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STATISTICAL DECISIONS UNDER NONPARAMETRIC A PRIORI INFORMATION

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The basic module of a statistic analysis applied programs package is described. By means of this module tasks of choosing theoretical model most adequately fitting to experimental data, selection of events of definite type, identification of elementar particles are carried out. For mentioned problems solving, the Bayesian decision rules, one-leave out test and KNN (K Nearest Neighbour) adaptive density estimation are utilized.

Yerevan Physics Institute
Yerevan 1985

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СТАТИСТИЧЕСКИЕ РЕШЕНИЯ ПРИ НЕПАРАМЕТРИЧЕСКОМ СПОСОБЕ ЗАДАНИЯ АПРИОРНОЙ ИНФОРМАЦИИ

Приводится подробное описание основного модуля пакета программ прикладного статистического анализа АНИ . С помощью модуля решаются задачи выбора теоретической модели, наиболее точно описывающей экспериментальные данные, выделения событий определенного типа, идентификации элементарных частиц и процессов взаимодействия. Для решения этих задач применяются байесовские решающие правила, процедура скользящего экзамена по обучающей выборке, NNC (N - ближайших соседей) адаптивное оценивание плотности вероятности.

Ереванский физический институт
Ереван 1986

Key words - nonparametric methods, pattern recognition, classification, Bayes risk estimation, multidimensional analysis, probability density, local estimation.

Characteristics of physical problems - choice of theoretical model most precisely describing experimental data, extraction of events of the definite type, identification of elementar particles and interaction processes.

Characteristics of statistical problems- quantitative comparison of multidimensional distributions, classification of distribution mixture, training with the teacther, probability density local estimation.

Procedures used - Bayesian decision rules, Bayes risk estimation, "one leave out" test over the training sample, KNN(K-nearest neighbours) adaptive method.

Long Write up

1. Introduction

The scientific method is characterized by the data classification, the study of their interrelation and the relation to the past experience, accumulated in various theories and hypotheses. Usually, it is impossible either to prove or to refute the statements concerning the extent of confirming various hypotheses, by the deductive method. However, the purposeful observation of the data leads to the empirical statements, that may be connected with the theoretical ones by means of the rational inductive conclusion rules /1/. In the general case these statements are always probability ones, the inductive conclusion may prove to be true in the given concrete case, though this certainty does not grow into the logical truth, as in the case of the deductive conclusion.

The Bayesian approach allows to express numerically the confidence to the alternative hypotheses. The Bayesian procedures are operational and applicable for the purpose of analysing practically the wide spectra of models and problems (see, e.g.2). Having estimated the posterior densities one may organize the procedure calculating the Bayesian risk which is used as the numerical characteristic of the theoretical model and empirical data closeness.

In the majority of applied regions the apriori information is given in the form of training samples (TS) corresponding to the alternative types or hypotheses. The basis of statistical procedures using such a nonparametric method of giving an a priori information is the density local estimation. The module, realizing the density adaptive local estimation and the calculation of the Bayesian risk by the training samples is the basic

one in the ЯNI applied statistical analysis programme package/3/, intended to interpret the experimental data and to plan the experiments in cosmic ray physics. By means of the package the processing of data from the X-ray-emulsion chambers is performed with the purpose of determining the chemical composition of the cosmic radiation primary component and choosing the model of strong interaction at superhigh energies /4/; determining the type of the cascade process in the calorimeter installations of the PAIR-METER type /5/ and identifying the cosmic radiation hadrons registered by the transition radiation detector system /6/.

2. The comparison of the alternative hypotheses. The measure of the empirical data and model closeness

In view of the measurements complexity and indirectness the only possibility to compare the experimental data and various hypotheses on the type of strong interaction of the high energy particles with the atmosphere atoms or on the chemical composition of the cosmic radiation primary component is the imitation experiment with the models of the radiation passage through the atmosphere and detectors. The bases of the statistical analysis are the training samples corresponding to the alternative models representations. It is necessary to determine the model wich is most close to the experimental data. The term closeness refers to the coincidence, similarity, correlation, to the extent of overlapping or any other variable used as the measure of similarity or distance. The most natural measure of closeness of W_1 and W_2 classes characterized by the density functions $p(\vec{x}/\omega_1)$ and $p(\vec{x}/\omega_2)$, is the probability of misclassification of events according to the distribution mixture:

