Intelligent Systems: Reasoning and Recognition
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Non-Parametric Models for Bayesian Recognition
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Bibliographical sources:"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). an observation. |
| N | The number of possible values for $X$ |
| $\vec{x}$ | A vector of D variables. |
| $\vec{X}$ | A vector of D random variables. |
| D | The number of dimensions for the vector $\vec{x}$ or $\vec{X}$ |
| $C_{k}$ | The class k |
| k | Class index |
| K | Total number of classes |
| $\omega_{k}$ | The statement (assertion) that $\mathrm{X} \in \mathrm{C}_{\mathrm{k}}$ |
| $P\left(\omega_{k}\right)=P\left(X \in C_{k}\right)$ Probability that the observation X is a member of the class k. |  |
| $M_{k}$ | Number of examples for the class k. |
| $M$ | Total number of examples. |
|  | M $=\sum_{k=1}^{K} M_{k}$ <br> $\left\{\vec{x}_{m}\right\}$ |
| $\left\{y_{m}\right\}$ | A set of training samples of indicator vectors for the training samples in $\left\{\vec{X}_{m}\right\}$ |
| $p(X)$ | Probability density function for a continuous value X |

## Bayesian Classification

Our problem is to build a box that maps a set of features $\vec{X}$ from an observation, X to a class $C_{k}$ from a set of $K$ possible classes.


Let $\omega_{\mathrm{k}}$ be the proposition that the event belongs to class k: $\omega_{k}=\vec{X} \in C_{k}$

In order to minimize the number of mistakes, we will maximize the probability that $\omega_{k} \equiv X \in C_{k}$

$$
\hat{\omega}_{k}=\underset{\omega_{k}}{\arg -\max }\left\{P\left(\omega_{k} \mid \vec{X}\right)\right\}
$$

Our primary tool for this is Bayes Rule: $\quad P\left(\omega_{k} \mid \vec{X}\right)=\frac{P\left(\vec{X} \mid \omega_{k}\right) P\left(\omega_{k}\right)}{P(\vec{X})}$

To apply Bayes rule, we require a representation for the probabilities $P\left(\vec{X} \mid \omega_{k}\right), P(\vec{X})$, and $p\left(\omega_{k}\right)$. Today we will look at some simple, non-parametric models for probability.

Today will look at three non-parametric representations for $P\left(\vec{X} \mid \omega_{k}\right)$ and $P(\vec{X})$ :

1) Histograms
2) Kernel Density Estimators
3) K-Nearest Neighbors

## Classification with a Ratio of Histograms

Consider an example of K classes of objects where objects are described by a feature, $X$, with N possible integer values from $[1, \mathrm{~N}]$. Assume that we have a "training set" of M samples $\left\{x_{m}\right\}$ along with indicator variables $\left\{y_{m}\right\}$ where the indicator variable is the class, k , for each training sample.

For each class k, we allocate a histogram, $h_{k}()$, with $N$ cells and count the values in the training set.

$$
\begin{aligned}
& \forall_{m=1}^{M}: \quad h\left(x_{m}\right) \leftarrow h\left(x_{m}\right)+1 \\
& \text { IF } y_{m}=k \text { THEN } h_{k}\left(x_{m}\right) \leftarrow h_{k}\left(x_{m}\right)+1 ; M_{k} \leftarrow M_{k}+1
\end{aligned}
$$

Then

$$
\begin{aligned}
& P(X=x)=\frac{1}{M} h(x) \\
& P\left(X=x \mid X \in C_{k}\right)=P\left(X \mid \omega_{k}\right)=\frac{1}{M_{k}} h_{k}(x)
\end{aligned}
$$

and $P\left(\omega_{k}\right)$ can be estimated from the relative size of the training set.

$$
P\left(X \in C_{k}\right)=P\left(\omega_{k}\right)=\frac{M_{k}}{M}
$$

giving: $P\left(\omega_{k} \mid X\right)=\frac{P\left(X \mid \omega_{k}\right) P\left(\omega_{k}\right)}{P(X)}=\frac{\frac{1}{M_{k}} h_{k}(X) \frac{M_{k}}{M}}{\frac{1}{M} h(X)}=\frac{h_{k}(X)}{h(X)}$
This can also be written as: $\quad P\left(\omega_{k} \mid X\right)=\frac{h_{k}(X)}{\sum_{k=1}^{K} h_{k}(X)} \quad$ because $\quad h(X)=\sum_{k=1}^{K} h_{k}(X)$
The ratio of histograms can be represented by a lookup table. $P\left(\omega_{k} \mid X\right)=T(X)$
To illustrate, consider an example with 2 classes ( $\mathrm{K}=2$ ) and where X can take on 8 values ( $\mathrm{N}=8, \mathrm{D}=1$ ).


