One of the earmarks of progress in a discipline is the shift from impressionistic description to the more objective practice of qualitative categorization and eventually to the rigorous procedures of quantitative evaluation. In the field of physical medicine, for example, gross observation originally gave rise to the classification of all diseases in which a wasting of tissue took place as consumption. Castiglioni (1947) traces the gradual analysis of consumption into the disease entities known today as diabetes, leprosy, tuberculosis, cancer, etc., from the discovery by Thomas Willis in 1670 that the urine of some consumptives was sweet (op.cit., p. 541), to the recognition by Gaspard Laurent Bayle in 1810 of six kinds of consumption (op.cit., p. 700), to the first accurate description of leprosy by M.C.C. Leloir in 1886 (op.cit., p. 737) after the discovery of the leprosy bacillus by A. Hansen in 1875 (op.cit., p. 817), and to the discovery by Koch in 1882 of the tuberculosis bacillus (op.cit., p. 817). Thus, each group of patients with one or more unique characteristics in common, not found in the other subgroups, was finally identified as a separate entity.

Psychiatric medicine, however, has not quite reached this level of specificity. The classification which brought the nosology of physical disorders into being began in the 18th century soon after the abandonment of the ancient notion that all disease was caused by disturbances of the four bodily humors. In psychiatry, the term insanity still lingers as a vestige of the earlier
conception of mental disease. It was not until late in the 19th century that the modern nosology of separate mental disorders was evolved by Emil Kraepelin (1893).

One of the disease entities which Kraepelin delineated was dementia praecox, which Bleuler (1950) later broadened into schizophrenia. In the earlier literature, during the period when Kraepelin's diagnostic procedures were followed, much more regularity was reported in such characteristics of schizophrenia as incidence rates, release rates, etc. With the broadening of the concept by Bleuler, the earlier consistencies seemed to disappear. Perhaps Bleuler's attempt was a step in the wrong direction -- apparently science proceeds by narrowing rather than widening concepts.

Kraepelin had hoped that by studying large populations with the aid of psychological tests he could discover those who were prone to become mentally ill. He wrote as follows:

As soon as our methodology has sufficiently proved itself through experience with healthy individuals, it would be possible to approach the actual ultimate goal of these efforts, the investigation of sick personality, especially of the inborn pathological disposition. In an investigation of many individuals we will always find some who deviate profoundly from the behavior of the vast majority in one or another aspect. If this deviation appears to be damaging to the mental life, and if it reaches a certain degree -- which admittedly can only be arbitrarily determined -- then we tend to regard it as an illness. Experience teaches us that persons with pathological traits of this kind are, on the whole, in greater danger of a general mental disturbance than those personalities (natures) whose characteristics are in the middle range.
We therefore have first of all to investigate whether it is possible by means of psychological tests to determine individual deviations which cannot be recognized by ordinary observation. If that succeeds, we would be in the position, through the quantitative determinations at our disposal, to establish the borderline between health and disease much more precisely and more validly than has been possible so far (Kraepelin, 1896, p. 77).

If one were to follow Kraepelin's suggestion, he would use such well-identified groups as registrants for military draft, random samples of birth registers, or entire populations for psychological investigation, and pick off the deviant individuals for scrutiny. Until such time as these plans are possible, however, one is forced to use the available diagnoses as starting points, apply a variety of psychological and other tests, and use statistical techniques for determining the subgroups that exist.

One of the acute problems now facing the research biometrician in the field of psychopathology arises from the fact that most diagnoses are based on subjective judgments whose reliability is often not very high. Consequently, any particular group of patients who carry a specific diagnostic label is often found to contain individuals who differ from each other both in level of performance on a given series of tests, and also in the interrelationships among these performances, some individuals showing positive trends while others show negative trends on the same set of variables. As a result, comparisons of one diagnostic group with another, or with a normal control group, often yield insignificant differences because of the high interindividual variability within these diagnostic groups. Indeed, studies in which samples of normals were compared with samples of schizophrenics, from more than twenty-five years ago (Jellinek, 1936) to the present (Sutton, Roehrig & Kramer, in press),
have invariably found that schizophrenics are more variable in performance than are normals. While this difficulty is not uncommon in medical, psychological and social diagnoses, the frequent absence of any objective indicators for making diagnoses in psychopathology makes the heterogeneity in this field a particularly serious problem.