$$p(\vec{x}) = p(\omega_1)\cdot p(\vec{x}/\omega_1) + p(\omega_2)\cdot p(\vec{x}/\omega_2) \qquad (1)$$

where $p(\omega_1)$ and $p(\omega_2)$ are the a priori probabilities, that may be assumed to equal 0,5, if the number of events in the class ω_1 equals to the number of events in class ω_2. Naturally, for the classification, one must choose an optimal decision rule, providing minimum errors at using the $\vec{x}$ feature complex. Such is the Bayesian rule of the posterior density maximum

$$p(\omega_1/\vec{x}) \lessgtr p(\omega_2/\vec{x}) \rightarrow \vec{x} \in \begin{cases} \omega_1 \\ \omega_2 \end{cases}, \qquad (2)$$

where

$$p(\omega_i/\vec{x}) = \frac{p(\omega_i) \cdot p(\vec{x}/\omega_i)}{p(\omega_1) \cdot p(\vec{x}/\omega_1) + p(\omega_2) \cdot p(\vec{x}/\omega_2)} \qquad (3)$$

$p(\vec{x}/\omega_i)$ is the conditional density, or, if it is considered as function of ω_i - the likelihood function, $p(\omega_i/\vec{x})$ is the posterior density, in which the optimal synthesis of the a priori and experimental information is realized. The probability of misclassification, at applying the Bayesian decision rule, coincides with the Bayesian risk as we use the simple function of losses (the losses are equal to zero for the correct classification and are equal 1 for any error). The risk at the point $\vec{x}$ is equal to

$$r^B(\vec{x}) = \min\left[p(\omega_1/\vec{x}), p(\omega_2/\vec{x})\right], \qquad (4)$$

finally the Bayesian risk is determined by the expression:

$$R^B = \int_\Gamma r^B(\vec{x})\, p(\vec{x})\, d\vec{x}, \qquad (5)$$

where $p(\vec{x})$ is the distribution mixture (I), and Γ is the feature space.

However, it is impossible to use the formula 4,5 for cal-

culating R^B as the analytical expression of the conditional densities and, hence, the posterior ones, is unknown. Therefore, instead of unknown densities we shall use their local estimations. But, first of all let us distinguish four types of estimations connected with calculating R^B /7/. R_M^α is the value obtained with given T S of M value and a definite α classifiers. $E\{R_M^\alpha\}$ is the mathematical expectation of that value, the averaging is performed by the M size possible samples taken from the general set. R_∞^α is the asymptotic value of the TS infinite increase, and, at last, R^B is the value corresponding to the "ideal" case of the known conditional densities. R^B depends only on the densities, R_∞^α on the classifier α too, $E\{R_M^\alpha\}$ on the TS size as well, R_M^α besides, on the concrete TS with the fluctuations inherent to it. In the subject region of interest one may not expect estimations of the R_∞^α type or the effective averaging of $E\{R_M^\alpha\}$ type, therefore it is necessary to choose a nonbiased and effective estimation procedure. In calculating R^B to the classification-errors coused by the overlapping of distributions there are added the errors connected with the TS scarsness and the errors in the classifier training due to that scarsness-the errors in the density nonparametric estimation. The method of density estimation will be considered in the next paragraph, and now we shall consider another main question - the method of using the training sample in the procedure of the Bayesian risk calculation.

The three main methods are distinguished /8/: P-method: the classifier is both trained and examined on the same sample, i.e., first the conditional densities $p(\vec{x}/\omega_i)$ are determined by TS, and then the classification is carried out; H-method: the TS devided into two equal parts, with one half the training

is performed, with the other-the examination. The P -method decreases the Bayesian risk, the H -on the contrary decreasied . Besides, the H -method does not use effectively the TS. The U - method (leave one out) is free of such defects. One element is removed from the sample, the training is performed without it, then this element is classified and replaced in the TS etc, until all the TS elements are executed.

