Center for Quality and Productivity Improvement
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Report No.30

DISCRIMINANT UPSET ANALYSIS

P. M. Berthouex, George E. P. Box, and A. Darjatmoko

May 1988

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PRACTICAL SIGNIFICANCE

Feedback and feedforward control are two strategies for keeping a process under control. Feedback control makes corrective adjustments on the basis of measurements on the output characteristics of primary interest. Feedforward is anticipatory. Rather than rely on measurements of the final product, it uses measurements on input and processing conditions. This paper presents discriminant analysis as a means of anticipating conditions that will lead to process upsets. Upsets are predicted by linear combinations of variables that characterize the inputs and the operating conditions. The method holds promise for diagnostic investigations and as an upset early warning system. It might be part of a feedforward control strategy. The method is illustrated for a wastewater treatment plant. This makes a good case study because (1) timely measurements of some important final effluent variables are not available and process control, therefore, must be based on influent and process variables and (2) upsets, once established, are persistent even when proper corrective actions are taken so an early warning of upsetting conditions is especially valuable.

Key Words: discriminant analysis, early warning, feedforward control, process upsets, wastewater treatment

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INTRODUCTION

Feedback and feedforward control are the two basic possibilities for keeping a process under control. Feedback control is corrective. It might be described as "wait for trouble and then fix things up." The typical use of quality control charts to detect deviations from targeted quality is part of a feedback control system. An advantage of this method is that decisions are made using measurements of the characteristic of primary interest, the final product. A disadvantage is that the control system always lags the process; the upset is detected after it has already occurred and the corrective action is applied even later. If the lag is great enough, feedback control becomes problematic and feedforward control becomes more attractive. Anticipation is better than reaction.

Feedforward control tries to anticipate upsets by detecting troublesome conditions before they enter the process and by making adjustments that will avoid the potential upset from becoming reality. Doing quality control on raw materials is a simple and powerful realization of the feedforward quality control philosophy.

Anticipatory control, of necessity, does not depend on measurements of product quality. Implementation, therefore, requires identification of variables that can be used in a model to compute a "measure of anticipated success." This measure may be useful for computing a corrective adjustment to the process. The process model may be mechanistic or empirical; it could be a dynamic model, for example an ARIMA time series model. Having to identify the key variables and the model are disadvantages of this method and present difficulties that often explain the popularity in practice of feedback control.

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There are two situations when anticipatory control is highly desirable: (1) when the results of key measurements on the final output are delivered too slowly to be useful and (2) when an upset, once established, cannot be quickly rectified (for example, in a process that has a long residence time, great inertia, or strong "memory").

In this report, we present preliminary work on using a discriminant function to compute a "score" from multivariate anticipatory measurements. A set of variables is used to characterize the process and to classify conditions as "normal" or "upset". The method holds promise as an "early warning system."

It also has an attractive diagnostic property, and so may be helpful in systems where early warning is not required. In this context, the discriminant analysis helps us identify which of several variables are associated with problems. Such a diagnosis, by pointing out which variables appear to be important, could lead to intelligent experimentation with the process. This experimentation might be evolutionary process (EVOP), an online strategy of collecting information about the system while the system continues in production.

DISCRIMINANT ANALYSIS

Discriminant analysis is a process of deriving classification rules from samples of classified objects. These rules can then be used for classification of new objects of unknown class [6],[7]. The objects are day-to-day outputs of a process which can be classified as being produced by either a normal operating condition or an upset. An upset is a signal that the plant is out of control and that something must be done to put it back to normal operation [2],[3]. It is desirable that the development of upsetting conditions can be determined before the upset happens, so the operator can be alerted to take preventive actions, if possible. The prediction is done by applying a set of rules or functions to plant operation attributes, e.g. influent and process parameters, and use the result to determine the class of that particular operation.

The discriminant analysis technique has been evolving since it was first introduced by Fisher in 1936. It has developed from the intuitive approach of Fisher to the probabilistic approach by Welch and Rao, followed by the Waldian approach based on statistical decision theory, and more recently to using nonparametric techniques [7].