The statistical techniques for dealing with this problem are in a rather primitive state of development. While several methods are available for finding the best set of weights to apply to a series of variables in order to discriminate between two or more populations, they are not applicable to the problem considered since there are no segregated populations to begin with. Instead, the natural lines of cleavage within the diagnosed group must be found so as to separate it into its natural subgroups.

Existing Techniques

As a first step in the direction of partitioning a population into homogeneous groups, Zubin (1938a; 1938b) provided the method of like-mindedness analysis, which is suitable for finding individuals who tend to cluster on such discrete variables as response to dichotomous or trichotomous items. In dealing with quantitative data, however, the like-mindedness method cannot be applied without loss of information due to dichotomization or trichotomization.

A solution to the problem of separating a population into subgroups on the basis of one variable was proposed by K. Pearson (see Rao, 1952, pp. 300-304). For the case of two hypothesized groups, the method consists of equating the first five sample moments to weighted averages of the subgroup moments, and solving the resulting equations for the subgroup means, the subgroup variances, and the proportion of mixture. The distribution of the variable is assumed
to be normal in each subgroup, so that the subgroup moments are functions only of the mean and variance. The subjects in the sample may then be assigned to one or the other group, and the groups can be studied to see what other characteristics the subjects within them tend to have in common. Rao (1952, p. 300) states that a solution based on the method of maximum likelihood also exists, but that the computations involved are very complicated.

The techniques based on the method of moments and on maximum likelihood can, at least theoretically, be extended to cases where more than two groups are assumed to exist, and to cases where more than one variable is involved. The number of parameters to be estimated, and the complexity of the set of equations to be solved, however, increase quite rapidly.

Each of these two procedures, it should be realized, is concerned with the problem of estimating the parameters in the subgroups assumed to exist. The problem at hand, however, is more one of classification than estimation. It would therefore follow that a procedure which aims primarily at clustering subjects, and which places little or no emphasis on the matter of estimation, will be most efficient in terms of time and labor, in spite of its perhaps being less efficient than other methods in a statistical sense.

One such method is that of Q technique, or so-called inverse factor analysis. For descriptions of this procedure see Cattell (1952); Cronbach (1953, pp. 376-388); Mowrer (1953, pp. 316-375); Nunnally (1955); Sakoda (1954); Stephenson (1935); Stephenson (1952). Applied to the problem being discussed, the method consists of measuring each subject in a sample on a number of tests, obtaining standard scores, and computing a correlation coefficient for each pair of subjects across all tests. The techniques of factor analysis are then applied to the matrix of inter-individual correlations, and the factors found are generally taken to define the subgroups. In view
of the many theoretical criticisms of factor analysis, in addition to the fact that a correlation between two persons does not have any simple interpretation, there is serious doubt as to the validity of this approach. Monro (1955) applied inverse factor analysis to a sample of 200 patients, and he was able to specify some thirteen "types" of mentally ill. The number of patients in each group varied, however, from three to thirty-five, while fifty of the 200 patients could not be classified at all. These facts, together with the fact that the basic measure of similarity was tetrachoric correlation, would tend to make any description of these types tenuous at best.

Factor analysis has also been applied to a matrix of distances rather than correlations by Nunnally (1962), but the theoretical arguments against factor analysis in general apply here too.

Two techniques which have recently been proposed use, as the basic measure of proximity between persons, the distance between the points which these persons determine, when the set of scores is viewed as determining a point in Euclidean space of as many dimensions as there are tests. For a discussion of the superiority of distance measures over correlation-like and other measures of similarity, especially in regard to the fact that distance preserves information on both shape and level differences, while correlation ignores the latter, see Cronbach and Gleser (1953). One such clustering technique is that given by Sawrey, Keller, and Conger (1960). Briefly, the procedure is to establish potential nucleus groups by grouping profiles whose distances one from another are less than some specified maximum distance, and then to add systematically to these nucleus groups the remaining profiles, by gradually increasing the maximum allowable distance.
This method suffers from a number of deficiencies, not the least of which is the fact that the problems of correlated variables and unstandardized tests are not faced. Also, the possibility exists that the groups ultimately found will be so homogeneous as to be a little usefulness. Finally, there are no suggestions given for determining whether the original sample is sufficiently homogeneous on the given variables to vitiate any fractionation.

