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INTERACTIVE DIAGNOSTIC PLOTS FOR MULTIDIMENSIONAL SCALING WITH APPLICATIONS IN PSYCHOSIS DISORDER DATA ANALYSIS

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Abstract: Multidimensional scaling (MDS) represents objects as points in an Euclidean space so that the perceived distances between points can reflect similarity (or dissimilarity) between objects. To be practical, the dimension of the projected space usually is kept as low as possible. Thus, it is unavoidable that part of the information in the original proximity matrix will be lost in the MDS plot. To assess the overall quality of projection, classical MDS diagnostic indices and plots are available. However, these global-fitness methods do not address another issue: how well represented is a specified individual object or a pair of objects in the projected space? Here, via the concept of color-linkage, a dynamic graphical system is developed for revealing the subtle spatial lack-of-fit pattern for any specified individual object. The proposed method is illustrated by using a data set from a psychopathological research project.

Key words and phrases: Colored linkage, dynamic graphics, model checking, outliers, proximity, stress.

1. Introduction

This paper is motivated by a psychopathological study, the Taiwan Inpatient Epidemiological Project (TIEP) (Liu, Hwu, Yeh, Chung, Rin and Lin (1995)). Of concern is the analysis of a data set consisting of 95 patients with 50 variables. Each variable records one symptom scale, see Section 2 for more detail in this regard. Multidimensional scaling (MDS) is an established method for addressing the fundamental issue of the grouping structure among symptoms.

To begin with, one should provide a similarity measure δ_{rs} between any two symptoms, r and s, the correlation coefficient between two variables for example. This gives an $n \times n$ $(= 50 \times 50)$ matrix of proximity between $n = 50$ objects (each object being a symptom). MDS aims at representing objects in a low-dimensional space so that users can study symptoms through their spatial relationship. Such configuration plots are often restricted to 2 or 3 dimensions.

In applying MDS, one frequently asked question is how well a specified symptom is represented in the configuration plot. Clearly the answer is not to be found in the configuration plot itself because the original information about the similarity between the specified symptom and other symptoms is partially lost during the dimension reduction process. One possibility is to turn to the available MDS diagnostic indices and plots as to be reviewed in Section 3. However, these global-fitness diagnostic methods do not address the more subtle spatial lack-of-fit pattern at the individual object level.

Our goal is to use a dynamic graphical system for addressing the above issue. Color linkage is the major concept in this proposed interactive system. The values in the input proximity matrix are projected as color dots onto the configuration space. When a point in the configuration space is clicked, the proximities in the column (row) related to the clicked point are projected through a color spectrum as color dots and then painted onto the corresponding configuration points to represent the proximity measurements between the clicked point and all other points. This colored configuration plot is called the conditional configuration plot for the point being clicked. A technique called color-smearing, using ideas from nonparametric smoothing, is used to fill up the space between all colored configuration points.

To see how well a specified object is represented in the configuration plot, we compare the static distance pattern related to the clicked point with the dynamic color contour pattern on the conditional configuration plot. When these two pieces of information match well with each other, the concerned object fits well into the MDS model. Otherwise, this object must be a potential stress contributor. Section 4 describes our method in detail. A simulation study is carried out to illustrate the versatility of the proposed method in Section 5. Section 6 further provides guidance on using the proposed method. Some further remarks are in Section 7.

2. The Psychosis Disorder Data

The data set consists of the Andreasen's positive and negative symptom scales (Andreasen (1983, 1984)) for 95 first-time hospitalized psychosis disorder patients. Among the 95 patients, 69 patients were diagnosed as schizophrenic and 26 patients were diagnosed as bipolar disorders. The system of Andreasen's symptom scales include the Scale for Assessment of Positive Symptoms (SAPS) with 30 items, and the Scale for Assessment of Negative Symptoms (SANS) with 20 items (see Appendix). SAPS includes four subgroups: hallucinations (AH1-6), delusions (DL1-12), behavior (BE1-4) and thought disorder (TH1-8). SANS has five subgroups: expression (NA1-7), speech (NB1-4), hygiene (NC1-3), activity (ND1-4) and inattentiveness (NE1-2). The available data set has 95 subjects (patients) with 50 variables (symptoms).

Psychiatrists in TIEP address three fundamental issues: the grouping structure among symptoms, the clustering structure of patients and the general behavior of patient-clusters in each symptom-group. In this paper, we consider only the first issue with respect to grouping structure among symptoms. The remaining two issues will be discussed elsewhere. For the symptoms grouping structure, researchers usually apply factor analysis (Andreasen, Arndt, Alliger, Miller and Flaum (1995), Stuart, Malone, Currie, Klimidis and Minas (1995)) or MDS (Minas, Stuart, Klimidis, Singh and Copolov (1994)) to identify the possible grouping of the symptoms and to study the structures within and between groups. We initially applied the MDS method to the TIEP data and identified some problems in using the algorithms. This work presents an interactive diagnostic plotting system to remedy some unsatisfying features of MDS.

3. MDS Algorithms and Classical Diagnostic Tools

Multidimensional scaling (MDS) of similarity (or dissimilarity) judgments has been widely applied to many disciplines, ranging from the medical, biological, and behavioral sciences to education, product development and marketing research. There are many programs available for performing different types of MDS model fitting. To name a few, MINISSA appeared in Roskam and Lingoes (1970); ALSCAL was developed by Takane, Young and De Leeuw (1977); KYST was designed by Kruskal, Young and Seery (1977); MULTISCALE adopted a maximum likelihood approach in Ramsay (1977); SMACOF was based on the majorization algorithm first proposed by De Leeuw (1977). ViSta-MDS, developed by McFarlane and Young (1994) is the only MDS program performing model exploration in an interactive fashion. This list is certainly not complete. Further discussion of MDS theories, algorithms, and programs can be found in the books by Cox and Cox (1994) and Borg and Groenen (1997), and in the review papers by Springall (1978) and Mead (1992).

In this article, we apply the ALSCAL (Alternating Least squares SCALing) program to illustrate the proposed method for diagnosing the general MDS model fitting. We do not intend to modify any of the ALSCAL program settings. The results can be easily adapted to other MDS programs.

3.1. Glossary for multidimensional scaling

There are some common notations used in general MDS framework:

The input target set of objects $\boldsymbol{O}$: a set of n individuals or variables among which the associations are to be studied. Only degree of relationship can be observed among the objects.

The proximity of a pair of objects $(o_r, o_s), \delta_{rs}$: a distance or similarity measurement used to represent the relationship between two objects.

The dimensionality of output configuration space q: a prespecified number for the desired dimension of the MDS solution space.

The output configuration set $\mathbf{X} = \mathbf{X}(q)$: a set of n q-dimensionl MDS solution configuration points, usually in Euclidean space, to represent the set of input objects $\boldsymbol{O}$.

The distance $d_{rs} = d_{rs}(\mathbf{X})$ of a pair of configuration points (r, s) in $\mathbf{X}$: the distance, usually Euclidean, between the points representing objects r and s in the configuration space to represent δ_{rs} in the input set.

The transformation function, $f : \delta_{rs} \rightarrow d_{rs}$: a function for specifying how the proximities should be related to the distances. The characteristics of f determine the type of MDS model. Due to the existence of noise in the observed proximities, f is usually only used to map proximities to approximate distances as closely as possible. Only the type (ratio, interval, logrithmic, exponential, ordinal, spline, etc.) of f is prespecified (see Borg and Groenen (1997) for more discussion), the exact form (parameters) of f is part of the MDS solution.