Recall that the number of cells in the histogram is $\mathrm{Q}=\mathrm{N}^{\mathrm{D}}$.
Having $\mathrm{M} \gg \mathrm{Q}$ is NECESSARY but NOT Sufficient.
Having $\mathrm{M}<\mathrm{Q}$ is a guarantee of INSUFFICIENT TRAINING DATA.

## Number of samples required

Problem: Given a feature $x$, with N possible values, how many observations, M , do we need for a histogram, $h(x)$, to provide a reliable estimate of probability?

The worst case Root Mean Square error is proportional to $O\left(\frac{Q}{M}\right)$.

This can be estimated by comparing the observed histograms to an ideal parametric model of the probability density or by comparing histograms of subsets samples to histograms from a very large sample. Let $p(x)$ be a probability density function. The RMS (root-mean-square) sampling error between a histogram and the density function is

$$
E_{R M S}=\sqrt{E\left\{(h(x)-p(x))^{2}\right\}} \approx O\left(\frac{Q}{M}\right)
$$

The worst case occurs for a uniform probability density function.

For most applications, $\mathrm{M} \geq 8 \mathrm{Q}$ ( 8 samples per "cell") is reasonable (less than $12 \%$ RMS error).

So what can you do if you do not have $\mathrm{M} \gg \mathrm{Q}$ ?
Adapt the size of the cell to the data!

## Variable Sized Histogram Cells

Suppose that we have a D-dimensional feature vector $\vec{X}$ with each feature quantized to N possible values, and suppose that we represent $p(\vec{X})$ as a D-dimensional histogram $h(\vec{x})$. Let us fill the histogram with M training samples $\left\{\vec{x}_{m}\right\}$.

Let us define the volume of each cell as 1 .
The volume for any block of V cells is V .
Then the volume of the entire space is $\mathrm{Q}=\mathrm{N}^{\mathrm{D}}$.

If the quantity of training data is too small, ie if $M<8 Q$, then we can combine adjacent cells so as to amass enough data for a reasonable estimate.

Suppose we merge $V$ adjacent cells such that we obtain a combined sum of $S$.

$$
S=\sum_{\vec{x} \in V} h(\vec{x})
$$

The volume of the combined cells would be V.
To compute the probability we replace $h(\vec{x})$ with $\frac{S}{V}$.
The probability $p(\vec{X})$ for $\vec{X} \in V$ is:

$$
p(\vec{X} \in V)=\frac{1}{M} \cdot \frac{S}{V}
$$

This is typically written as: $\quad p(\vec{X})=\frac{S}{M V}$

We can use this equation to develop two alternative non-parametric methods.

Fix $V$ and determine $S=>$ Kernel density estimator.
Fix $S$ and determine $V=>K$ nearest neighbors.
(note that the symbol " K " is often used for the sum the cells.
This conflicts with the use of K for the number of classes.
Thus we will use the symbol $S$ for the sum of adjacent cells).

## Kernel Density Estimators

For a Kernel density estimator, we represent each training sample with a kernel function $k(\vec{X})$.

Popular Kernel functions include
a hypercube centered of side w
a triangular function with base of w
a sphere of radius w
a Gaussian of standard deviation $\sigma$.

We can define the function for the hypercube as

$$
k(\vec{u})=\left\{\begin{array}{cc}
1 & \text { if }\left|\mathrm{u}_{\mathrm{d}}\right| \leq 1 / 2 \text { for all } \mathrm{d}=1, \ldots, \mathrm{D} \\
0 & \text { otherwise }
\end{array}\right.
$$

This is called a Parzen window.
Subtracting a point, $\bar{z}$, centers the Parzen window at that point.
Dividing by w scales the Parzen window to a hyper-cube of side w.

$$
k\left(\frac{\vec{X}-\vec{z}}{w}\right) \text { is a cube of size } \mathrm{w}^{\mathrm{D}} \text { centered at } \vec{z} \text {. }
$$

The M training samples define M overlapping Parzen windows.
For an feature value, $\vec{X}$, the probability $p(\vec{X})$ is the sum of Parzen windows at $\vec{X}$

$$
S=\sum_{m=1}^{M} k\left(\frac{\vec{X}-\vec{x}_{m}}{w}\right)
$$

The volume of the Parzen window is $V=w^{D}$.
Thus the probability $p(\vec{X})=\frac{S}{M V}=\frac{1}{M w^{D}} \sum_{m=1}^{M} k\left(\frac{\vec{X}-\vec{x}_{m}}{w}\right)$
A Parzen window is discontinuous at the boundaries, creating boundary effects. We can soften this using a triangular function evaluated within the window.