The second technique, titled syndrome analysis, was proposed by Saunders & Schucman (1962). The procedure begins by specifying pairs of subjects such that within every pair each subject is closer to his partner than to any other person. It continues by adding to each cluster those subjects who are closer, on the average, to the subjects comprising the cluster than to any others, but in such a way that each of the subjects originally in the cluster must also be closer to the others in it than to any others. This notion of mutual proximity is used throughout the clustering procedure until everyone, except for a few "mavericks," has been assigned to a specific cluster.

This method likewise has built into it some of the drawbacks cited in reference to the technique of Sawrey et al. (1960). Specifically, it starts from the perhaps unwarranted assumption that the tests considered can in fact determine meaningful subgroups. Unlike the technique of Sawrey et al. (1960), in which standardization is left more or less to the whim of the investigator, syndrome analysis is properly performed on variables which have been standardized by division by the population standard deviations. But this standardization introduces some logical difficulties, for, dividing by a standard deviation implies that the dispersion of any variable within each of the subgroups is the same. Syndrome analysis as it stands, however, permits some of the subgroups to be much more coherent and homogeneous than others,
which means that the standard deviations need not be the same. A final
difficulty with the presentation of this method, one which is shared by
the other, is that not only is the question of correlated tests not faced
squarely, but also that the problems encountered when the standard deviations
are estimated from the sample data are not mentioned. These points will be
discussed below.

Preliminary Considerations

Before any procedure for segregating the members in a population into
homogeneous subgroups may be applied, it is essential that certain properties
of the variables used in the fractionation procedure be known. First, it
must be known that the tests are reliable, i.e. that they are subject to
minimal random variation, and also valid, i.e. that they indeed measure the
traits they were designed to measure. Thus, in studying schizophrenia, the
tests to be used should tap the physiological, sensory, perceptual,
psychomotor, and conceptual levels of performance, as accurately and precisely
as possible. If possible, these tests should have been administered to
relatively homogeneous samples of subjects, both with a view to determining the
variability of each test in such samples, and also with a view to determining
their interrelationships, i.e. the correlations between them.

The knowledge of the test standard deviations and intercorrelations is
especially important from the point of view of decreasing the misclassifications
inevitably to be expected in any clustering procedure. For, consider first
the possibility that the variables are correlated within the subgroups
ultimately to be identified. It is then naturally desired to locate these
clusters with their proper contours. In order to achieve this, the proper
distance measure is not simply the square root of

\[ \begin{align*}
    d^2_{xy} &= \frac{K}{\kappa} \left( \frac{X_i - Y_i}{\sigma_i} \right)^2, \\
    i &= 1
\end{align*} \]

where \( X_i \) and \( Y_i \) denote the raw scores on test \( i \) for subjects \( X \) and \( Y \), \( \sigma_i \) denotes the standard deviation of test \( i \) within a subgroup and \( K \) denotes the number of tests, but is rather the square root of

\[ \begin{align*}
    d^2_{xy} &= \frac{K}{\kappa} \sum_{i=1}^{K} \sum_{j=1}^{K} \sigma_{ij} (x_i - y_i)(x_j - y_j),
\end{align*} \]

where \( \sigma_{ij} \) denotes the \( i, \ j \)th element in the inverse of the matrix of test variances and covariances within the subgroups. In matrix notation, this becomes

\[ \begin{align*}
    d^2_{xy} &= (X - Y)' \Sigma^{-1} (X - Y),
\end{align*} \]

where \( X \) and \( Y \) denote the column vectors of raw scores of subjects \( X \) and \( Y \), \( (X - Y)' \) denotes the transpose of the vector of difference scores, \( \Sigma \) denotes the variance-covariance matrix of these tests assumed to be common to all subgroups, and \( \Sigma^{-1} \) denotes the inverse of this matrix. Equations [2] and [2'] are valid only if the elements of \( \Sigma \) are known. If they are not known, and if they are estimated from the available sample, then serious biases may result.