In this paper, we will use only the classical Fisher discriminant analysis which will produce linear discriminant functions. The criterion of Fisher discriminant analysis is identifying the linear surface which best discriminates between two classes. This is equivalent to finding the direction (the normal to the above surface) along which two groups are best separated. Fisher defined the separation between two groups in a particular direction as the distance between the means of the two groups standardized for within-group variance in the specified region.

The criterion can be satisfied by maximizing the ratio of between-class scatter to within-class scatter. In other words we want to maximize

$$C = \frac{\text{distance between sample means}}{\text{standard deviation within sample}}$$

DISCRIMINANTS AS EARLY WARNING INDICATORS OF PROCESS UPSETS

One question is whether early warning indicators can be found to predict likely occurrence of operating difficulties.

Suppose that on day t we record various measurements, such as temperature, x_{1t}; flow rate, x_{2t}; blower pressure, x_{3t}; solids concentration, x_{4t}; etc. We denote the aggregate of all measurements made on the t^{th} day by the vector $\mathbf{X_t}$.

Suppose now we look through the records and isolate a number of **n** instances occurring at times t = r, t = s, . . . , where a particular problems *has* occurred, and a number of **m** instances occurring at times t = u, t = v, . . . , where it *has not* occurred, and that we use $y_t = +1$ to indicate occurrence and $y_t = -1$ to indicate non-occurrence at time t.

Then we will have data of the form

	...	$\mathbf{X_{r-2}}$,	$\mathbf{X_{r-1}}$,	$\mathbf{X_r}$	$y_r = +1$
n observations	...	$\mathbf{X_{s-2}}$,	$\mathbf{X_{s-1}}$,	$\mathbf{X_s}$	$y_s = +1$
(problem occurred)	.	.	.	.	.
	.	.	.	.	.
	...	$\mathbf{X_{u-2}}$,	$\mathbf{X_{u-1}}$,	$\mathbf{X_u}$	$y_u = -1$
m observations	...	$\mathbf{X_{v-2}}$,	$\mathbf{X_{v-1}}$,	$\mathbf{X_v}$	$y_v = -1$
(no problem occurred)	.	.	.	.	.
	.	.	.	.	.

Such data may be solved using discriminant function analysis.

If we assume that a *linear* discriminant function is appropriate, standard procedures allow us to estimate a discriminant function

$$\ldots \mathbf{a}_2'\, \mathbf{X}_{t-2} + \mathbf{a}_1'\, \mathbf{X}_{t-1} + \mathbf{a}_0'\mathbf{X}_t = \mathbf{Y}_t$$

which may be computed at any time t such that:

if $y_t > y_0$ then occurrence of the problem at time t is indicated

if $y_t < y_0$ then occurrence of the problem at time t is not indicated.

This is called the *lead-zero predictor*. Also, it will be possible to compute the probability of problem occurrence for each set of predictor **X**'s.

Now we want to be able to predict problems ahead of time. We can therefore repeat the analysis omitting the last column of X's from the data. This will yield a discriminant function that uses data up to time (t-1) and predicts possible trouble at time t, thus answering the question "What is the best linear discriminant function of predicting trouble one day ahead?" This is called the *lead-one predictor.*

An analysis omitting the last two columns of **X**'s from the data provides the *lead-two predictor*, answering the question "What is the best linear discriminant function for predicting trouble 2-days ahead?" and so on.

Formally the analysis at each stage is like a regression analysis of the ± 1's of the y's onto the X's. One difficulty is the very large number of individual coefficients in $\mathbf{a}_0'$, $\mathbf{a}_1'$, $\mathbf{a}_2'$, etc. that need to be estimated, possibly from rather scanty data. Now the objective is only to find a good predictor (not necessarily to understand why it works).

Geometrically the concept of a linear discriminant function involving p predictors x_1, $x_2, x_3, \ldots, x_p$, is to find a hyperplane

$$a_1 x_1 + a_2 x_2 + a_3 x_3 + \cdots + a_p x_p = y_0$$

in p dimensions which best separates occurrences (+'s) from non-occurrences (–'s). We are also concerned with which set of p predictors give best separation. Figure 1 illustrates the situation for $p = 3$.