The error empirical calculation /8/ was one of the first estimation procedures. Let us introduce a random variable

$$\varepsilon(\vec{x}_i) = \begin{cases} 0 \text{ , if } \vec{x} \text{ is classified} \\ \text{correctly,} \\ 1, \text{ in the opposite case} \end{cases} \qquad (6)$$

Let the empirical risk be determined by means of $\varepsilon(\vec{x}_i)$

$$R^{э}_{M} = \frac{1}{M} \sum_{i=1}^{M} \varepsilon(\vec{x}_i) = \frac{mezz}{M} \qquad (7)$$

where mezz is the number of misclassifications.

The estimate varianse equals

$$\sigma^2_{R^э} = \frac{1}{M} R^{Б}(1 - R^{Б}) \qquad (8)$$

Another type of estimate is connected with the approximation of the formula 5, the posterior densities in formula 4 are obtained by local estimation of the conditional densities.

$$R^{Б} = E\left\{r(\vec{x})\right\} = \int_{\Gamma} r(\vec{x}) p(\vec{x}) d\vec{x} \approx \frac{1}{M} r(\vec{x}_i) \equiv R^{P} \qquad (9)$$

It is interesting to note, that the variance of this estimate proves to be less than that of the previous one.

$$\sigma^2_{R^p} = \frac{1}{M}(1-R^5) - 1/2\, R^5/M \qquad (10)$$

This result seems to be paradoxical, as in the second case the information on the $\vec{x}$ vector true class is not used. This contradiction is explained by that R^p may take any rational value approaching R^5 while R^3 may take only the values equal to the ratio of integers m_{ez}/M, this causing a large spread around R^5.

3. The Probability Density Local Estimation.

The density estimation nonparametric methods have received recently a large development effort /see, e.g. 9 / mainly owing to their simplicity and the absence of excessive requirements to the distribution function form. The estimation histogram method develops in two main directions. Firstly these are the Parzen methods, in which the histogram function single step is changed by a certain nuclear function, and, secondly, the KNN (K-nearest neighbour) methods that adapt the cell size. The cells in that case contain exactly K represenatives of TS and, hence, the density estimation in the point $\vec{x}$ will be obtained in the form of:

$$p_{K,M}(\vec{x}) = \frac{K}{M \cdot V_{K,M}(\vec{x})}\ , \qquad (11)$$

where

$$V_{K,M}(\vec{x}) = \frac{2\pi^{N/2} d_K^N(\vec{x})}{N \cdot \Gamma(N/2)} \qquad (12)$$

is the volume of the region containing K representatives of TS, nearest to the point $\vec{x}$, M is the number of TS vectors (the TS size or volume), N is the feature space dimensionality, $\Gamma(N/2)$ the gamma-function, d_K - the distance to the K^{+h}- nearest neighbour of the point $\vec{x}$ in any suitable metric. Two metrics are

are used: the usual Euklidian and the Mahalonobis /10/, where the distance between points $\vec{x}$ and $\vec{y}$ is equal to:

$$D_M^2 = (\vec{x} - \vec{y})^T \Sigma^{-1} (\vec{x} - \vec{y}) \qquad (13)$$

where Σ is the TS covarians matrix. The use of the Mahalonobis metric allows one to take into account the correlation informa - tion; besides, the distances, calculated in this metric are invariant with respect to the linear transformations of coordina - tes, this allowing not to take care of the scale of features.

The presence of unknown parameters in the nonparametric method. prevents to apply them successfully. In the histogram method these are the cell number and size, in the KNN methods - the K parameter, in the Parzen methods - the nucleus type and width. These parameters depend on the unknown density and volume of TS, therefore, practically, the recommendations on their values are often contradictional, depend on the concret type of data and have an iterative character of the cut-and-try. We have stated a problem of such an development of KNN methods that the procedure should weakly depend on the parameter heuristic choice.