The disparity of a pair of objects $(o_r, o_s), \hat{d}_{rs} = f(\delta_{rs})$: the realization of the transformation of δ_{rs} .

Stress $= \sigma^2 = \sigma^2(X, f(\delta)) = \sigma^2(d, \hat{d})$: a loss function for measuring the closeness of the mapping from proximities to distances: a measure of badness-of-fit for evaluating the quality of representation of the set of transformed proximities $\hat{d}_{rs}$ by the set of distances d_{rs}, usually in some weighted form of $\sum_{(r,s)}(d_{rs} - \hat{d}_{rs})^2$.

The nature of MDS technique differs from other topics of multivariate analysis in the following manner. For multidimensional scaling, given a set $\mathbf{O}$ of n objects (individuals or variables), only a degree of relationship can be observed among the objects yielding $C(n, 2)$ pairs of between-object proximities. (In our case study of psychosis disorder data, there are 50 objects (symptoms) and $C(50, 2) = 1225$ between-symptom correlation coefficients.)

MDS procedure attempts to find an appropriate transformation f and a set of points in a configuration space $\boldsymbol{X}$, such that the stress is as small as possible. There are many different types of scaling for MDS. However, we only briefly describe two major categories of scaling in this article: metric and non-metric scaling. For detailed discussion of other types of scaling, see Cox and Cox (1994) and Borg and Groenen (1997).

3.2. Metric scaling and nonmetric scaling

Metric scaling models assume that the disparities $\hat{d}_{rs}$ satisfy metric conditions. The transformation f usually takes a continuous monotonic functional form

$$\hat{d}_{rs} = f(\delta_{rs}) = a + b \cdot g(\delta_{rs}), \tag{1}$$

where a and b are parameters to be estimated, and $g(\cdot)$ can be partially or completely predetermined. An important case is interval MDS with free parameters

a and b, and identity $g(\cdot)$. When $a = 0, b = 1$, and $g(\cdot)$ is the identity, we have the simplest case of absolute MDS. A ratio MDS with $a = 0, b < 0$, and $g(\cdot)$ the identity can be used to transform similarity proximities δ_{rs} to distance disparities $\hat{d}_{rs}$. For some psychological measurements of δ_{rs}, the logaritnmic or exponential form of $g(\cdot)$ may be quite meaningful.

If the metric properties of the transformation for the proximities are released, we have nonmetric MDS. No particular function form of f is required as long as the monotonicity constraint

$$\delta_{rs} < \delta_{uv} \Rightarrow f(\delta_{rs}) < f(\delta_{uv}) \qquad \text{for all} \quad 1 \leq r, s, u, v \leq n, \tag{2}$$

is preserved. Thus, the transformation in nonmetric MDS models represents only the ordinal properties of the data. In our case study, f transforms the correlation coefficients to distance measurements with the same order as the original rank in the correlation matrix. This transformation is usually obtained by using monotone regression with Kruskal's algorithm (1964b).

Nonmetric scaling was first studied by Shepard (1962a, b) using an iterative approach since there is no analytic solution. Kruskal (1964a, b) introduced the idea of minimizing a loss function to the framework of nonmetric scaling and gave it a sounder foundation.

3.3. MDS configuration plot

After the coordinates of the q-dimensional configuration of the objects, $\mathbf{X} = \mathbf{X}(q)$, has been found, these objects can be plotted as n points in the low-dimensional Euclidean space. This is called the MDS configuration plot or the stimulus plot. In doing so, the set of proximities $\{\delta_{rs}\}$ is transferred to visualized distances $\{d_{rs}^{(q)}\}$. This plot is the most important output of most MDS methods. When the stress score is insignificant, most of the structure embedded in the input proximities is well-represented by the distances in this configuration plot. Many useful pieces of information can be seen in the configuration plot. These include the grouping effect of the configuration points, the between-group relationships, and the relative position of each object to all other objects. The configuration plot for our case study is displayed in Figure 1a.

In the process of dimension reduction, some information is lost. Occasionally, the loss is severe. When this is the case, the structure in the MDS modeling and the configuration plot provide only a rough approximation to the structure embedded in the input proximities. In the literature, there are several indices and plots available for showing how well the MDS model fits.

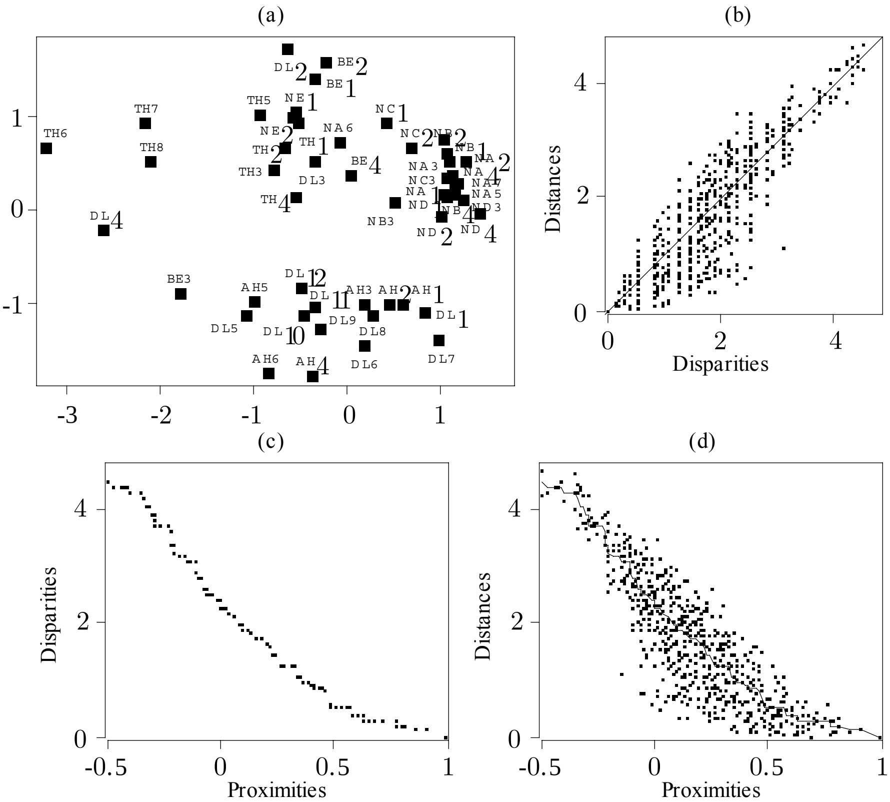

Figure 1. Classical graphic tools for MSD. (a) Configuration plot; (b) Plot of linear fit; (c) Plot of transformation; (d) Plot of nonlinear fit.

3.4. Classical diagnostic indices

Kruskal (1964a) proposed a scheme for measuring how much a lower-dimensional geometrical representation falls short of a perfect match. The measurement, called stress (STandardized REsidual Sum of Squares), is defined as

$$STRESS(q) = \Big\{\sum_r \sum_s (d_{rs}^{(q)} - \hat{d}_{rs}^{(q)})^2 \Big/ \sum_r \sum_s (d_{rs}^{(q)})^2\Big\}^{1/2}. \tag{3}$$

For each q, a configuration with the minimum stress can be obtained. As q increases, the minimum stress decreases. This is usually referred to as STRESS1. An alternative stress function used in nonmetric MDS which employs a different normalizing factor is

$$STRESS(q) = \Big\{\sum_r \sum_s (d_{rs}^{(q)} - \hat{d}_{rs}^{(q)})^2 \Big/ \sum_r \sum_s (d_{rs}^{(q)} - d_{\cdot\cdot}^{(q)})^2\Big\}^{1/2}, \tag{4}$$

where $d_{\cdot\cdot}^{(q)}$ is the mean over all pairs of the distances $\{d_{rs}\}$. This is referred to as STRESS2.