More generally, some nonlinear discriminant

$$f(x_1, x_2, x_3, \ldots) = y_0$$

in which the +'s and –'s are separated by some non-plane surface might be sought.

Three possible approaches are:

(1) to use subset regression: We could for example set the computer the task of finding the best equation employing only p individual predictors $x_{i,t-d}$ (where i = 1, 2, 3, . . ,p). This could be done using some canned method and canned program or simply by evaluating all possibilities.

(2) to use summary statistics: Such statistics could be used to describe the local properties of the series and we could then perform our regression on these. They could, for example, be local moving averages, exponentially weighted moving averages (EWMA), cumulative sums (Cusum), trend indicators, or residuals from any of the above.

(3) to combine these two approaches.

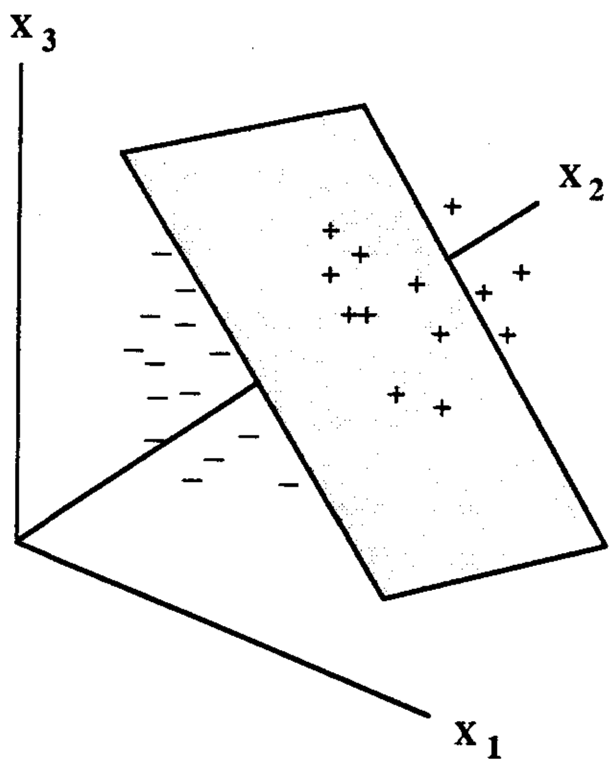

Figure 1. The geometrical concept of a linear discriminant

EXAMPLE - WASTEWATER TREATMENT PLANT UPSETS

As an example we have used a wastewater treatment plant. It has several characteristics that make application of traditional control methods problematic [11],[12]:

(a) There is no control possible on process inputs; the system must process what comes, when it comes.

(b) The process has a long "memory" and detecting an upset after it has occurred may mean several days of unacceptable performance.

(c) A key measure of effluent quality required by law, the 5-day BOD, is worthless for process control purposes, because it is not available until five days later. Possible surrogates for the 5-day BOD have been considered flawed in various ways and are generally not measured.

(d) The process is mechanistically complicated and building an adequate model is, at best, difficult . Even when a model has been developed, it contains many parameters that are difficult to estimate and the parameter values change with environmental conditions.

(e) The process mechanisms, while difficult to capture in a model, are understood well enough to know which variables are likely to be useful as indicators and how these variables affect process behavior. So, while the method is empirical in some respects, it is possible to interpret the information mechanistically, though qualitatively.

This report discusses only the construction of the discriminant function and evaluates its potential for classifying process conditions. The applications to process control have not been made, but it will be shown how the function might be inverted to identify the variables that are most influencing the process.

The example under study is an activated sludge treatment process. It consists of a biochemical stage and a separation stage. The biochemical reactions that are exploited in this process are the same that would occur naturally in a stream. The "activated sludge" is a mass of bacteria that is mixed with the incoming wastewater and aerated. These bacteria consume the organics in the wastewater, converting it to new bacterial cells, carbon dioxide, and water. These biochemical reactions are accomplished in an aeration basin. The bacterial mass is separated by quiescent gravity settling in a final clarification basin. When the process is healthy, the bacteria grow in clumps that will quickly settle from the liquid to leave a crystal clear effluent that can be safely discharged into a stream.