For the KNN density estimates not to depend so strongly on the K parameter it was suggested to calculate the estimates simultaneously for the parameter several values. By means of a series of estimates $\{P_{i,M}(\vec{x})\}, i = 1, Q$, the averaged KNN3 estimate is constructed:

$$\hat{P}_{Q,M}(\vec{x}) = \frac{1}{Q} \sum_{i=1}^{M} P_{i,M}(\vec{x}), \qquad (14)$$

$$\hat{P}_{i,M}(\vec{x}) = \frac{i}{M \cdot V_{i,M}(\vec{x})} \qquad (15)$$

This estimate uses a more detailed information on the $\vec{x}$ point neighbourhood and provides the estimates that are more stable to the fluctuations in the TS and to the Q parameter choice. However, in the row of estimates there may be significant deviations from the true value, that distort the averaged estimate. Therefore we have suggested to apply the order statistics /I2/. By transformation of the row $\{P_{i,M}(\vec{x})\}$ into a variational one $\{P_{(i),M}(\vec{x})\}$ we shall obtain a density estimate in the form of order statistics linear combination

$$\hat{P}_{(Q),M}(\vec{x}) = \sum_{i=1}^{Q} a_i \hat{P}_{(i),M}(\vec{x}), \tag{16}$$

$$\sum_{i=1}^{Q} a_i = 1 \tag{17}$$

At the corresponding choice of a_i coefficients this estimate is more stable to the fluctuations in the TS. The particular case of estimations are the median estimates at which:

$$a_i = \begin{cases} 1, & \text{if } i=[Q/2]+1, Q \text{ is odd} \\ 0, & \text{in the opposite case} \end{cases}$$

If Q is even the two middle order statistics are given the weight 0,5. The introduction of adaptive estimates is connected with that, for the periphery points (being far from the distribution mode) the simple KNN estimates with $K = 2 \div 5$ (for the TS of 25 - 400) are optimal. As the density around the mode is high, the K parameter increase will not lead to any significant increase of the KNN containing region volume. Hense, the values of the most terms of the variation row will be overestimated with respect to the true density and the median estimates will not be

able to "choose" the best one. Therefore, at the periphery points, that are chosen according to the value of the local region relative size, the density is calculated according to the 3NN rule. The peripherality criterion is represented by the ratio

$$\eta_M(\vec{x}_i) = \rho_M(\vec{x}_i) / \bar{\rho}_M \,, \tag{18}$$

where

$$\rho_M(\vec{x}_i) = \frac{1}{\sqrt{M}} \sum_{j=1}^{\sqrt{M}} d_j(\vec{x}_i) \tag{19}$$

and

$$\bar{\rho}_M = \frac{1}{M} \sum_{i=1}^{M} \rho_M(\vec{x}_i) \,, \tag{20}$$

where $d_j(\vec{x}_i)$ is the distance to the j^{th} - neighbour of the $\vec{x}_i$ point.

Finally the KNN adaptive rule takes the form of:

$$P_{AD,M}(\vec{x}) = \begin{cases} P_{i,M}(\vec{x}) \text{ if } \eta_M(\vec{x}) > \alpha, \ \alpha = 3, \ i = 3 \\ \hat{P}_{[a/2]+1,M} \quad \text{in the opposite case, } a = M/2 \end{cases} \tag{21}$$

Thus, the uncertainty in the K and a parameters choice is overcomed. In the adaptive method the i, α, a parameters choose does not depend on the unknown densities and the TS volume. In fact, we carry out the method triple adaption by the TS. First, by means of calculating the auxiliary parameter - the local region size - we select the estimation regime, then with the help of the order statistics we choose the K parameter optimal value and then select the cell size according to the K parameter.

4. The Information Input and Output.

With KNN2 module the tasks of comparing the theoretical

models with the experimental data, of the high energy particle identification, of obtaining the probability density smooth estimates etc. are developed. The exchange of data with the module is realized by means of formal parametrs. Though, it leads to a rather long list of parameters, the undesirable collateral effects of the module on the main programme are practically excluded, and the module operation high obviousness is provided. The module is given the training sample $B(N,M,L)$ where N is the space dimensionality, M is the TS volume, L is the class number (for the simplicity, here it is assumed that various classes are presented by the TS with equal volumes), $T(N,MP)$ is the control sample, MP the control vectors number.

