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Utilization of Interactive Computer Graphics in Analyzing 3-dimensional Data Sets

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Effective analysis of 3-dimensional data derived from ordination methods is facilitated by convenient and accurate means of viewing the results. The efficiency of utilizing an existing, operational interactive computer graphics system for this purpose is evaluated herein. An example of system use for principal components analysis of 21 samples is included. INDEX DESCRIPTORS: Interactive computer graphics, Multivariate analysis.

Ordination methods such as principal components analysis and canonical analysis are frequently used in biological studies as dimension reducing procedures. Interpretation of these analyses is usually done graphically and oftentimes requires graphic representations upon 3 axes to facilitate interpretation. Typically, such representations are depicted as perspective views of 3-dimensional drawings (see for example, Schmidly and Hendricks, 1976). Ball and stick models and photographs of these models have also been used but only with limited success. Rohlf (1968) proposed the use of stereograms for depicting the 3-dimensional relationships among points plotted to represent the results of such analyses. However, this and the former two methods possess certain disadvantages. Both ball and stick model construction and preparation of perspective drawings involve inaccuracy in preparation and are somewhat tedious to construct, especially as the number of samples increases. The use of a computer plotting routine for stereograms can alleviate both of these problems but does not afford the user a convenient means of choosing those views that are most revealing. In this paper, we describe the use of an interactive computer graphics system which prepares 3-dimensional projections accurately, rapidly and flexibly. An example of its use in the analysis and interpretation of a set of taxonomic data is also presented.

SYSTEM COMPONENTS AND SOFTWARE

A detailed description of the Biographics system can be found elsewhere (Meyer, et al., 1974). Its main components are a Digital Equipment Corporation PDP 11/40 minicomputer and a Vector General display unit. Real time interaction with the graphics display is achieved through the use of 10 dials which control such functions as rotations, pointers and relative intensities of displayed files. The dials are usually pre-assigned to a particular set of functions but may be easily changed to the operator's specifications. Although the Biographics system is designed primarily for interactive molecular fitting problems such as the fitting of macromolecular models to electron density maps or substrates to enzyme active sites (Collins, et al., 1975), it is readily adaptable to any 3-dimensional data set.

A particular data set is read into memory from cards, tape or directly from the keyboard. It can then be displayed either as points in 3-dimensional space or as projections from such points to a plane. Axial systems can be drawn and labelled and, for smaller data sets, each individual point may be labelled as well. The display program used (PIXMOV, Swanson, unpublished) allows viewing of up to 10 separate display files (for example, axis, labels, projections, etc.) with dial control of the relative intensity of each. Rotation around each axis, accomplished by rotation of 3 controlling dials, enables unobstructed viewing from any direction. This rotation also conveys the 3-dimensional nature of the data display. Additionally, options for stereo viewing have also been incorporated which heighten the 3-dimensional effect, especially in viewing stationary, non-rotating displays. A pointer is available which can consecutively bounce through the data set and be positioned at any particular point. Since it sequentially follows the data set display list, the operator can obtain the coordinates of each point and a numerical label. For larger data sets, this provides a convenient means of identifying individual projections as labelling complicates the image and for very large data sets produces discernible image flicker.

The program also allows computer control of both photographs and movies for documentation of results. Movie features include a record and playback scheme which enables the operator to compose, record and preview the movie prior to filming. A film illustrating the various capabilities of the display program has been prepared and presented (Legg, 1978).

AN EXAMPLE OF SYSTEM USE

The results of a principal components analysis on 21 samples of *Thomomys bottae*, Botta's pocket gopher, from Trans Pecos, Texas illustrates the utility of the Biographics system. The original data set was comprised of 13 cranial measurements recorded from 205 individual female gophers (Schmidly, ms in preparation). The first 3 principal components extracted from the variance-covariance matrix, using the NT-SYS program (Rohlf, et al., 1972), accounted for 87.63%

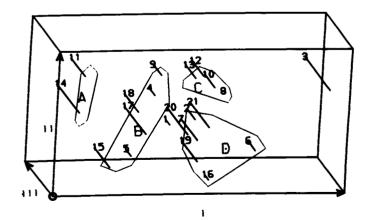


Fig. 1. Projections of 21 samples of T. bottae onto their first 3 principal components. (I, II, III). Origin (O) is most conveniently viewed as the lower left corner of the cell with principal component III pointing upward. Boundaries of groups A to D lie at the base of the projections in the plane formed by I and II.