For, depending on the relative positions of the subgroup centroids, true correlations which are positive may be estimated to be negative, true negative correlations might be estimated to be positive, and true zero
correlations might be estimated to be far different from zero. For a demonstration of this latter possibility, see Cramer (1955, pp. 144-145, prob. 5). Thus, in the absence of any knowledge concerning the test correlations, where this knowledge would have to be based on samples from homogeneous groups, it is obvious that the sample correlations may be badly biased estimates of the true subgroup correlations if subgroups in fact exist. It is therefore suggested that, if the correlations are not known, and there is reason to suspect that they are non-zero, then the investigator should not attempt any clustering with these variables. If there are a priori grounds for believing the correlations to be small, then the investigator may proceed, ignoring the correlations in the computations. To summarize, if no numerical information is available concerning the magnitudes of the test correlations, then proceeding to cluster is justified only if there are strong grounds for assuming the correlations to be negligible. If the tests are correlated, then biases are almost inevitable no matter what one does, that is, either estimate the correlations from the sample or ignore them. In view of this, it would be difficult to justify any clustering.

Biases are also possible when the variances are estimated from the sample. For, if two groups underlie the total population in the proportions \( p \) and \( 1-p \), if the variance of a test is \( \sigma^2 \) for each group, and if the means on the test are \( \mu_1 \) and \( \mu_2 \) for the two groups, then the variance computed for the total sample will, for large sample sizes, be approximately equal to \( \sigma^2 + p(1-p) (\mu_1 - \mu_2)^2 \). The effects of this bias on the power of any technique to detect subgroups are evident. For, the proper weight which squared differences on a test should receive is \( 1/\sigma^2 \), while using the sample standard deviation as the standardization factor will result in the weight
being approximately $1/(\sigma^2 + \rho(1-\rho)(\mu_1 - \mu_2)^2)$, which is less than the proper
weight. As $\mu_1$ and $\mu_2$ diverge, i.e. as the two groups are more and more
separated on this variable, then the smaller this weight will become. But
it is precisely a variable such as this, namely one on which the two groups
are disparate, which should receive the fullest weight in the clustering. Thus,
by the seemingly innocuous procedure of standardizing the observations by the
sample standard deviations, the very purpose of the entire clustering program
may be defeated. The solution is not simply to ignore the standard deviations,
since the tests will most likely be scored in different metrics. The
possibility exists, in fact, that no satisfactory solution can be found to
this problem of bias when independent variance estimates are unavailable. It
is hoped, however, that the procedure to be described will overcome the
effect of these biases, at least when certain conditions are met.

There will be no discussion of methods appropriate to the case when
independent variance and covariance estimates are available, since such
cases are, at present, nonexistent. Tiedman (1955, pp.1-14) has rightly
pointed out that much research has yet to be conducted on the experimental
variables before they can be applied to the resolution of a heterogeneous
population into homogeneous components. But to wait, as Tiedman (1955, p.12)
implies, until these variables are known almost completely, is to lose much
information along the way.

A Method for Fractionating a Population

One deficiency shared by the clustering methods currently reported
in the literature is that they do not allow for the possibility that the
population studied is homogeneous to begin with on the variables chosen,
so that clustering will not only be wasteful of time, but will end with
end with trivial results. Just what is meant by homogeneity will, of course, depend on notions varying with the specific problem.

The definition of homogeneity which will be made in this paper is that, in order for a group to be declared homogeneous, the subjects within it must be distributed in a manner at least approximating the multivariate normal distribution. For discussions of this distribution, see Mood (1950, pp. 165-188); Rao (1952, pp. 51-57); Anderson (1958, pp. 5-39). There is no guarantee that this definition will have validity in any given study, but it does seem to be reasonable in view of the fact that measurements on many psychological variables, after suitable transformation if necessary, are distributed approximately normally. If these tests are independent, then their joint distribution will approximate the multivariate normal law, for in this case the joint distribution is the product of the marginal distributions. There is no guarantee that this will hold in the general case of nonindependent tests (see Anderson, 1958, pp. 37-38), so that this is a second reason for working with independent variables, for, not only may the problem of biased estimates of the correlations then be ignored, but also the assumption of joint normality may be made with confidence. Note, however, that the demand is for independent tests; this is formally a stronger requirement than that the tests be uncorrelated.