The Module Control Parameters are:

KCL corresponds to the Q parameter in the formulae 14,16,21, usually $KCL = M/2$, $NL(N)$ is the code combination, by means of which the feature complex selection from the primary information is realized - the N dimensionality array, where code 1 in i^{th}-position means the i^{th}- feature inclusion in the set under investigation.

$AP(L)$ the L dimensionality array - the a priori probabilities of the models being studied.

$F(KCL)$- the KCL dimensionality array - the coefficients of the order statistics, it corresponds to the formula 17. Usually,

$$F_i = \begin{cases} 1 & \text{if } i = [Q/2]+1,\ Q \text{ is odd} \\ 0{,}5 & \text{if } i = [Q/2],[Q/2]+1,\ Q \text{ is even} \\ 0 & \text{in the opposite case} \end{cases} \qquad (22)$$

KL1 is the code of choosing the metric in which the distances between the $\vec{X}$ point and TS poins are calculated. The $KL1=0$ value corresponds to the Mahalonobis metric (13). KL2 parameter, controlling the selection of the periphery points, corresponds to α of formula 21. Usually $KL2=3$. $R1(N,N,L)$,

is the covariation matrix of the TS classes.

During the operation in"one leave out" regime for Bayesian risk calculation, the number of TS classes $L=2$, and in the main programme the control sample is substituted by the training one.

The number of events, separately, of the 1 and the 2 class, classified as the representatives of the 1 and the 2 class by means of the KNN method various modifications, are placed in the $CL(L, KCL+2, L)$ array

$$CL(L,i,L)=\begin{cases} i=1,2,\ldots,KCL & \text{is the simple KNN classification} \\ i=KCL+1 & \text{is the averaged KNN 3 formula 14.} \\ i=KCL+2 & \text{is the adaptive KNN formula 21.} \end{cases} \quad (23)$$

The values of the Bayesian risk calculated by means of averaging the posterior risk (formula 9) are restored in the $DFM(KCL+2)$ array. The R^3 values calculated with the method of empirical calculation of misclassifications are restorted in the $G(KCL+2)$ array. The order of values in the arrays is analogous (23).

In the classification regime the numbers of classes to which the control vector are referred, are placed in the array $LUM(MP)$.

In the regime of constructing the density smoothed estimates, the density values for the L classes of TS, are placed in the $R(L,KCL+2)$ array. The coordinates in which the density is estimated, are transferred to the module in the $T(N,MP)$ array.

Besides the presented arrays the module uses the operational ones $D(M,L)$, $C(KCL+2)$, $R2(N,N)$, $R3(N,N,L)$

The C, CN, AP, DFM arrays are of double precision.

5. Programm Testing

The programm testing was performed with the application of samples from the normal (Gaussian) distribution. The choice of this distribution is due to its exstensive use as a simple test to compare various estimation methods, as well as due to the simplicity of calculating the Bayesian risk for the normal sets.

$$R^{5} = \Phi(-D_M/2), \qquad (24)$$

where Φ is the cumulative normal distribution function, and D_M is the Mahalonobis distance (13) between the mathematical expectationsof two classes. Usually several samples of the fixed volume were generated (10 or 25), the density was estimated at 50 points of the interval (-5 - 5), the mean-square error MSE and the integrated mean-square error IMSE were calculated by the formula

$$MSE(x) = E\left\{[\hat{P}(x) - p(x)]^2\right\} \approx \frac{1}{J}\sum_{j=1}^{J}[\hat{P}_j(x) - p(x)]^2 \qquad (25)$$

$$IMSE = E\left\{\int MSE(x)dx\right\} \approx \frac{1}{J}\sum_{j=1}^{J}\left(\sum_{i=1}^{I} MSE(x_i)\Delta x\right) \qquad (26)$$

The choice of X points is performed uniformly over the X variation region. The figure shows the results of testing for the comparison of KNN, KNN3 and adaptive estimation. The standard normal Density N(0,1) was estimated. Obviously, the adaptive estimations are much more precise than the ones could be obtained with any K fixed parameter.