Instead of using Kruskal's stress score, the ALSCAL algorithm minimizes a loss function called SSTRESS (Takane, Young and De Leeuw (1977)), which is defined as

$$SSTRESS(q) = \Big\{\sum_r\sum_s \Big((d_{rs}^{(q)})^2 - (\hat{d}_{rs}^{(q)})^2\Big)^2 \Big/ \sum_r\sum_s (d_{rs}^{(q)})^4\Big\}^{1/2}. \tag{5}$$

These stress scores help determine the dimensionality of the configuration space. They range from zero (perfect fit) to one (worst possible fit). The STRESS1 and SSTRESS scores are 0.220, and 0.284, respectively, in our case study.

While the stress scores function like the residual mean square in a regression context, the R^2 measure in MDS is the squared correlation between distances $\{d_{rs}\}$ and the transformed proximities $\{f(\delta_{rs})\}$ (or the disparities $\{\hat{d}_{rs}\}$). It can be interpreted as the proportion of variation of the transformed proximities $\{f(\delta_{rs})\}$ that can be accounted for by the distances $\{d^q_{rs}\}$ of the MDS model. The value of R^2 is 0.779 in our study.

3.5. Classical diagnostic plots

There are three diagnostic plots of interest. The first is the plot of linear fit (Figure 1b): a scatterplot of distances $\{d^q_{rs}\}$ versus transformed proximities $\{f(\delta_{rs}) = \hat{d}_{rs}\}$. The closer to the 45^o line, the better the fit.

For nonmetric analysis and some metric MDS with nonlinear transformations, two more plots can be made. The transformation plot (Figure 1c) is a scatter plot of the transformed proximities $\{f(\delta_{rs}) = \hat{d}_{rs}\}$ versus original proximities $\{\delta_{rs}\}$. The transformation plot can be interpreted as the monotonic regression line that minimizes the error when error is measured vertically.

The plot of nonlinear fit (Figure 1d) is a scatter plot of the distances $\{d^q_{rs}\}$ versus original proximities $\{\delta_{rs}\}$. If this plot is identical to the transformation plot, then the MDS model fitting is a perfect match. For metric analysis with a linear transformation, the nonlinear-fit plot is the same as the linear-fit plot.

3.6. Limitations of classical diagnostic tools

The aforementioned diagnostic tools are concerned mainly with the effects of overall model fitting. They do not provide information on an individual object's behavior. We address the following two problems.

Nonzero stress. When we find an MDS configuration plot with $R^2 = 80\%$, roughly 20% of the relationship information contained in the input proximity matrix is incorrectly represented by the plot. The plot and the diagnostic indices can only be read as a whole. The 20% information loss cannot be recovered from the original input measurements by standard diagnostic tools.

Zero stress. The output configuration has a stress score equal to zero, but the complete picture of the underlying relationship structure is not yet understood. One such problem is an MDS analysis with a correlation proximity matrix. When applying MDS to a correlation proximity matrix, the range of correlations are usually transformed from $[-1,1]$ to [0, 2], with the matrix treated as a regular similarity proximity matrix. If some of the correlation coefficients are negative, variables with positive correlation coefficients are viewed as more similar than variables with negative correlation coefficients. This can be very misleading.

3.7. Classical MDS result for the psychosis disorder symptoms

From the classical MDS plots in Figure 1 and diagnostic indices, we have the following conclusions about the grouping structure of the symptoms of the psychosis disorder study: most of the negative symptoms, SANS (see Appendix) except NA6, NB3, NC1-2, and NE1-2, form a coherent cluster on the upper right corner; mania symptoms (DL4, TH6-8) form a small but distinct group, with only four symptoms, located opposite to negative symptoms; the cluster of thought disorder (TH1-5)with some behavior (BE1, 2, 4) and delusion (DL2,3) symptoms and NA6 form an intermediate symptom group between the two previous clusters; the stretching out symptom group of all hallucination symptoms(AH1-6) and most delusion symptoms(DL5-12), with BE3 located at the bottom of the plot, has relatively equal distances to all three other symptom clusters. The proposed method is employed to further understand the embedded structure of the correlation matrix in Section 4.

4. An Interactive Diagnostic System for Multidimensional Scaling

There are three different aspects in a diagnostic procedure for a statistical model fitting: (1) evaluation of the performance of the model fitting; (2) identification of potential problems of the model fitting; (3) action to change the model fitting. The first aspect is covered by classical diagnostic indices and plots. For the identification of potential problems, the construction of confidence regions (Ramsay (1978), Weinberg, Carroll and Cohen (1984)) in the configuration plots provides users a technique for diagnosing the relative location of points in an MDS space. For the third aspect, McFarlane and Young (1994) cleverly used a computer program called ViSta-MDS to graphically examine the sensitivity of changes of parameters in the model fitting and to study the problem of local minima in the computation of stress score.

There is a fourth aspect not usually covered in model checking, namely the retrieval of information lost during the process of model fitting. The diagnostic method for MDS model fitting to be proposed in this section covers the first two aspects mentioned above. We do not change or improve the model fitting in an MDS problem. Instead, we assume that the MDS model fitting has already reached its optimal solution, that model fitting cannot be improved. Our effort is then focussed on the recovery of the information lost during the MDS model fitting and dimension reduction procedure.

To resolve the problems raised in Section 3.6, we link the MDS configuration plot and the classical diagnostic plots to the input proximity matrix through color linkage. This concept is implemented in the XLISP-STAT (Tierney (1990)) environment. The discussion of linkage in interactive graphics can be found in Fisherkeller, Friedman and Tukey (1974), Newton (1978), McDonald (1982), Becker and Cleveland (1987), Stuetzle (1987), Buja, McDonald, Michalak and Stuetzle (1991), Wegman and Carr (1993), and Buja, Cook and Swayne (1996).

4.1. Color linkage

Conventional configuration plots are black and white. We can use color to represent the values of the input proximity measures. For instance, our case study uses red for positive correlation coefficients and blue for negative correlation coefficients. The darker the color, the larger the absolute value of correlation coefficient. For different types of proximity, users can select appropriate color spectrums to represent the measurements. When clicking any point, e.g. the r-th point in the plot, colors of all points on the plot will be changed to represent the correlation coefficients from the r-th row (or column) of the proximity matrix. Figures 2a and 2b illustrate this concept of color linkage. When the point representing symptom NB1 is clicked, the column of correlation coefficients between NB1 and all other symptoms are projected as colored dots and then painted on all corresponding configuration points.

4.2. Conditional configuration plot

When a user clicks at object o_r on the configuration plot, the colors displayed on all n configuration points represent the proximities $\{\delta_{rs}, s = 1, \ldots, n\}$ (correlation coefficients) with the point o_r. We refer to this colored configuration plot as the conditional configuration plot for o_r. There are n conditional configuration plots, one for each object. If there is not much stress related to the clicked point, as NB1 in Figure 2b, the point is initially surrounded by a layer of darker red (high positive correlation) points, then by a layer of lighter red (low positive correlation) points, followed by a layer of lighter blue (low negative correlation) points and, perhaps, by a layer of darker blue (high negative correlation) points. As stress rises, the pattern of the colors surrounding the point being clicked reveals some disturbance. Figures 6a and 7a provide such examples.