Given the above definition of homogeneity, the hypothesis that the study sample is sufficiently homogeneous with respect to the variables under consideration to obviate any clustering may be tested as follows. The statistic $\Delta^2$ is computed for each subject in the sample, where, in matrix notation,

$$\Delta^2 = (X - \bar{X})' S^{-1} (X - \bar{X}),$$

where $\bar{X}$ is the vector of sample means and $S^{-1}$ is the inverse of the matrix of sample variances, the covariance being assumed to be zero. Under the hypothesis of normality, and given a
from normality will not lead to rejection), then it is to be inferred that the tests employed do not discriminate among the subpopulations assumed to exist, in which case other variables will have to be employed in a subsequent study. If the hypothesis of normality is rejected, there is cause for proceeding with the clustering. The hypothesis of normality may also be rejected if the sample is excessively homogeneous, but this is unlikely with subjects such as schizophrenics.

The problem of the dispersion of the variables within the groups must now be faced. If the true within cluster variances are equal, then it is perhaps reasonable to expect that the biases in the total sample variances will not seriously distort the proper assignment of subjects to the groups. If, however, the test variances for one group differ greatly from the variances for the others, then it is possible that the clusters which are found will bear little resemblance to the true subpopulations. If the investigator is willing to assume that what differentiates the subpopulations is only a difference in centroid location, with no differences in dispersion, then the procedure to be described should be adequate. If he is not willing to make such an assumption, then the procedure is inappropriate, and the investigator will have to turn to one of the other methods which have been proposed, or invent his own.

A method of clustering which seems most efficient under the above assumptions, in the sense of being able to identify subgroups which exist, and which will guard against the detection of spurious clusters, i.e. those which do not in fact exist, is one which proceeds first by separating the sample into two groups, then testing them for homogeneity, and, depending on the result of this test, either declaring the groups to be homogeneous or starting over again and separating the sample into three groups. The procedure
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the result of this test, either declaring the groups to be homogeneous or
starting over again and separating the sample into three groups. The procedure
is continued either until homogeneous groups are found or until the number of
groups to be found grows so large as to make them virtually meaningless.

In order to find two subgroups, one should proceed in such a way that
for each subject in the sample, the average squared distance from him to the
other members of his subgroup should be less than the average squared distance
between him and the members of the other subgroup. This criterion may be
achieved as follows. The matrix of intersubject $d^2$'s (see equation [1])
is scanned, and the largest entry in this matrix is identified. Suppose
it happens that the squared distance between subjects X and Y is greater than
the squared distance between any other pair of subjects. Subjects X and Y
will then form the foci of the subgroups. About each of these foci separately
is clustered each of those subjects whose distance squared from the focus is
less than the fifth percentile of all the squared distances. It is very
unlikely that, at so early a stage in the procedure, a subject will be so
close to each focus that he is assigned to both clusters. If this should
happen, however, then the average squared distance from him to the other
members should be computed for each cluster and he should be assigned to
the cluster for which this average is smaller.

These two clusters of subjects are then taken as the nuclei for further
clustering. About each of these nuclei are now clustered those subjects
whose average distance squared from the members of the nucleus is less than
the tenth percentile of all distances. If a subject meets this criterion
with respect to both clusters, then the average squared distances from him
to the other members of the clusters, both those in the nuclei and those
clustered uniquely about them, are computed and compared, and he is assigned
to the cluster for which this average is smaller.
These two larger clusters of subjects are then taken as the nuclei for the next step in clustering, which differs from the previous step only in that the criterion for assigning a subject to a cluster is that his average squared distance from the nucleus be less than the fifteenth percentile of all distances. The clustering continues in this way with the criterion for inclusion constantly being relaxed, until every subject in the sample has been assigned to one of the two subgroups. It should be noted that once a subject has been assigned to a cluster, he is irrevocably a member of it, so that only those subjects not yet assigned are considered for clustering at each step. No allowance is made for the possibility that there are subjects in the sample who belong to neither of the hypothesized groups, for just as these are atypical normals, so should there be atypical members of a group of mentally ill.