Table 1 presents the results of comparing the adaptive

method with the Parzen method and the maximum likelihood with the penalty functions (the results of the latter two are taken from the monograph 9). IMSE and it variance (figure in brackets) are calculated by 2 5 independent random samples from the distribution $N(0,1)$ and the bimodal distribution $0{,}5N(-1{,}5,1) + 0{,}5N(1{,}5,1)$. The density was estimated in 50 points of the interval (-5-5). The adaptive KNN estimation has shown somewhat worse results. However, it should be noted that the parameters of both the Parzen and ML methods have been chosen applying the information on the true density, while the KNN method use only the sample information. Therefore the slight deterioration of accuracy is compensated with usury by the procedure stability, as in processing the real data, of course, the density analytical form is unknown.

The Bayesian risk was calculated for the samples from the normal distribution at various feature space dimensionalities and Mahalonobis distances. The calculations were performed with the use of ten independent samples. Table 2 presents the varianses theoretical values, calculated by the formula 8 and 10, the sample means and mean-square deviations MSE . A good agreement of sample and theoretical values is apparent, and though the varianses of R^p values is less than that of R^3 , their bias leads to that, their mean-square deviation is greater. Therefore, the method of error empirical calculation is more preferable, especially, at the feature space great dimensionalities.

IMSE of Various Methods Density Local Estimation

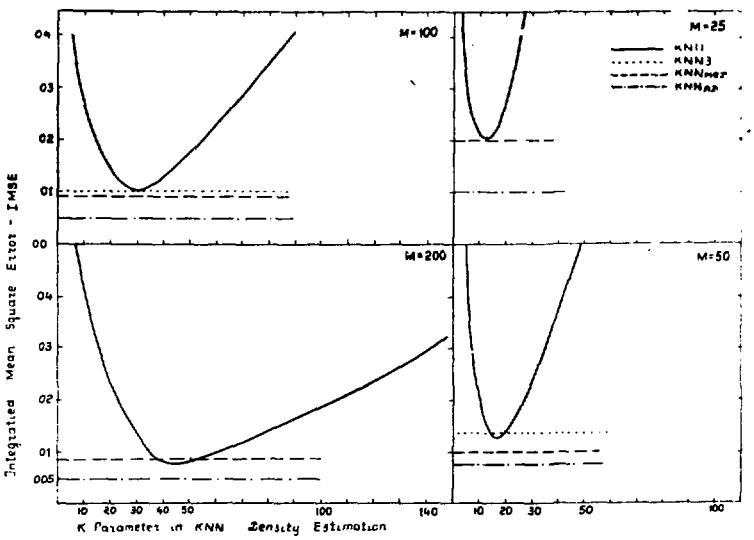
Table 1

distribution	TS size	MLM with the penalty func.	Parzen method with Gaussian Kernel	Adaptive KNN
N (0,I)	M = 25	0.10	.016	0.014
		(.008)	(.012)	(0.010)
N (0,I)	M = 100	.0037	.0050	0.0052
		(0.0021)	(.0027)	(0.002)
N (0,I)	M = 400	.0015	.0020	0.0032
		(.0008)	(.0009)	0.0012
Bimodal	M = 25	.010	.009	0.012
		(.003)	(.007)	(0.003)
Bimodal	M = 100	.0036	.0036	0.0048
		(.0007)	(.0020)	(0.0017)

Comparison of the Bayesian Risk Estimation Methods with the Application of the Density Adaptive KNN Estimation

Table 2

N	M	R^B	σ_{R^B}	σ_{R^P}	$\hat{\sigma}_{R^B}$	$\hat{\sigma}_{R^P}$	MSE_{R^B}	MSE_{R^P}
I	100	0.3085	0.046	0.024	0.039	0.026	0.0005	0.0013
I	200	0.3085	0.033	0.017	0.026	0.015	0.0003	0.0008
2	50	0.2340	0.048	0.031	0.044	0.027	0.0030	0.0039
8	50	0.5	0.07	0.05	0.05	0.012	0.005	0.044
10	50	0.5	0.7	0.047	0.047	0.017	0.004	0.046



Comparison of different modifications of KNN method

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СТАТИСТИЧЕСКИЕ РЕШЕНИЯ ПРИ НЕПАРАМЕТРИЧЕСКОМ СПОСОБЕ ЗАДАНИЯ АПРИОРНОЙ ИНФОРМАЦИИ
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