Each conditional configuration plot conveys two pieces of information: the information about the input proximities $\{\delta_{rs}\}$ and the information about the output distances $\{d_{rs}^{(q)}\}$. Information on $\{d_{rs}^{(q)}\}$ is what the original black-and-white configuration plot can display. The information about $\{\delta_{rs}\}$ is given by color. After clicking a point, we can see if the proximity measurements, as represented by colors, match well with the distances or not. If the match is good, then this point will not contribute much to stress. Otherwise, a potential stress contributor is detected. By performing a similar comparison for each configuration point, we can identify the stress contributors and obtain a comprehensive understanding about the quality of fit of the classical MDS result.

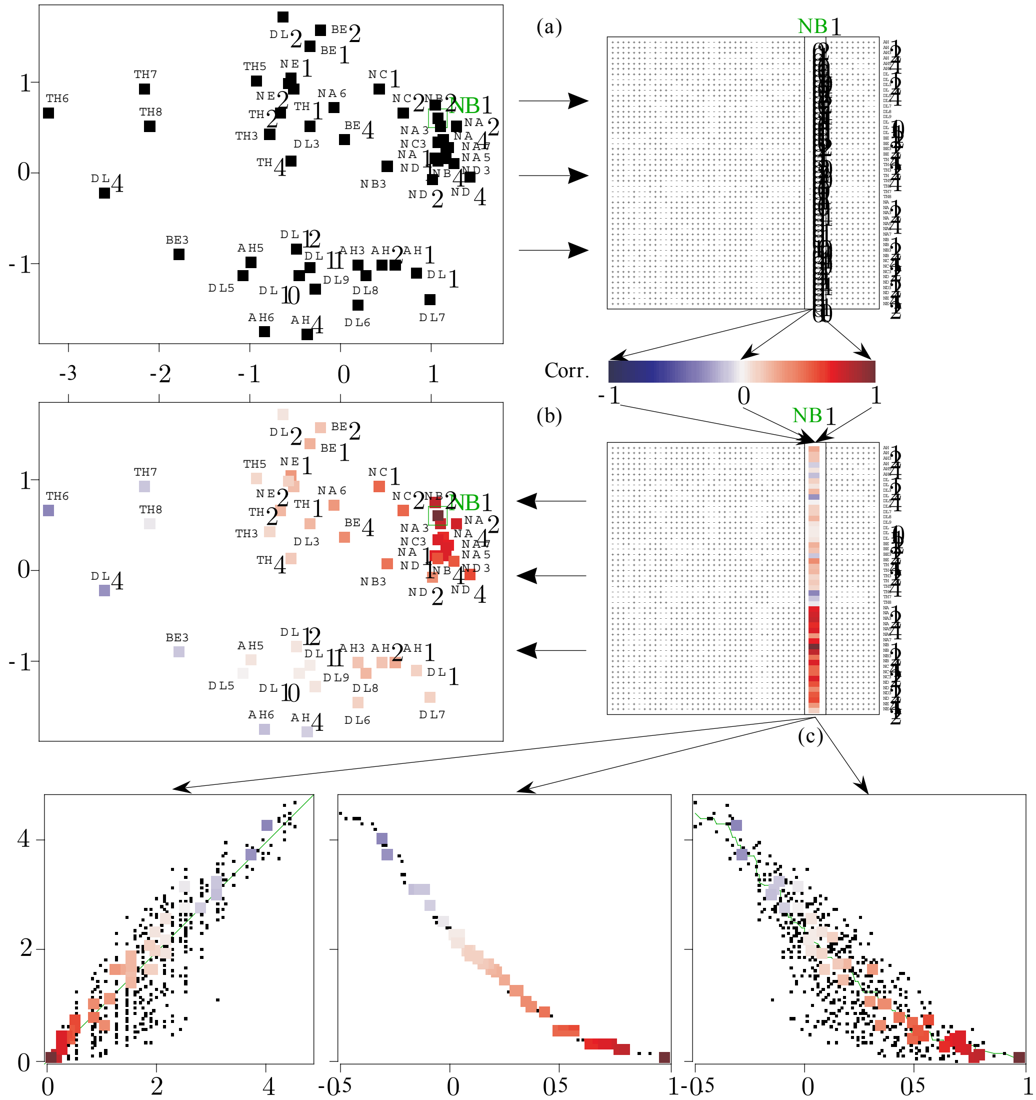

Figure 2. Concept of color linkage for interactive diagnostic plots for MDS, case study: symptom NB1. (a) User clicks at a point (symptom NB1 in this case) on the configuration plot. Action links back to the column of proximities associated with the clicked point (NB1) in the proximity matrix. (Only the signs of proximities are shown for clarity for columns other than NB1). (b) The n proximities of the column (NBl) are projected through a selected color spectrum (blue-red in this case) to create n color dots. These n color dots are then painted onto the corresponding n points on the configuration plot. (c) The n color dots are also painted onto the n points associated with the clicked point in all three diagnostic plots.

4.3. Conditional diagnostic plots

The static diagnostic plots can also be equipped with linking function similar, but not identical, to the linking function used in the dynamic configuration plot. There are $C(n, 2)$ points in any of the three static diagnostic plots. Instead of clicking at points in these diagnostic plots, these diagnostic plots are linked to the configuration plot. When a user clicks at a point o_r in the dynamic configuration plot, the same n colors used to display the n configuration points are used to display the corresponding n (among $C(n, 2)$) points related to o_r on these diagnostic plots. Figure 2c summarizes the linking effect of these three conditional diagnostic plots for symptom NB1.

This linkage possesses two advantages over the dynamic configuration plot itself. First, the pattern of the n points in these diagnostic plots can be used to reconfirm the result derived from the configuration plot. When all n points in the diagnostic plots stay close to the perfect fit line, the clicked point in the configuration plot fits the MDS model; when they depart from the perfect fit line, the clicked point is a possible stress contributor. Second, the pattern displays the relative positions of proximities, disparities and distances for these n pairs of relationship related to the point being clicked among all $C(n, 2)$ pairs. With these two pieces of information from the dynamic configuration plot and the diagnostic plots, the MDS model can be diagnosed in a more informative and accurate way.

4.4. Color-smearing

In our colored configuration plot, colors are only given to the configuration points. There is no color for the space between points. Patterns can be more easily found if we can fill the space with colors. There are two ways to fill up the space using ideas from nonparametric smoothing.

q-Dimensional Color-smearing. For the conditional configuration plot of object o_r, the colors on the plot represent the column of proximities $\{\delta_{rs}, s = 1, \ldots, n\}$ between other objects and o_r. Let the q-dimensional MDS output configuration for each point be $\{x_s, s = 1, \ldots, n\}$. We compute the estimated proximity from every point x on the configuration space to object o_r, $\hat{\delta}_r(x)$, by the usual nonparametric kernel regression estimator

$$\hat{\delta}_r(x) = \frac{1}{n} \sum_{s=1}^{n} \delta_{rs} \kappa_{h_x}(x - x_s) \Big/ \frac{1}{n} \sum_{s=1}^{n} \kappa_{h_x}(x - x_s). \tag{6}$$

The same color spectrum is then used to fill up the configuration space with the estimated proximity $\hat{\delta}_r(x)$. If no stress exists for the conditioned object, this plot of color-smearing displays contours with a peak centered at the conditioned point and smoothly descends to the boundary of the configuration space with appropriate distance/disparity matching ratio as displayed on the colored spectrum bar. When stress is substantial, the color-smearing plot has a twisted pattern or a smooth pattern with an inappropriate distance/disparity matching ratio.