$$
k(\vec{u})=\left\{\begin{array}{cc}
1-2\|\vec{u}\| & \text { if }\|\vec{u}\| \leq 1 / 2 \\
0 & \text { otherwise }
\end{array}\right.
$$

Even better is to use a Gaussian kernel with standard deviation $\sigma$.

$$
k(\vec{u})=\frac{1}{(2 \pi)^{D / 2} \sigma} e^{-\frac{1}{2} \frac{\|\vec{u}\|^{2}}{\sigma^{2}}}
$$

We can note that the volume (or integral) of $e^{-\frac{1}{2} \frac{\|\vec{u}\|^{2}}{\sigma^{2}}}$ is $V=(2 \pi)^{D / 2} \sigma$
In this case $p(\vec{X})=\frac{S}{M V}=\frac{1}{M} \sum_{m=1}^{M} k\left(\vec{X}-\vec{x}_{m}\right)$

This corresponds to placing a Gaussian at each training sample and summing the Tails at $\vec{X}$.
The probability for a value $\vec{X}$ is the sum of the Gaussians.

In fact, we can choose any function $k(\vec{u})$ as kernel, provided that

$$
k(\vec{u}) \geq 0 \text { and } \int k(\vec{u}) d \vec{u}=1
$$

## K Nearest Neighbors

For K nearest neighbors, we hold $S$ constant and vary V. (We have used the symbol $S$ for the number of neighbors, rather than $K$ to avoid confusion with the number of classes).

For each training sample, $\vec{x}_{m}$, we construct a tree structure (such as a KD Tree) that allows us to easily find the $S$ nearest neighbors for any point.

To compute $p(\vec{X})$ we need the volume of a sphere in D dimensions that encloses the nearest S neighbors. Suppose the set of S nearest neighbors is the set $\left\{X_{s}\right\}$.

This is D dimensional sphere of radius $R=\underset{\left\{X_{s}\right\}}{\arg -\max \{ }\left\{\left\|\vec{X}-\overrightarrow{x_{s}}\right\|\right\}$

$$
V=\frac{\pi^{\frac{D}{2}}}{\Gamma\left(\frac{D}{2}+1\right)} R^{D}
$$

Where $\quad \Gamma(\mathrm{D})=(\mathrm{D}-1)!$

For even D this is easy to evaluate

For odd D, use a table to determine $\Gamma\left(\frac{D}{2}+1\right)$
Then as before: $\quad p(\vec{X})=\frac{S}{M V}$

## Probability Density Functions

A probability density function $p(X)$, is a function of a continuous variable $X$ such that

1) $X$ is a continuous real valued random variable with values between $[-\infty, \infty]$
2) $\int_{-\infty}^{\infty} p(X)=1$

Note that $p(X)$ is NOT a number but a continuous function.

A probability density function defines the relatively likelihood for a specific value of $X$. Because $X$ is continuous, the value of $p(X)$ for a specific $X$ is infinitely small. To obtain a probability we must integrate over some range of $X$.
To obtain a probability we must integrate over some range $V$ of $X$.
In the case of $\mathrm{D}=1$, the probability that X is within the interval $[\mathrm{A}, \mathrm{B}]$ is

$$
P(X \in[A, B])=\int_{A}^{B} p(x) d x
$$

This integral gives a number that can be used as a probability.

Note that we use upper case $P(X \in[A, B])$ to represent a probability value, and lower case $p(X)$ to represent a probability density function.

Classification using Bayes Rule can use probability density functions

$$
P\left(\omega_{k} \mid X\right)=\frac{p\left(X \mid \omega_{k}\right)}{p(X)} P\left(\omega_{k}\right)=\frac{p\left(X \mid \omega_{k}\right) P\left(\omega_{k}\right)}{\sum_{j=1}^{K} p\left(X \mid \omega_{j}\right) P\left(\omega_{j}\right)} \quad \text { because } p(X)=\sum_{j=1}^{K} p\left(X \mid \omega_{j}\right) P\left(\omega_{j}\right)
$$

Note that the ratio $\frac{p\left(X \mid \omega_{k}\right)}{p(X)}$ IS a number, provided that $p(X)=\sum_{k=1}^{K} p\left(X \mid \omega_{k}\right) P\left(\omega_{k}\right)$

Probability density functions are easily generalized to vectors of random variables.
Let $\vec{X} \in R^{D}$, be a vector random variables.
A probability density function, $p(\vec{X})$, is a function of a vector of continuous variables

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