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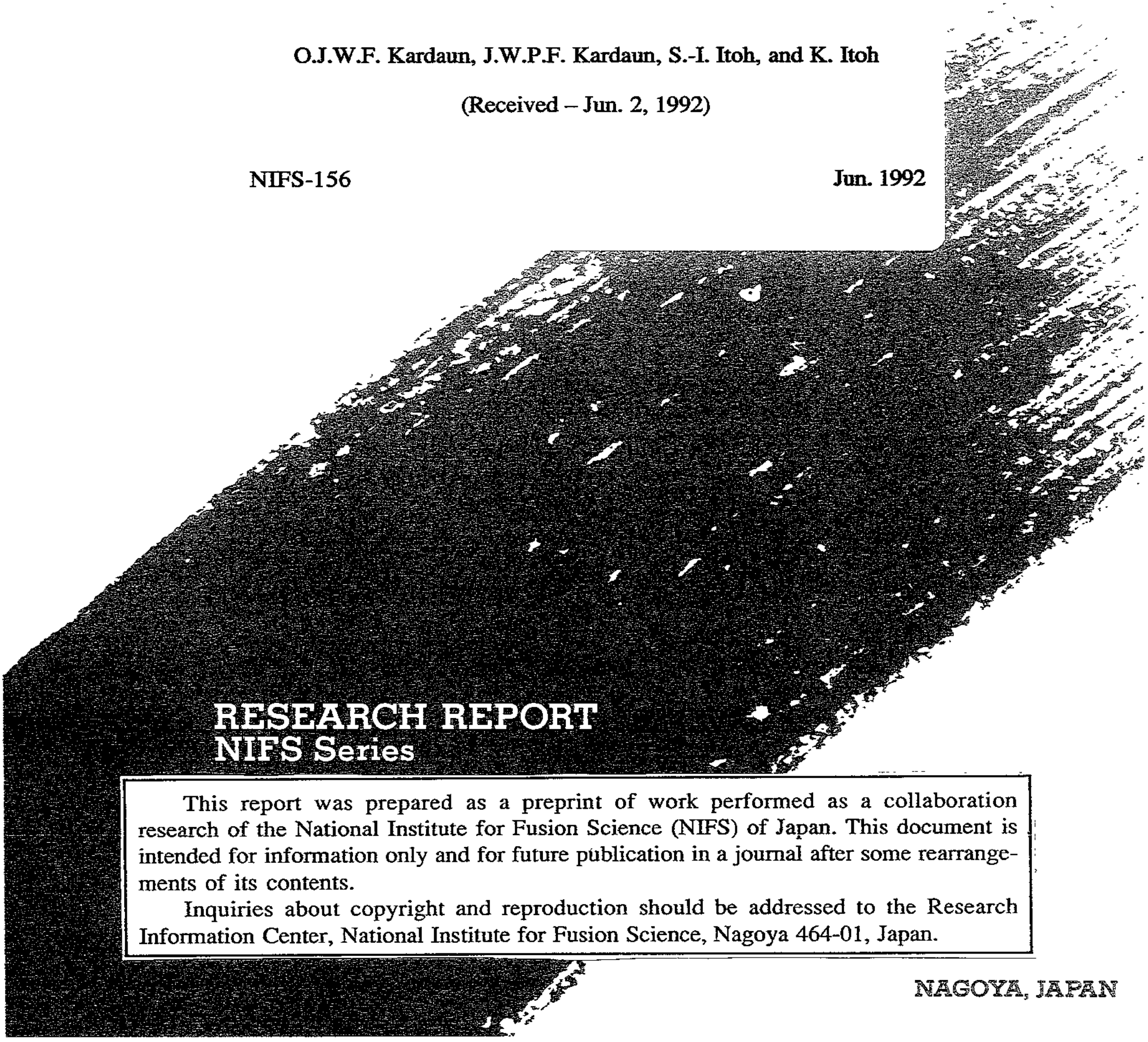

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Discriminant analysis of plasma fusion data

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Keywords
Quadratic discriminant analysis, SAS, multinomial independence model, INDEP, triangular plots, decision analysis, plasma fusion data.