The conditional color-smearing plot of symptom NB1 is overlaid with the conditional configuration plot in Figure 3a. A smooth pattern with appropriate distance/disparity matching ratio reconfirms that symptom NB1 fits the model well as in earlier observation. From the contrast between the colors on the configuration points and the color pattern on the color-smearing plot, we do notice a slight disturbance near the peak of the contour. This shows some advantage of overlaying the color-smearing plot on the conditional configuration plot over the configuration plot alone.

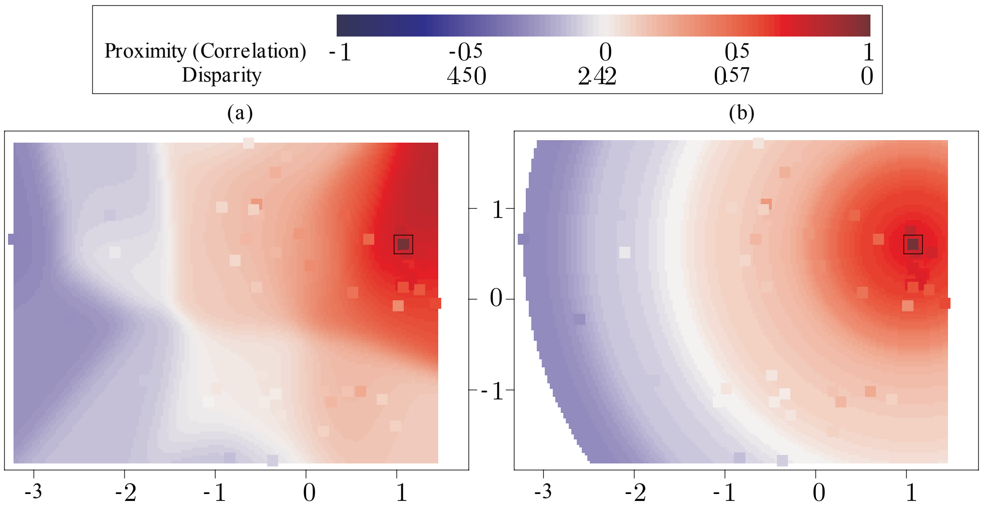

Figure 3. Color smearing for conditional configuration plot, case study: symptom NBl. (a) Two-dimensional color-smearing plot; (b) One-dimensional color-smearing plot.

One-Dimensional Color-smearing. The notion of color-smearing was demonstrated with a two-dimensional MDS configuration space. With a higher-dimensional MDS configuration space, the concept can be adapted to a display in a three-dimensional rotation plot or a scatterplot-matrix. However, the loading of the computation can be quite heavy with a high dimensional nonparametric kernel regression estimator. When instant interactive diagnosing is necessary, the following one-dimensional color-smearing can be performed.

Conditioned on object o_r, we perform the following one-dimensional version of (6):

$$\hat{\delta}_r(d) = \frac{1}{n}\sum_{s=1}^{n} \delta_{rs}\kappa_{h_d}(d - d_{rs}^{(q)}) \Big/ \frac{1}{n}\sum_{s=1}^{n} \kappa_{h_d}(d - d_{rs}^{(q)}). \tag{7}$$

With this much simplified computation, we need to compute only the one-dimensional $\hat{\delta}_r(d)$ within the range, $0 \leq d \leq \max_{s=1,\ldots,n}(d_{rs}^{(q)})$. The next step is to plot a series of circles (spheres), centered at x_r, with radius d and color $\hat{\delta}_r(d)$, within the range $0 \leq d \leq \max_{s=1,\ldots,n}(d_{rs}^{(q)})$. Figure 3b displays the one-dimensional color-smearing plot overlaid on the conditional configuration plot for symptom NB1. Since this is only a one-dimensional color-smearing plot, the pattern always contains continuous circles (spheres) centered at the clicked point. Of relevant concern is the continuum of colors of the circles (spheres): if the pattern matches that on the color spectrum bar, no stress arises; otherwise, we identify a stress contributor. This one-dimensional color- smearing plot is definitely less informative than the higher-dimensional one since the direction of the contour is now meaningless, but the computation is extremely simple. Users can obtain an instant response and the missing piece of information about the direction can be retrieved from the contrast of the color pattern of the color-smearing plot with the overlaid color dots on the conditional configuration plot.

4.5. The decomposed stress proportion plot

In our case study, the psychiatrists know in advance which symptoms may not fit well in the lower dimensional MDS configuration space. More attention can be paid to diagnostics for those particular symptoms. This prior knowledge about possible stress contributors or potential outliers may be unavailable when we use MDS as an initial data analysis tool. Then it can be quite time consuming to go through all dynamic plots for every object in the model. We need guidance on which objects must be examined first. We propose a decomposed stress proportion plot for this situation. The notion is to obtain a picture of the possible distribution of the stress score for all objects. Using the SSTRESS formula in (5), we compute the stress proportion for each object as

$$STRESS_q(o_r) = \sum_{i=1}^{n} \left((d_{ri}^{(q)})^2 - (\hat{d}_{ri}^{(q)})^2\right)^2 \Big/ \sum_{i=1}^{n}\sum_{j=1}^{n} \left((d_{ij}^{(q)})^2 - (\hat{d}_{ij}^{(q)})^2\right)^2, \; r = 1, \ldots, n. \tag{8}$$

In this quantity, each pair (i, j) is counted twice while computing all the n stress proportions. The stress proportions can also be computed using the STRESS1 or STRESS2 formula. The decomposed stress proportions are then sorted by their magnitudes and plotted in a descending order. Users can then begin examining those objects with higher proportion of stress contribution.

Figure 4 identifies symptom DL2 as having the highest portion of contributed stress followed by symptoms BE3, TH6, DL7 and BE2. On the opposite side, NA1, NA5, NA3, NB1, and NA7 share the smallest portions of stress. With this plot of decomposed stress proportion, we can understand the stress distribution structure. However, we still need the dynamic conditional configuration plot with color-smearing and the diagnostic plots to understand the detailed source and types of the possible stress.

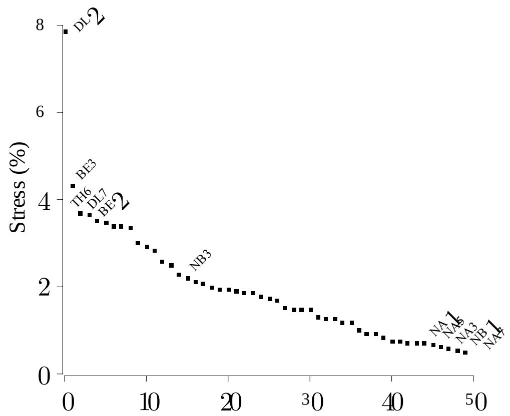

Figure 4. The decomposed stress proportion plot, case study.