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of the total variation in the original sample (54.02, 18.62 and 14.99% of the variation respectively). Mean values of the 1st 3 principal components for each of the 21 samples were obtained and these values were plotted as projections onto the 1st 3 principal components using the Biographics system (Figure 1). The relative distance between samples in this newly derived character space is a measure of the overall morphological similarity between samples.

Rotations help elucidate the structure and relationships among samples in this character space. Figure 2 illustrates a sequence of rotations around an arbitrary axis roughly coincident with principal component III. Examination of these projections on the Biographics system led to the recognition of 4 groups of samples with 1 outlier (sample 3) and 1 sample (1) whose affinity was uncertain (Figure 2-E). This particular grouping was made primarily on the basis of differentiation along the 1st 2 principal components. However, rotation to a position viewing the I, III plane indicates that alternative groupings are possible with this data set as a result of sample differentiation along the 3rd principal component (Figure 3). It should be noted that the 2nd and 3rd principal components each explained approximately the same portion of the total variation in the original data set suggesting that alternative groupings may be equally viable. In general, decisions concerning relationships among samples are made by interactively viewing the projections on the Biographics system from a variety of vantage points. Stereo projections are readily obtainable (Figure 4) and are a more effective way of viewing 3-dimensional systems of this type.

SYSTEM ACCESSIBILITY AND REMARKS

The utilization of computer graphics, and in particular of interactive graphics systems, is rapidly increasing. Several realtime interactive systems, similar in capability to the Biographics system at Texas A&M University described herein, are presently available.

Use of the Biographics system at Texas A&M requires only the purchase of computer time as the system is already well-developed with regard to programming software. This expense is comparable to using Texas A&M's Amdahl 470V/6 to plot stereograms. Its use has the additional advantage of not requiring trial and error selection of the viewing angle. The full capability of the system has not been realized even with respect to the plotting of simple 3-dimensional diagrams. Other immediate applications, for example, could include the construction of 3-dimensional minimum spanning trees and the plotting of

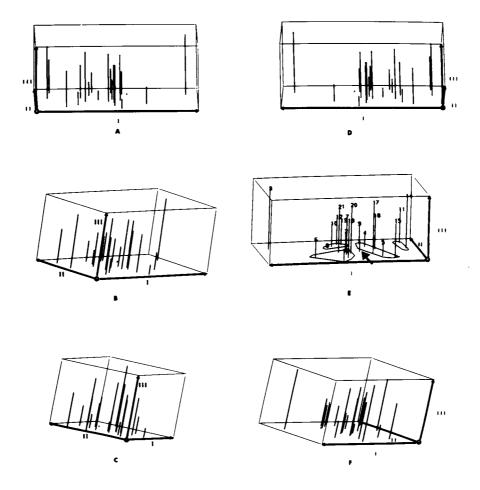


Fig. 2. Sequential views (A-F) of a rotation of the projections of 21 samples of T. bottae onto their first 3 principal components. A through D show an approximately 180° clockwise rotation of the plane formed by components I and II. E includes a demarcation of four groups separated along principal components I and II. Sample 1, indicated by an arrow, is intermediate between two groups.

COMPUTER GRAPHICS AND 3-DIMENSIONAL DATA SETS

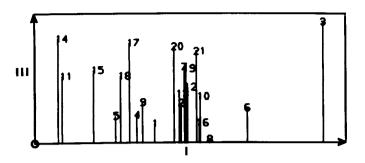


Fig. 3. Projections of 21 samples of T. bottae onto principal components I and III.

3-dimensional standard deviation ellipsoids. Potentially the system offers a novel and effective technique for examination of a wide range of problems of biological significance.

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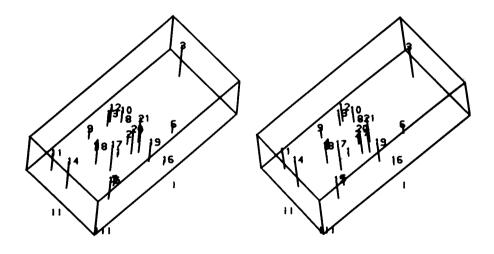


Fig. 4. Stereogram of the projections of 21 samples of T. bottae onto principal components I, II, and III. To achieve the stereo effect, projections should be viewed with a stereo viewer.