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1. INTRODUCTION

Discriminant analysis is a branch of statistics with applications in many fields [9,11,12]. One of these (a relatively new one) is nuclear fusion research, where one is interested in various types of plasma discharges produced in toroidal devices. In many instances, one has a small number, say 2 or 3, of different types of discharges under investigation. For instance, L-mode and H-mode discharges (L stands for Low confinement, and H for High confinement), or: H-mode discharges without ELM's, with 'small' ELM's, and with 'large' (giant) ELM's. The abbreviation ELM's stands for Edge Localised Modes, which are detected by light recording instruments. They enhance the outward transport of the plasma, including the plasma impurities (which is a good thing), but if they are large, they produce a heavy heat load on material contacts of the plasma with the wall (which is not so good). There are typically 4 or 5 continuous variables, for instance plasma current I_p, magnetic field B_t, plasma electron density n_e, input heating power P_{inj}, that influence the type of discharge ('shot') that will occur. In addition, there may be a few (2 or 3) discrete variables that are physically expected to be important. Finally, there are a number of wall conditioning aspects, which influence the type of shots that will be produced.

In the framework of the ITER project, a collaborative effort between Europe, GUS, Japan and the USA, an international fusion reactor device is being designed which

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is due to operate at the beginning of the next century. In this context, a database (ITERH.DB1) has been assembled containing plasma confinement data of about 1000 H-mode discharges from 6 different Tokamaks [2]. These data have been released for general use by plasma physicists and other interested scientists. We will use part of these data to illustrate various discriminant analysis techniques.

Several discriminant analysis methods are applied and compared in [8] to predict the type of ELM's in H-mode discharges: (a) quadratic discriminant analysis (linear discriminant analysis being a special case), (b) discrimination by non-parametric (kernel-) density estimates, and (c) discrimination by a product multinomial model on a discretised scale. Practical evaluation was performed using SAS in the first two cases, and INDEP [6,7], a standard FORTRAN program, initially developed for medical applications, in the last case. We give here a flavour of the approach and its results.

2. THEORY

Consider a decision rule d: $\mathbb{R}^p \rightarrow \{a_1, \ldots, a_k\}$, and its associated losses $\ell(h, d(\underline{x}))$. The action a_j consists in assigning to group j $(j = 1, \ldots, k)$. The Bayes decision rule with respect to prior probabilities $\rho_1, \ldots, \rho_k$ is a decision rule that minimises, for each $\underline{x} \in \mathbf{R}^p$, the 'risk densities'

$$\sum_{h=1}^{k} \ell(h, d(\underline{x}))\rho_h f_h(\underline{x}).$$

For 0-1 losses, no doubt regions, and normal probability densities this reduces to: assign to that group h for which

$$D_h^2(\underline{x}) = (\underline{x} - \underline{\mu}_h)^t \underline{\underline{\Sigma}}_h^{-1} (\underline{x} - \underline{\mu}_h) + \log(det(\underline{\underline{\Sigma}}_h)) - 2\log\rho_h \tag{1}$$

is minimal, where $\underline{\mu}_h$ and $\underline{\underline{\Sigma}}_h$ denote the mean value and the dispersion matrix, respectively, of the distribution of group h. Inasfar as unknown, these parameters are replaced by estimators. For every pair (h, j) of groups, the set $\{\underline{x} | D_h(\underline{x}) = D_j(\underline{x})\}$ is a quadratic surface (possibly a hyperbola with two branches), which is linear only in the case that $\underline{\underline{\Sigma}}_h = \underline{\underline{\Sigma}}_j$. Even if the distribution of the data is not multivariate normal, one can use this rule as an approximate descriptive method.

Alternatively, the densities may be estimated nonparametrically, for instance by using kernel density estimates [10], or projection pursuit methods [3]. (To the authors' knowledge, the last approach is not yet implemented in the major standard statistical packages.) In these cases, the complexity of the boundary description is of the same order as that of the dataset itself, whereas for the quadratic surface it is of the same order as that of the covariance matrix of the datset. Therefore, as there are a large number of observations, the nonparametric methods in this case are used mainly to benchmark the performance of the quadratic allocation rules.