The process can be "upset" in several ways [2],[3]. The most serious, because it takes a long time to correct, is to destroy the ecological balance of the activated sludge such that it loses the property to separate from the liquid. When this happens the effluent quality will be poor. Poor effluent quality can also be caused by exceeding the organic or hydraulic processing capacity, by providing too little aeration, or by letting the mass of activated sludge fall below a critical level.

The process will be characterized as being "normal" or "upset" according to the measures of effluent quality that are required by the Clean Water Act. These are biochemical oxygen demand (BOD) and suspended solids (SS). Both measures should be low. Most plants are required to discharge, based on the 30-day averages, less than 30 mg/L of BOD and 30 mg/L of SS. A well operated plant will have levels between 10 and 20 mg/L for each variable. When the process is unhealthy, both variables tend to increase. The BOD takes five days to measure and so is worthless as a control variable. Here we have used a record of past BOD data to construct the discriminant function and to test the method. SS, on the other hand, can be measured within 1-2 hours and is useful.

The processing conditions are measured in terms of:

Influent characteristics:

- RSFLOW is raw sewage *flow rate*,
- RSPH is raw sewage *pH*
- RSTEMP is raw sewage *temperature*, and
- RSSS is raw sewage *suspended solids*

Process operating conditions:

- MLSS, or *mixed liquor suspended solids*, is a measure of the concentration of bacteria working in the system. A high value generally improves treatment efficiency and makes the process more stable.
- SLAGE indicates *sludge age*, a measure of the average length of time that the bacteria are kept in the system. A higher value usually makes the system more stable, i.e. better able to resist unfavorable conditions.
- DO is the *dissolved oxygen* concentration in the aeration basin. Too little oxygen and the bacterial metabolism will be insufficient to purify the waste; it may also allow poorly separable bacteria to infest the system.
- RAS indicates *return activated sludge*, a measure of how much of the bacterial mass is recirculated from the final clarifier back to the aeration basin.

- WAS is *waste activated sludge*, a measure of how much of the bacterial mass is removed from the system. Increasing WAS will decrease MLSS and SLAGE.
- SETTL indicates the *settleability* of the bacterial mass. A low value is desirable. The operator cannot set the value of SETTL; it is a consequence of the other operating conditions. It is very easy and fast to measure.

Increasing MLSS and SLAGE tend to make the system more efficient and more stable. Unfortunately, there are persuasive reasons for keeping them low. As they increase, the need for aeration increases. Aeration is expensive, usually the largest single cost of treatment. Small changes in MLSS and SLAGE may represents thousands of dollars in operating costs. Also, there is an operational constraint. If MLSS and SLAGE are pushed too high, it will become impossible to keep the DO above the critical level.

A one-year long record of daily performance data from a treatment plant in Saginaw, Michigan, will be used in this analysis. To reduce the noise caused by sampling and measurement error, the exponentially weighted moving averages (EWMA) are used instead of the original data set [8]. The EWMA can be easily calculated by the recursive formula [4] :

$$\mathrm{EWMA}(t) = \lambda * \mathrm{DATA}(t) + (1-\lambda) * \mathrm{EWMA}(t-1)$$

Choosing $\lambda = 0.3$ results in a reasonable smoothing effect similar to that of a 7-day moving average. The occasional variation is largely eliminated while the general pattern of fluctuation and trend is retained. Figure 2 shows the original and the smoothed data.

The data is split into two sets, namely the "design set" and the "training set". The design set contains all the attributes and the classification which means that each day of the set is assigned either normal or upset. As the name implies, the decision rules will be "designed" from this set. The training set contains days with all the attributes and also the classification. This training set will be classified using the rules produced by the design set, and the results are compared to the actual group membership. The misclassification rate or the error rate is the rate of being classified to the other group.

