} \sum_{m=1}^M X_m = \int_{-\infty}^{\infty} p(x) \cdot x dx$$

The second moment is

$$\sigma^2 = E\{(X - \mu)^2\} = \frac{1}{M} \sum_{m=1}^M (X_m - \mu)^2 = \int_{-\infty}^{\infty} p(x) \cdot (x - \mu)^2 dx$$

Note that

$$\sigma^2 = E\{(X - \mu)^2\} = E\{X^2\} - \mu^2 = E\{X^2\} - E\{X\}^2$$

Note that this is a "Biased" variance.

The unbiased variance would be

$$\tilde{\sigma}^2 = \frac{1}{M-1} \sum_{m=1}^M (X_m - \mu)^2$$

If we draw a random sample $\{X_m\}$ of M random variables from a Normal density with parameters (μ, σ)

$$\{X_m\} \leftarrow \mathcal{N}(x; \mu, \tilde{\sigma})$$

Then we compute the moments, we obtain.

$$\mu = E\{X_m\} = \frac{1}{M} \sum_{m=1}^M X_m$$

and

$$\hat{\sigma}^2 = \frac{1}{M} \sum_{m=1}^M (X_m - \mu)^2 \quad \text{Where } \tilde{\sigma}^2 = \frac{M}{M-1} \hat{\sigma}^2$$

Note the notation: \sim means "true", \wedge means estimated.

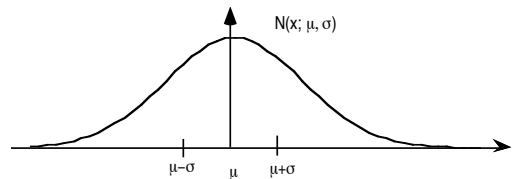
The expectation underestimates the variance by 1/M.

Later we will see that the expected RMS error for estimating p(X) from M samples is related to the bias. But first, we need to examine the Gaussian (or normal) density function.

The Normal (Gaussian) Density Function

Whenever a random variable is determined by a sequence of independent random events, the outcome will be a Normal or Gaussian density function. This is demonstrated by the Central Limit Theorem. The essence of the derivation is that repeated convolution of any finite density function will tend asymptotically to a Gaussian (or normal) 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.

This is often written as a conditional:

This is sometimes expressed as a conditional $\mathcal{N}(X | \mu, \sigma)$

In most cases, for any density $p(X)$:

$$\text{as } N \rightarrow \infty \quad p(X)^{*N} \rightarrow \mathcal{N}(x; \mu, \sigma)$$

This is the Central Limit theorem.

An exception is the dirac delta $p(X) = \delta(x)$.

Multivariate Normal Density Functions

In most practical cases, an observation is described by D features.

In this case a training set $\{\vec{X}_m\}$ can be used to calculate an average feature $\bar{\mu}$

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

If the features are mapped onto integers from $[1, N]$: $\{\vec{X}_m\} \rightarrow \{\vec{n}_m\}$ we can build a multi-dimensional histogram using a D dimensional table:

$$\forall m = 1, M : h(\bar{n}_m) \leftarrow h(\bar{n}_m) + 1$$

As before the average feature vector, $\bar{\mu}$, is the center of gravity (first moment) of the histogram.

$$\mu_d = E\{n_d\} = \frac{1}{M} \sum_{m=1}^M n_{dm} = \frac{1}{M} \sum_{n_1=1}^N \sum_{n_2=1}^N \dots \sum_{n_D=1}^N h(n_1, n_2, \dots, n_D) \cdot n_d = \frac{1}{M} \sum_{\bar{n}=1}^N h(\bar{n}) \cdot n_d = \mu_d$$

$$\bar{\mu} = E\{\bar{n}\} = \frac{1}{M} \sum_{m=1}^M \bar{n}_m = \frac{1}{M} \sum_{\bar{n}=1}^N h(\bar{n}) \cdot \bar{n} = \begin{pmatrix} \frac{1}{M} \sum_{\bar{n}=1}^N h(\bar{n}) \cdot n_1 \\ \frac{1}{M} \sum_{\bar{n}=1}^N h(\bar{n}) \cdot n_2 \\ \dots \\ \frac{1}{M} \sum_{\bar{n}=1}^N h(\bar{n}) \cdot n_D \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \dots \\ \mu_D \end{pmatrix}$$

For Real valued X:

$$\mu_d = E\{X_d\} = \frac{1}{M} \sum_{m=1}^M X_{dm} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} p(x_1, x_2, \dots, x_D) \cdot x_d dx_1, dx_2, \dots, dx_D$$

In any case:

$$\bar{\mu} = E\{\bar{X}\} = \begin{pmatrix} E\{X_1\} \\ E\{X_2\} \\ \dots \\ E\{X_D\} \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \dots \\ \mu_D \end{pmatrix}$$

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

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

This is often written

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

and gives

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

This provides the parameters for

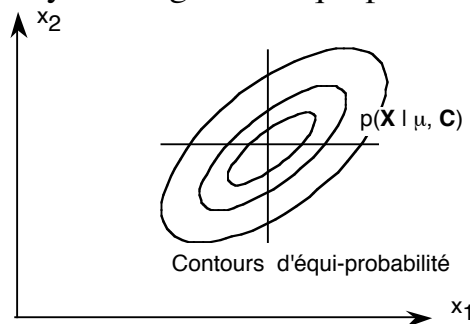
$$p(\vec{X}) = \mathcal{N}(\vec{X} | \vec{\mu}, \Sigma) = \frac{1}{(2\pi)^{\frac{D}{2}} \det(\Sigma)^{\frac{1}{2}}} e^{-\frac{1}{2}(\vec{X}-\vec{\mu})^T \Sigma^{-1} (\vec{X}-\vec{\mu})}$$

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

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

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 $x_1 = \text{height (m)}$ and $x_2 = \text{weight (kg)}$

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