One way to estimate the performance of a discrimination rule is to look at the error rate estimated from the sample at hand while using the jackknife (or leaving-one-out method) to avoid an optimistic bias. Although this estimator has a rather large variance (in comparison with some others), it does not depend on the assumption of normality, so it can effectively be used to compare the various methods.

Many statistical packages, such as SAS, ask for prior probabilities, and use priors proportional to the sample fractions as default. Using equal priors always gives a worse allocation table, at least if the jackknife is not used. In the present context the whole concept of prior probability is rather artificial, as future discharges can be performed (within the operating regime) at arbitrary values of the discriminating variables I_p, B_t, etc. Nevertheless, the default procedure has some justification. To simplify the notation, let us consider 0-1 losses and 2 groups. By choosing formally $\rho_j = n_j / \sum_j n_j$, $j = 1, 2$, and integrating over $\mathbf{R}^p$, one effectively minimises

$$n_1 \int_{R_2} f_1(\underline{x}) + n_2 \int_{R_1} f_2(\underline{x}), \tag{2}$$

where R_1 and R_2 denote the allocation regions. This is the estimated total number of misclassifications for the sample sizes n_1 and n_2 and sampling distributions as in the dataset under investigation. So the procedure has an objectivistic interpretation, somewhat akin to minimising the sum of squared residuals in OLS regression. Moreover, for $\underline{\underline{\Sigma}}_1 = \underline{\underline{\Sigma}}_2$ it is equivalent to logistic regression, and for $\underline{\underline{\Sigma}}_1 \neq \underline{\underline{\Sigma}}_2$ probably to quadratic logistic regression. However, one should bear in mind that in future experiments, one may choose the experimental points according to another distribution, say $ng(\underline{x})$, where $g(\underline{x})$ is some normalised deterministic density (discrete, or, for an approximate description, continuous). The predicted number of misclassifications is now n times

$$\int_{R_2} f(1|\underline{x}) g(\underline{x}) d\underline{x} + \int_{R_1} f(2|\underline{x}) g(\underline{x}) d\underline{x}, \tag{3}$$

where $f(1|\underline{x})$ and $f(2|\underline{x})$ are the estimated posterior densities. For $ng(\underline{x}) = n_1 f_1(\underline{x}) + n_2 f_2(\underline{x})$, it reduces to (2). In practice, in SAS, such an error rate can be estimated by summing all but the largest posterior densities of a user generated distribution of observations in the TESTDATA dataset. As the posterior densities are estimated, the predicted number of misclassifications is a random variable. The asymptotic theory for constructing corresponding confidence intervals is rather complicated, but developed in [1], and implemented in [13], albeit presently still without the above integration with respect to $g(\underline{x})$.

An explicit loss function formulation is useful in our case, since misclassifying 'Non HSELM' discharges as HSELM is usually considered several times more costly than the opposite type of error. Allocation of the losses is determined in discussion with the physicists involved. As the loss allocation depends on the situation and contains subjective elements, it is convenient to have the procedures laid out in such a way that the effects of allocating different losses can be made directly clear to the decision maker, though there is the philosophical objection that the allocation of the losses should not be substantially influenced by the discrimination rule that comes out.

Table 1.
Univariate statistics of ASDEX H-mode discharges (in DN configuration) with small ELM's (HSELM) and 'no or giant ELM's' (Non HSELM)

	Non HSELM N=134		HSELM N=72				Non HSELM N=134	HSELM N=72
log:	Mean	SD	Mean	SD	T	F	W1	W2
Pinj	1.07	0.16	0.91	0.17	6.7	.	5.5	5.1
Ip	-1.10	0.12	-1.22	0.16	5.4	**	6.9	2.2
Bt	0.77	0.07	0.77	0.07	-0.8	.	-0.95	-6.3
Nel	1.39	0.19	1.33	0.12	3.0	***	0.35	3.9

***: $P < 0.001$, **: $0.001 < P < 0.01$, .: $0.4 < P < 0.6$

The column F denotes the significance of the F test for the equality of the Standard Deviations.
The column T gives the t-value for the equality of the Means, in the equal or unequal variance case (determined by the column F).
The columns W1 and W2 give the weights of the linear discriminant functions based on the dispersion matrices of the 2 groups, respectively.