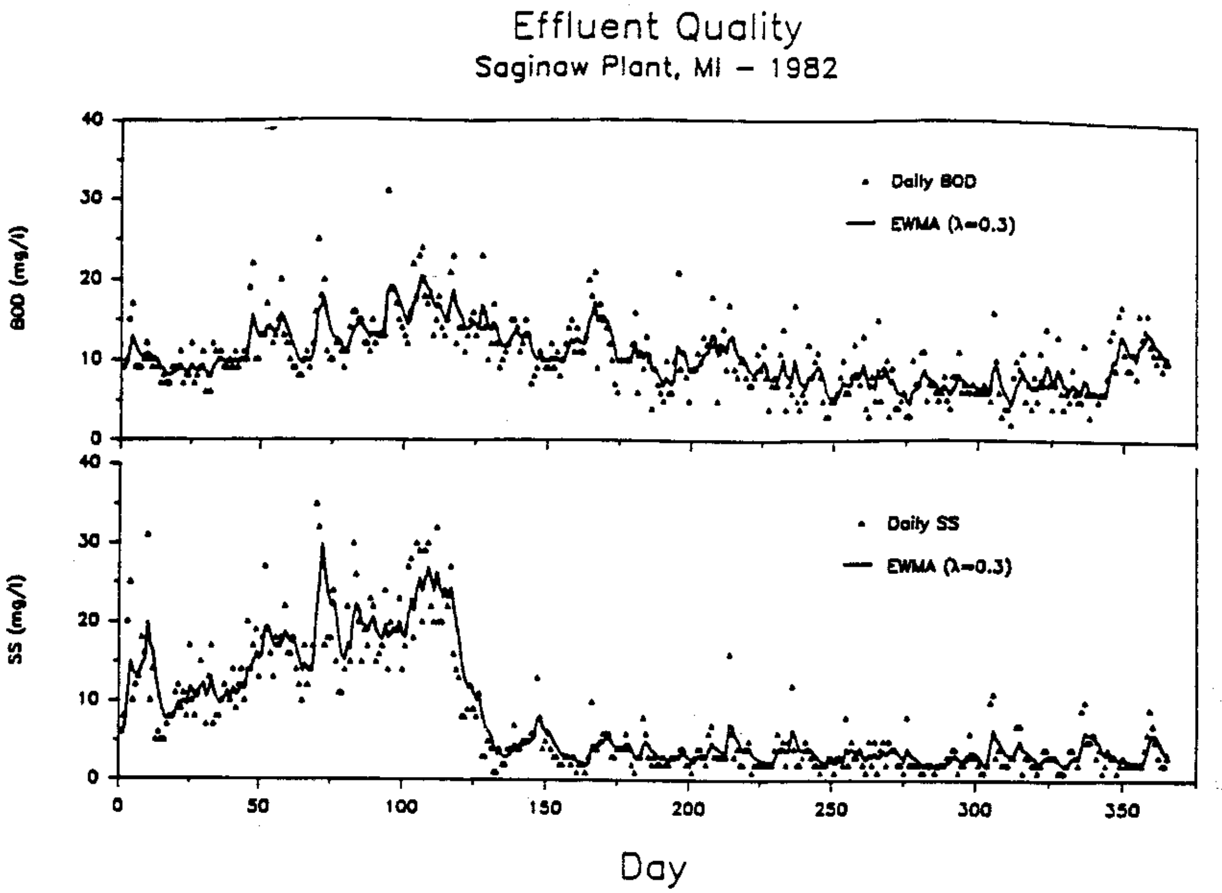

Figure 2: Plot of daily effluent BOD and SS and the associated EWMA with $\lambda=0.3$ (Data from Saginaw Treatment Plant, Michigan - 1982)

After studying a plot of effluent BOD vs SS, Figure 3, it seemed reasonable to consider that an upset exists if both BOD and SS are both high, so the following criterion was tried:

$$\begin{aligned} &\text{U(pset)} \quad \text{if } \text{BOD} + \text{SS} > 35 \text{ mg/l} \\ &\text{N(ormal)} \quad \text{if } \text{BOD} + \text{SS} < 35 \text{ mg/l} \end{aligned}$$

We note that "high BOD+ low SS" (or vice versa) could signal an upset according to this criterion. This may not be the expected behavior of the process, but we prefer to have such an occurrence brought to the operator's attention. It might be an unusual form of process upset, or it might indicate a problem in the measurement system.