4.6. The residual plot wih a link function

The decomposed stress proportions plot gives us the overall performance for each individual object in the MDS model fitting. On the other hand, the source of an individual stress or risidual $(d_{rs}^{(q)} - \hat{d}_{rs}^{(q)})$ may be of interest to the users. This piece of information can be obtained with an additional diagnostic plot. Instead of plotting the distances $\{d_{rs}^{(q)}\}$ versus the disparities $\{\hat{d}_{rs}^{(q)}\}$, as in the linear fit plot, we can plot the deviations $(d_{rs}^{(q)} - \hat{d}_{rs}^{(q)})$ from the $d = \hat{d}$ line as a residual plot (Figure 5a). This residual plot is then linked to the configuration plot in Figure 5b with a special linking function. We can then use the brushing function to

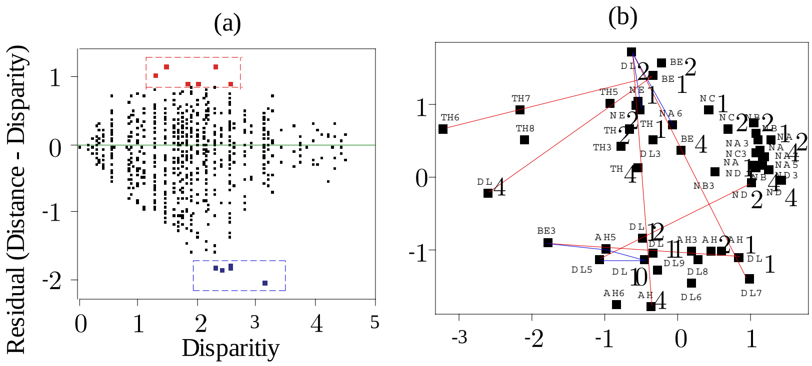

Figure 5. Residual plot with a link function, case study. (a) Residual plot; (b) Linked configuration plot. When user brushes through the residuals (distances - disparities) plot, the corresponding paired objects are connected by lines in the configuration plot.

locate the residuals in the residual plot. The corresponding pairs of objects in the configuration plot are connected by lines. in Figure 5b, red (blue) lines connect pairs of objects corresponding to the high positive (negative) residuals in the brushing windows in Figure 5a. Positive and negative residuals represent those distances that are over- and under-represented, respectively, in the configuration space. We see that symptom DL2 is responsible for both the highly over-represented and under-represented distances.

4.7. Examination of the individual symptom behavior and grouping structure with proposed method

In Section 3.7 we inferred from the classical MDS tools that there are four possible symptom groups. In this section, we use the proposed interactive MDS diagnosing system to further understand the overall structure and the detailed relationship between symptoms. For illustration, we examine the dynamic configuration plot and diagnostic plots for only 3 symptoms. Of particular emphasis is the possible conflict between the visualization of configuration distances $\{d_{rs}^{(q)}\}$ and the visualization of color pattern of the input proximities $\{\delta_{rs}\}$.

Symptom NB1. From Figure 4, we infer that symptom NB1 has one of the smallest proportions of stress among all 50 symptoms. Results obtained from more noticeable observations in Figures 2 and 3, rather than in Figure 1, of the classical MDS are as follows: (1) symptoms in the TH (thought disorder) group have low positive or zero correlations with symptom NB1, but the pattern of magnitude of correlation does not match well with the distance pattern; (2) the relationship of NB1 to the AH/DL group can be roughly divided into the following three parts: symptoms AH1-3, DL1 and DL6-8 on the right side, low positive correlations; symptoms AH5, DL5 and DL9-12 in the middle, zero correlations; symptoms AH4, AH6 and BE3 on the lower left part, low negative correlations; (3) the blue color on the left part of the plots indicates that the mania symptom group is negatively correlated to NB1. This information of negative correlation is not available in the classical MDS tools. The problem with a zero stress score raised in Subsection 3.6 is simply resolved by this color linkage function.

Symptom NB3. Figure 6 indicates that symptom NB3 actually does not belong to any of the four groups. It has similar relationships with groups of negative symptoms (NEG), thought disorder (TH) and hallucination/delusion (AH/DL). However, the configuration distances between NB3 and the symptoms in these three groups do not accurately represent the magnitude of correlation between them. Symptom NB3 has a relatively high correlation with some of the symptoms in all three groups, NB4 in NEG group for example. However, those symptoms, on the other hand, also have a strong relationship with other symptoms in their own groups. We conclude that NB3 is a unique symptom that deserves special attention.