Table 2.
Jackknifed misclassification tables of the ASDEX data, according to three different discrimination methods

Prior probability: HSELM = 0.35

	Allocated class: Non HSELM	HSELM	TOTAL	Non HSELM	HSELM	OTHER	TOTAL
True class:							
a) quadratic boundaries				b1) kernel density estimates (r=1)			
Non HSELM	114	20	134	130	4	0	134
Row %	85.1	14.9		97.0	3.0	0.0	
HSELM	34	38	72	43	29	0	72
Row %	47.2	52.8		59.7	40.3	0.0	
Total	148	58	206	173	33	0	206
Row %	71.8	28.2		84.0	16.0	0.0	
c) multinomial independence model				b2) kernel density estimates (r=0.5)			
Non HSELM	111	23	134	116	9	9	134
Row %	82.8	17.2		86.6	6.7	6.7	
HSELM	27	45	72	34	32	6	72
Row %	37.5	62.5		47.2	44.4	8.3	
Total	138	68	206	150	33	15	206
Row %	67.0	33.0		72.8	19.9	7.3	

3. PRACTICE

In Table 1, univariate summary statistics are given for the two groups of discharges (HSELM and non-HSELM), from which one can see that some discrimination will be possible, and that the covariance matrices of the two groups are not the same. The columns $\underline{W}_1$ and $\underline{W}_2$ display the weights of the linear discriminant functions utilising the sample covariance matrices of each of the two groups, respectively, i.e. $\underline{W}_j$ is an estimate of $\underline{\underline{\Sigma}}_j^{-1}(\underline{\mu}_2 - \underline{\mu}_1)$, $j = 1, 2$. At constant P_{inj} and B_t (see Fig. 1), the sets of linear boundaries are given by $6.9 \log I_p + 0.35 \log n_e = c_1$ and $2.2 \log I_p + 3.9 \log n_e = c_2$, respectively. For linear discrimination some pooled covariance matrix has to be taken, which lies 'somewhere between these two'. In this case, pooling is somewhat straining the discrimination, however, as the null-hypothesis of equal covariance matrices is rejected.

In Table 2, one sees the jackknifed (mis)classification tables of the quadratic discriminant analysis and of 2 non-parametric methods, applied to DN H-mode discharges from the ASDEX tokamak. As discriminators the four above mentioned plasma variables were used. Better discrimination is possible by including the time-history and the distance between the plasma and the wall into account [8]. One can see that less misclassifications for non HSELM discharges, but a few more misclassifications for HSELM discharges occur by using these uniform kernel density estimates. Note that for $r = 0.5$ some observations (those for which all other observations are at least 0.5 units away) are not allocated. Under the assumption of multivariate normality, which applies only approximately to these data, the 'optimal' values of r, according to a criterion by Rosenblatt, see [10], are not too far from 1, being 0.88 and 0.95 for the two samples, respectively.

For the multinomial independence model, each variable has been discretised into 10 groups (roughly according to the deciles). Except for one parameter describing the dependence between the variables, this model imposes an independent multinomial distribution, which is one way to avoid the explosion of the number of free parameters as the dimension and the number of classes increase. A bettter fit, albeit with a slightly more complicated interpretation, would be obtained by applying the multinomial independence model to the joint principal components, see [5], of the two datasets. At present we have not yet implemented this. To our knowlegde it is not standard available in any of the major statistical packages.

In Fig. 1, the quadratic discrimination is illustrated. The ellipses are sections of the 4-dimensional ellipses fitted to the data. In case of multivariate normal distributions, the 4-dimensional ellipses enclose about 95% of the data. The hyperbolae are sections of the quadratic discrimination surfaces. The values of *prat* denote the ratio of the posterior probabilities using the sample sizes as priors. The • symbols indicate the discrimination curve for equal losses. (There are 2 boundaries, only the left one goes through a region with sufficient data.) One can see that the two covariance matrices are not equal and that linear discrimination is expected to be somewhat less efficient (though possibly rather robust). If misclassifying non-HSELM is considered to be 3 times as costly than misclassifying HSELM discharges, then the discrimination curve is