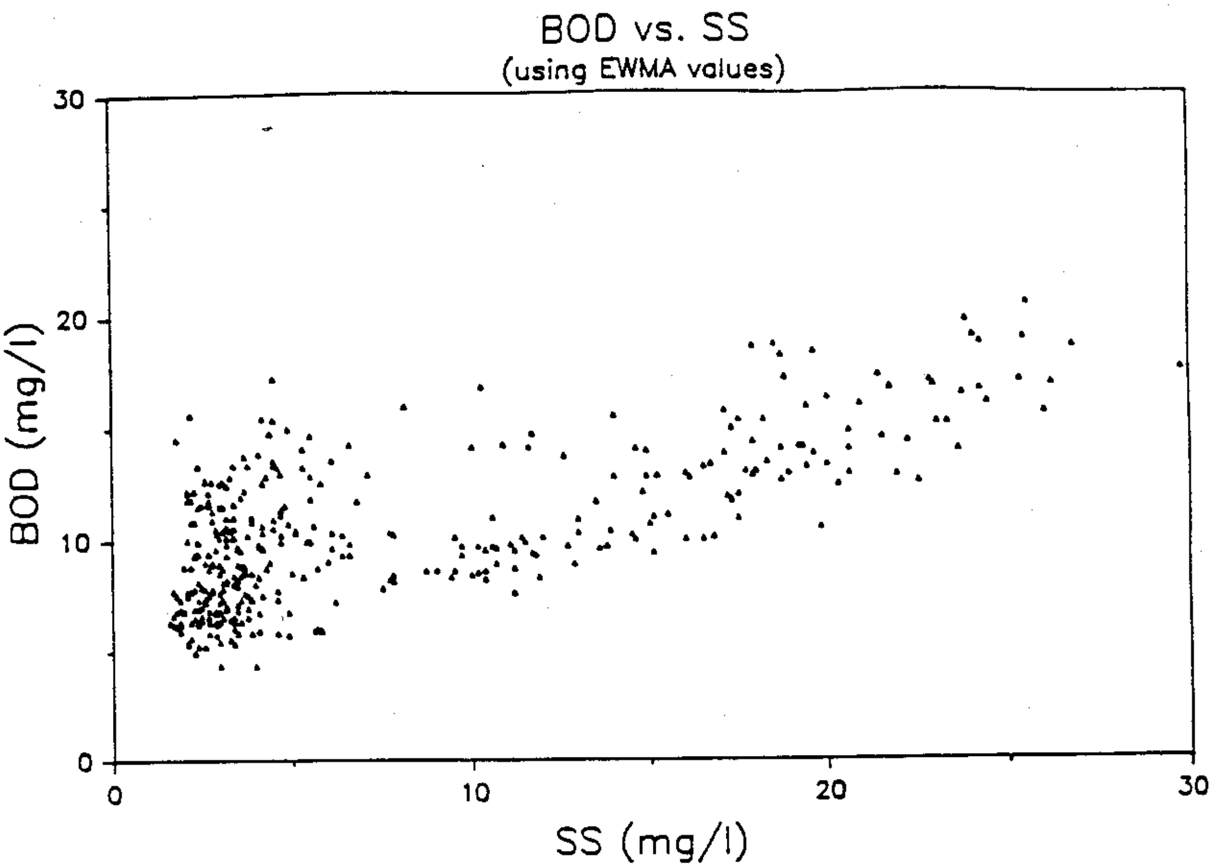

Figure 3: Plot of effluent BOD against effluent SS for Saginaw Plant - 1982

There are also some clusters of low BOD and low SS and it should be interesting to learn what combination of conditions yields such desirable performance. A third classification group was added, giving the following criterion:

U(pset)	if	BOD + SS	> 35 mg/l
N(ormal)	if	10 < BOD + SS	< 35 mg/l
L(ow)	if	BOD + SS	< 10 mg/l

There are 35 days of upset according to the above criterion. Since the occurrence of upsets is much less than that of normal operation, the proportion of upsets to normals was used as the prior probability of membership for calculating the posterior probability.