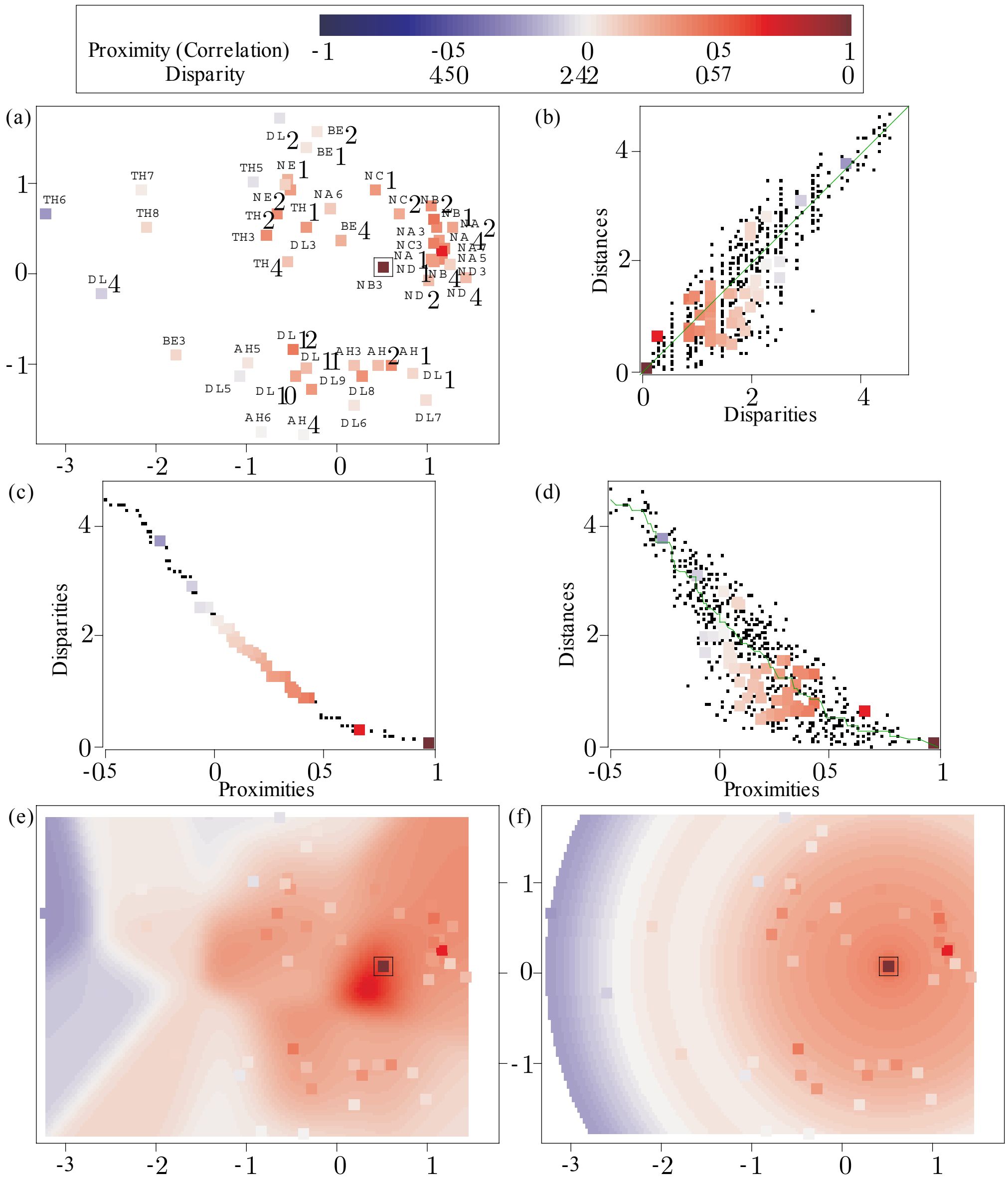

Figure 6. Interactive diagnostic plots for MDS, case study: symptom NB3. (a) Conditional configuration plot; (b) Conditional linear fit plot; (c) Conditional transformation plot; (d) Conditional nonlinear fit plot; (e) Two-dimensional color-smearing plot; (f) One-dimensional color-smearing plot.

Symptom DL2. Figure 4 reveals that symptom DL2 has the highest decomposed proportion of stress (8%) among all 50 symptoms. DL2 is a symptom which is sacrificed by the classical MDS modeling. Without the proposed method, symptom DL2 is obviously a member of the group of thought disorder.

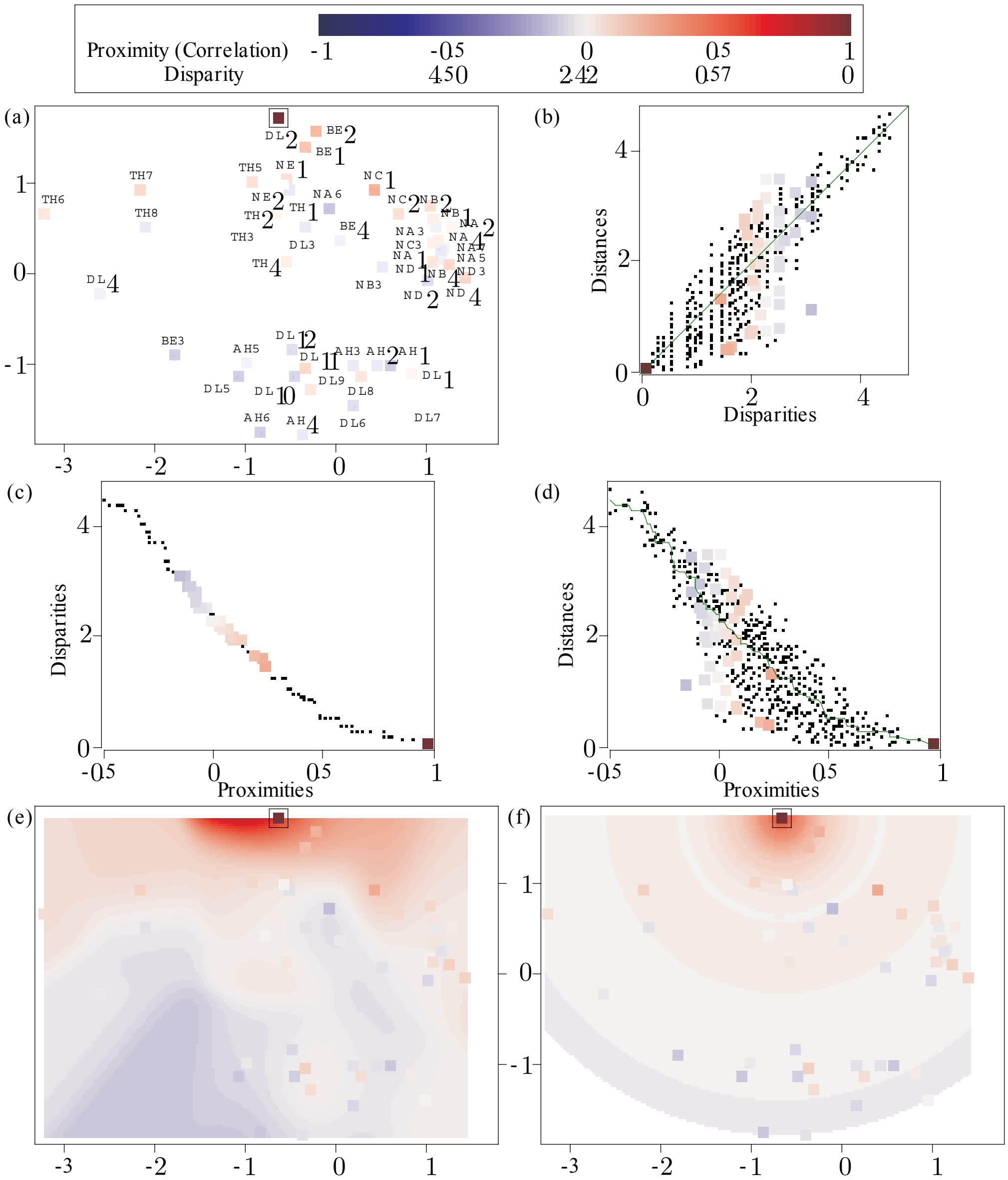

Figure 7. Interactive diagnostic plots for MDS, case study: symptom DL2. (a) Conditional configuration plot; (b) Conditional linear fit plot; (c) Conditional transformation plot; (d) Conditional nonlinear fit plot; (e) Two-dimensional color-smearing plot; (f) One-dimensional color-smearing plot.

From the dynamic conditional configuration and diagnostic plots in Figure 7, symptom DL2 is nearly uncorrelated with any other symptom. Even with BE1 and BE2, the correlation coefficients are as low as 0.2. It actually has negative correlations with NA6 and TH2, though high positive correlations are suggested by the configuration distances. Without diagnostics the misleading result of the MDS model fitting might well be accepted as the correct one.

Instead of accepting the classical MDS configuration as a whole and taking a $20 \sim 30\%$ discount on what we observe on the configuration space, our proposed diagnostic method can identify problems with MDS model fitting. A more detailed study should be made on those objects which are diagnosed as potential stress contributors to identify the actual underlying causes of problems.

5. A Simulation Study

In addition to our case study with the correlation matrix as the input proximity matrix, we conducted a simulation study with a different type of proximity to illustrate the versatility of our proposed method. A rainbow like color spectrum is used to represent the distance type input proximities $\{\delta_{rs}\}$.

5.1. The model

Three independent variables are involved in the simulation. The first two variables, x_1 and x_2, are drawn uniformly from the unit square. The third variable, x_3, takes only two distinct values: 0 and 0.5, with probabilities 0.95 and 0.05 respectively. The Euclidean distance matrix of the n observations in the 3-dimensional space is used for the input $\{\delta_{rs}\}$, and a 2-dimensional configuration space with a metric model is requested.

Fifty observations are generated from the model. Three observations, o_4, o_{20} and o_{32}, have x_3 equal to 0.5. The observations are plotted in Figures 8a and 8b. In a two-dimensional MDS modeling, the classical MDS algorithm is expected to neglect information about the third variable. Those observations are essential outliers to the 2-dimensional MDS model.