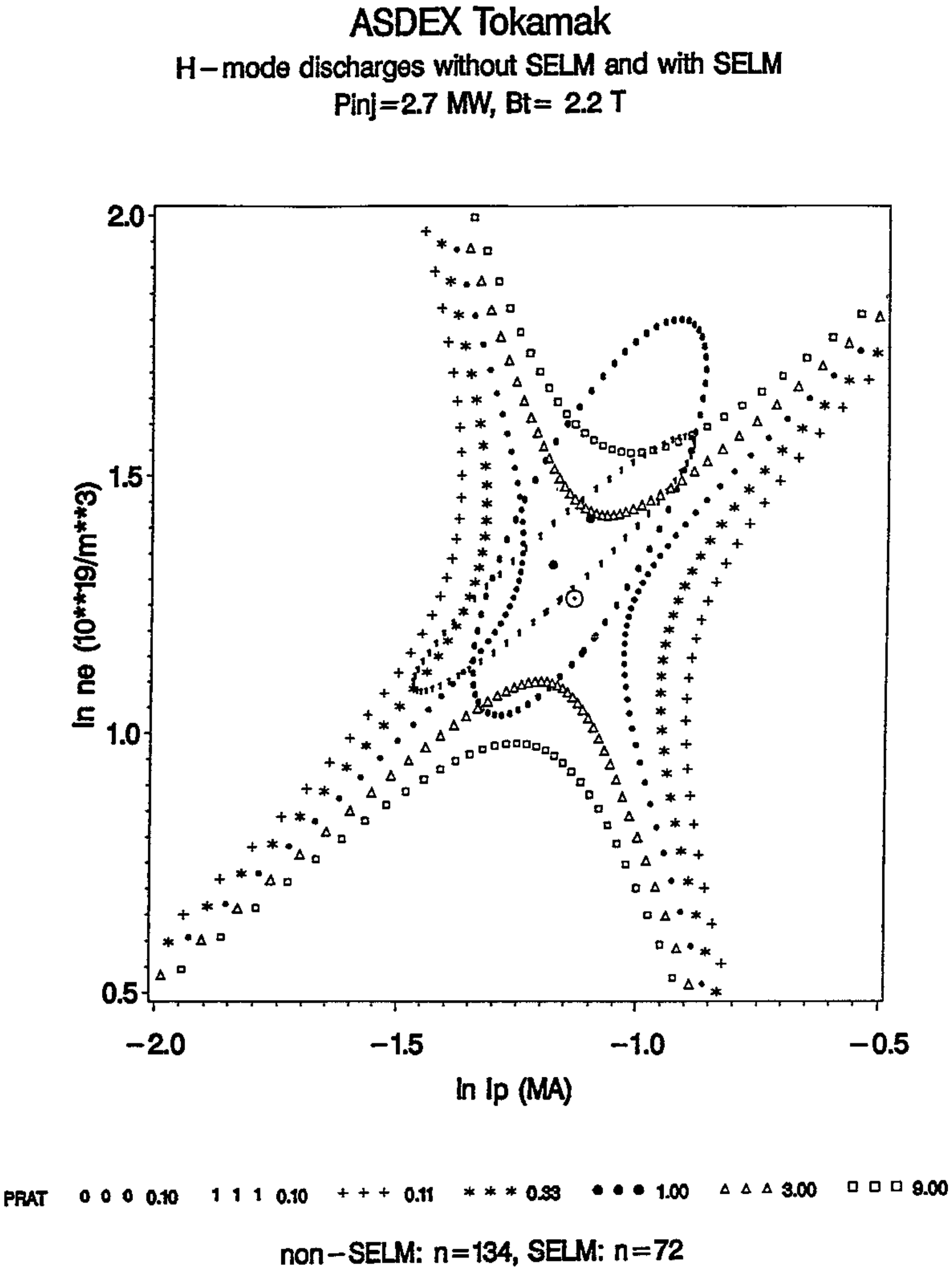

Fig. 1. Sections of fitted ellipses and hyperbolic discrimination surfaces for ASDEX DN discharges. Prat denotes the groups (non-HSELM=0 and HSELM=1), as well as the posterior probability ratio between non-HSELM and HSELM.

given by *prat* = 1/3. (For the values of n_e and I_p as specified in the plot, this reduces rather drastically the operating region where the desired HSELM's are expected to be producible). A general SAS/IML program has been written to produce these curves for arbitrary coordinate-plane sections, using a parametric representation. (At present it is not possible with PROC GPLOT in SAS/GRAPH to connect in an easy way the various contours separately. A two dimensional contour plot tends to give ragged curves, unless an immoderate number of points is generated.)