RESULTS

The discriminant analysis was performed using the Multivariate General Linear Hypothesis (MGLH) module in the SYSTAT statistical package [9],[10]. The design set was used to determine the best *lead one predictor* discriminant functions. Since we have specified three groups, two functions are needed to classify them. The discriminant coefficients, the weights for the linear combination function, are listed in Table 1.

Table 1. Weights, or Discriminant Coefficients, standardized by the conditional (within groups) standard deviations used to compute the *lead one predictor* discriminant scores.

Variable	Factor (1)	Factor (2)
RSFLOW	−0.054	−0.967
RSTEMP	−0.412	−0.111
RSPH	−0.348	−0.053
RSSS	0.077	0.169
SLAGE	0.092	0.205
MLSS	0.411	0.119
FMRATIO	0.173	0.224
SETTL	0.006	1.036
DO	0.088	0.601
RAS	−0.709	−0.895
WAS	−0.217	0.449

The discriminant scores are computed using the above discriminant coefficients and standardized discriminators, for example:

$$\text{Factor (1)} = -0.054 * \text{rsflow} - 0.412 * \text{rstemp} - 0.348 * \text{rsph} + \ldots\ldots$$
$$\text{Factor (2)} = -0.967 * \text{rsflow} - 0.111 * \text{rstemp} - 0.053 * \text{rsph} + \ldots\ldots$$

where the lower case indicates the standardized value of the original observation (e.g. rsflow is the standardized value of RSFLOW).

Factor (1) is dependent largely on RSTEMP, RSPH, FMRATIO, MLSS, RAS, and WAS. Factor (2) is most dependent on RSFLOW, SETTL, DO, RAS, and WAS. Canonical correlation coefficients of 0.765 and 0.430 for Factor (1) and Factor (2), respectively, show the