After the two subgroups have been identified, the variance of each test is computed for each group, and the estimates for the two groups are combined to yield a pooled variance for that test. If the estimated variance for test 1 in subgroup A is \( s_{iA}^2 \), in subgroup B is \( s_{iB}^2 \), and if the original sample of size \( n \) is so partitioned that \( n_A \) subjects are assigned to group A and \( n_B \) (\( = n - n_A \)) are assigned to group B, then the pooled variance for test 1 is

\[
s_i^2 = \left( \frac{(n_A-1)s_{iA}^2 + (n_B-1)s_{iB}^2}{n_A + n_B - 2} \right)
\]

The two group centroids are computed, and \( \bar{\Delta} \) is computed for each subject, the deviations being taken about the centroid of his group, and the pooled variances being the elements of the matrix \( S \) (see equation [3]).

Combining all \( n \) values of \( \bar{\Delta} \), the \( \chi^2 \) distribution with \( K \) degrees of freedom may again be fitted to the resulting distribution, and a \( \chi^2 \) goodness
of fit test may again be applied. This test is valid, since under the null hypothesis that the two groups are homogeneous, and assuming that $n_A$ and $n_B$ are each large, the set of $\chi^2$ values for each group separately should have approximately a $\chi^2$ distribution with $K$ degrees of freedom, so that the combined set should have this distribution. The number of degrees of freedom for the $\chi^2$ statistic is $N-2-3K$, where $N$ again is the number of classes into which the $\Delta^2$'s are distributed. Two degrees of freedom are subtracted because the numbers in the two groups are specified, and $3K$ more are subtracted because $K$ means have been estimated for group $A$, $K$ for group $B$, and $K$ variances have been estimated by pooling the within group variances. An insignificant value of $\chi^2$ is taken to mean that homogeneous clusters have been found, while a significant value of $\chi^2$ is interpreted as meaning that the clusters are not yet homogeneous, so that further clustering is necessary.

If further clustering is to be performed, it would be preferable that the pooled variances obtained during the preceding step be used in determining the distances between subjects, since presumably they are subject to less bias than the total sample variances. If this recomputation of distances is not feasible, then the original matrix of distances will have to be used, with its accompanying biases. Whichever matrix is employed, the next step consists of identifying that trio of subjects who are mutually further apart from one another than any other triplet of subjects, in the sense that the mean of the squared distances between them is greater than that for any other group of three. Subjects are clustered about each of these foci as previously, and the homogeneity of the resulting subgroups is tested as above, where within group variances are computed and then pooled, and where the goodness of fit statistic now has $N-3-4K$ degrees of freedom.
Given that at some stage of the procedure, the subgroups have been found to be homogeneous, the next step would be to find what other variables the subjects within them tend to have in common. The variables might be ones such as a measure of response to treatment, a measure of hospitalization status, the presence of certain premorbid factors, etc. At any rate, the availability of such information should form an integral part of the study.

Since the procedure described depends heavily for its validity on so many factors, namely the availability of a large sample, normality in the underlying groups, independent variables and equal covariance matrices, it is obvious that it could be applied only in rather special instances, specifically, where enough is known about the experimental variables so that these assumptions may be made with confidence. At Biometrics Research, for example, work is currently going on in obtaining valid measures of the dimensions underlying schizophrenia. For a review of this work, see Zubin, Sutton, Salzinger, Salzinger, Burdock and Peretz (1961). Along with this research, data are being collected which will be amenable to the techniques described. The results of the clustering procedure applied to these data will be described in the future.

Summary

The observation of a consistent disparity of measurements on samples of normals and schizophrenics, not only in level of performance but also in variability of performance, has led to the hypothesis that the persons currently classified as schizophrenics actually constitute discrete populations of mentally ill within the broad heading of schizophrenia. In the absence of any proven mathematical techniques for finding these populations, a method
has been described which should under certain specified conditions detect the subgroups which exist. While the specified conditions laid down in this approach might at present seem unduly restrictive (normal correlation surface between variables where the correlations are uniformly zero) they need not remain so restrictive in future developments of this approach. The variables to be used in an application of the method are currently being developed.
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