In Fig. 2, the posterior probabilities, according to the multinomial independence model, are plotted for the three groups (H, HSELM, HGELM). The length of a perpendicular onto one side of the triangle measures the estimated probability not to belong to the group indicated at the opposite edge. Outside the dashed triangle, one of the 3 posterior probabilities is larger than 50%. From the plot one can see that, with a few exceptions, many of the HSELM shots are correctly classified. There seems to be a group of HGELM shots that is difficult to discriminate from H, and another group that is difficult to discriminate from HGELM. There are a limited number of ELM-free H-mode points. It is more difficult to discriminate them from HGELM than from HSELM. The misclassification table 2^c can be viewed as a very collapsed version of this figure.

In summary, discriminant analysis can be used as a useful descriptive method of specifying regions where particular types of plasma discharges can be produced. Parametric methods have the advantage of a rather compact mathematical formulation. Pertinent graphical representations are useful to make the theory and the results more palatable to the experimental physicists.

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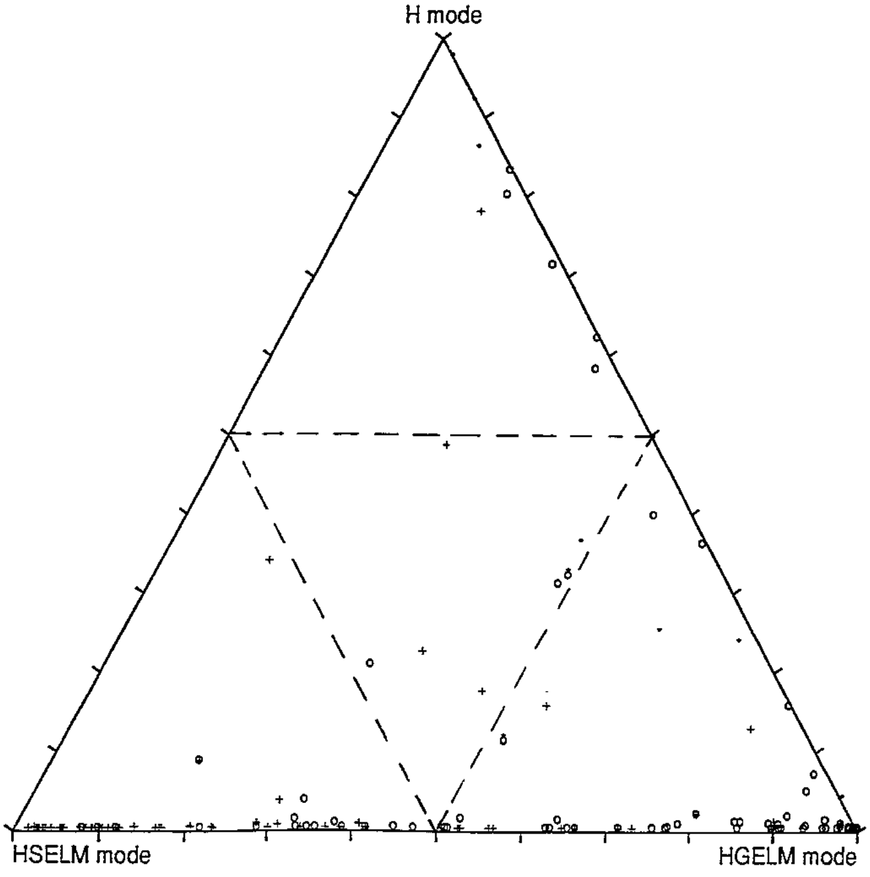

Fig. 2. Triangular posterior probability plot of ASDEX Double Null discharges (N=206), according to the multinomial independence model and using Bt, Ip, Pinj, and Nel as discriminating variables.

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