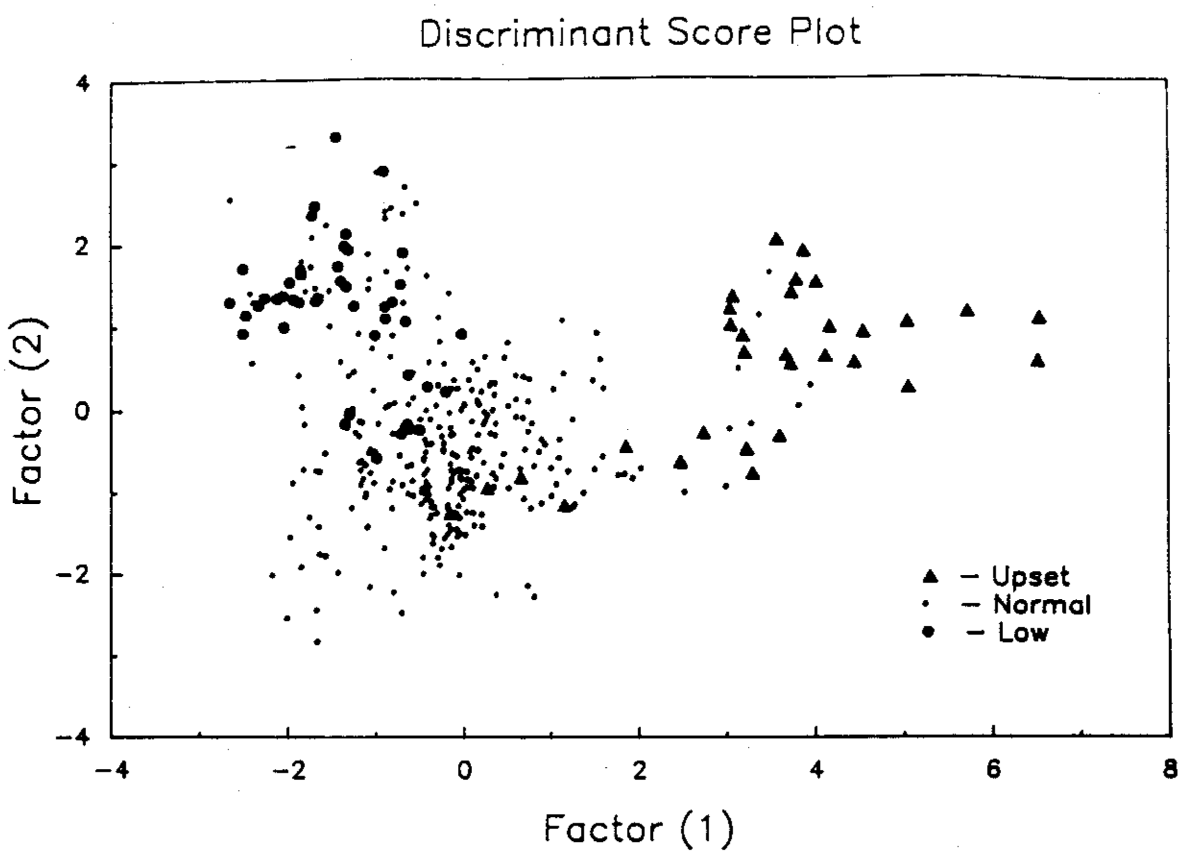

Figure 4: Plot of discriminant scores for 3-group classification.

relative contribution of each factor to the discriminating power.

Plotting each day as a function of Factor (1) and Factor (2), in Figure 4, shows the clustering of the three different groups.

The misclassification rates are given in the Tables 2a and 2b. Reclassifying the design set gives the error rate, often called the *apparent error rate*, of 2 out of 16 upsets. Two upsets were wrongly classified as normal, and five normals were classified as upsets.

The *true error rate* can be computed from classifying the training set data. Three out of 15 upsets are misclassified and 3 normals are classified as upsets.

The misclassification happens mostly on the boundary of a group, since there is seldom perfect separation of the groups. The distributions of the groups overlap somewhat in the tail areas. The misclassification of normals as upsets may not be a serious problem, since it is manifested only as "false alarm." Making an unnecessary control adjustment will do no harm and costs nothing. The reverse, however, is not true. Misclassification of upsets can be damaging because the operator misses the chance to prevent a loss, or perhaps even to prevent an even larger upset. An alternative solution to this ambiguity is done by treating the overlapping area of two adjacent groups (in this case: upset and normal) as another group. When a particular observation happens to fall in this area, the operator can be advised to look at the process closely before making any adjustment. By manipulating the size of this area, the impact of misclassification can be minimized [1],[5].

Table 2a. Classification Table for the Design Set

		(Predicted)			
		L	N	U	TOTAL
(Observed)	L	15	8	0	23
	N	11	127	5	143
	U	0	2	14	16
	TOTAL	26	137	19	182

Table 2b. Classification Table for the Training Set

		(Predicted)			
		L	N	U	TOTAL
(Observed)	L	11	12	0	23
	N	11	130	3	144
	U	0	3	12	15
	TOTAL	22	145	15	182

SUMMARY

The discriminant analysis has been performed on daily performance data of a wastewater treatment plant. Using most of the influent and process variables, a set of rules that determine the normal/upset condition can be found. These rules appear to correctly predict the proper condition of the plant. A plot is still needed to detect misclassification on the boundary between groups.

The method holds promise for diagnostic investigations and for giving an early warning of upsets. Measures of final product quality are not used. Instead the process is "scored" using a set of indicator variables. This approach is necessary when final product quality data are not available on a timely basis. It is desirable where foresight is better than hindsight.

FUTURE WORK

Variable selection will be the object of investigation in the future. If an adequate subset of original measurement can be found without degrading the accuracy of classification then only this subset need be measured on all future objects to be classified. This will result in a much simpler model and less cost to obtain data needed for classification.

The issue of normality and the effect of serial correlation existing in treatment data will also be investigated. Properly transformed data will satisfy the multi-normality requirement of the analysis, while considering the serial correlation effect may result in a more precise estimate of the true variance.

Future work will investigate the inverse problem of making control decisions based on the discriminant function classification. Some set of the indicator variables can be partitioned into "control variables" and "status indicators." The relative influence of each control and indicator variable needs to be assessed and adjustments proposed.

Most important, we believe that this method has application in other industries, in particular the manufacturing industry, and we look forward to trying it on such a problem. It is our hope that by making use of a collection of informative variables that upsets can be anticipated and that control can be based on foresight rather than hindsight.

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