5.2. Classical MDS result

Figure 10a (without color) reveals the 2-dimensional MDS configuration plot as nearly identical to the scatterplot of the original first two variables with a rotation of the coordinates. The STRESS1 and SSTRESS scores with R^2 are 0.092, 0.11692 and 0.952, respectively, leading us to believe that MDS does a good job on the model fitting. On the other hand the classical plot of linear fit (Figure 10b without color) does show some unusual pattern of disturbance. However, the source of the problem cannot be identified with a classical static plot of linear fit.

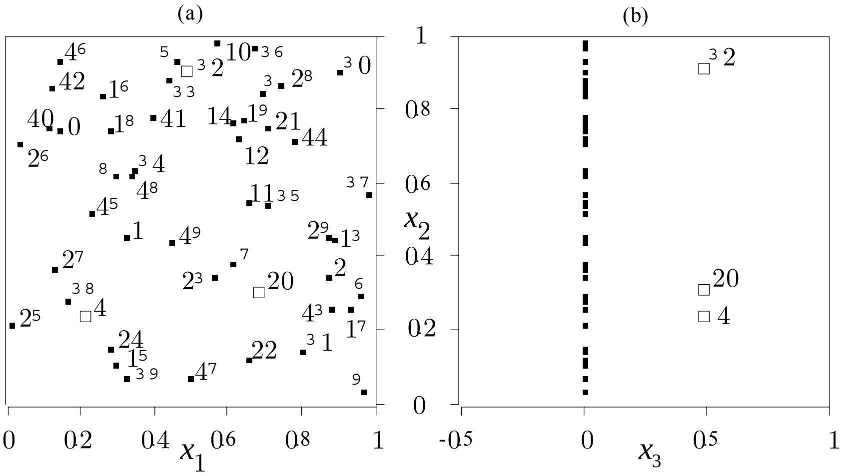

Figure 8. Plots of the fifty observations for simulation study. (a) x_2 versus x_1; (b) x_2 versus x_3.

5.3. Analysis with proposed diagnostic method

The individual stress proportion plot in Figure 9 picks up observations o_{32}, o_{20}, and o_4, which contribute more than half (50%) of the total stress score, as potential stress contributors.

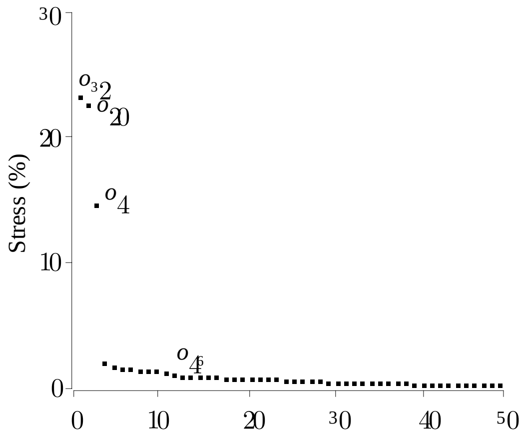

Figure 9. The decomposed stree proportion plot, simulation study.

Diagnosis on a non-stress-contributor. For a non-stress-contributor, o_{46} in this case, the conditional configuration plot (Figure 10a) displays layers of color dots which closely correspond to the color stripes on the spectrum except for a slight disturbance at the point located at the lower right corner of the plot, which is o_{32}, one of the outliers. The 2-dimensional color- smearing plot (Figure 10c) is a smooth one except for a disturbance due to the same observation. The

1-dimensional color-smearing plot (Figure 10d) resembles a target board with the bull's-eye at o_{46}. The circles with colors identical to that on the spectrum bar are laid out in a perfect manner where any possible outlier can be easily identified from the colored dots on the overlaid conditional configuration plot.

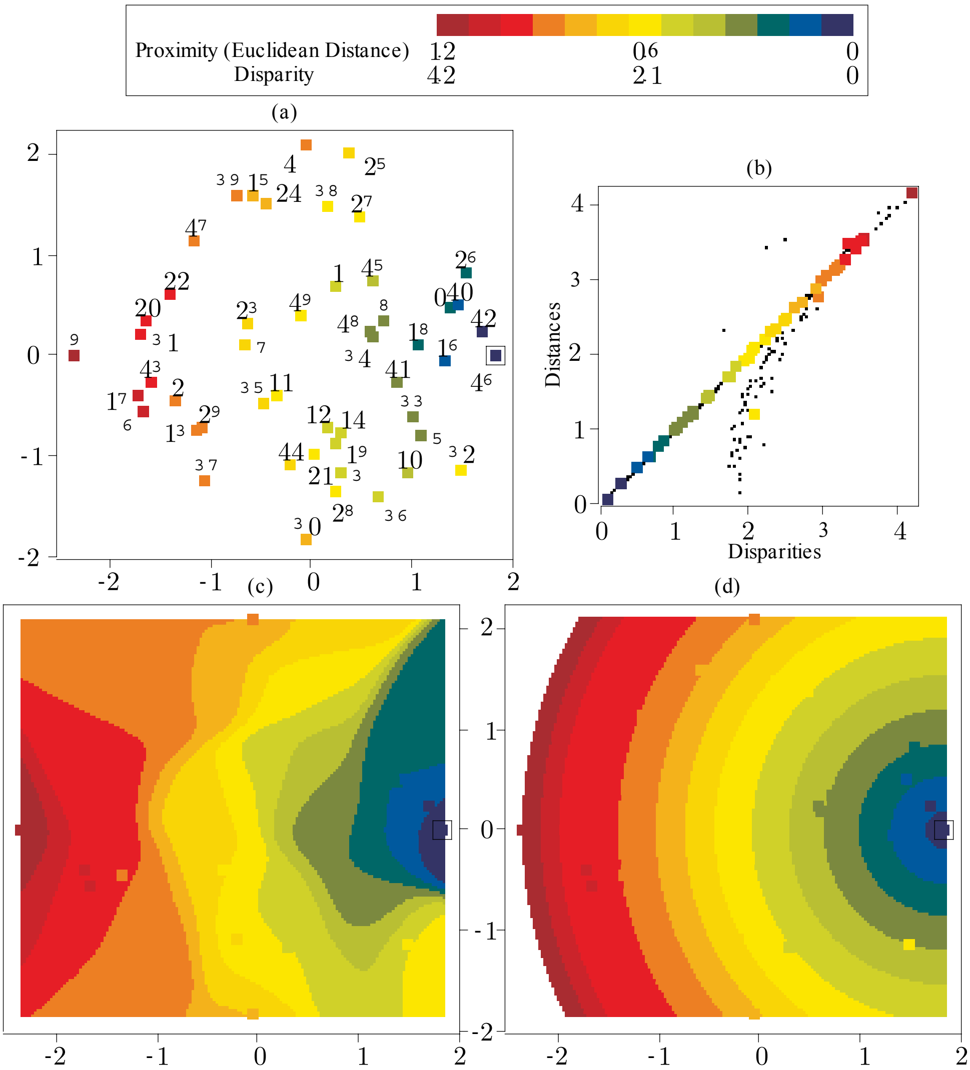

Figure 10. Interactive diagnostic plots for MDS, simulation study : O_{46}. (a) Conditional configuration plot; (b) Conditional linear fit plot; (c) Two-dimensional color-smearing plot; (d) One-dimensional color-smearing plot.

In Figure 10b all corresponding distance/disparity pairs for o_{46} remain on the perfect fit line except for the one associated with o_{32}. These two points are close to each other on the first two coordinates (see Figure 8a), and the difference on the third variable was ignored by the MDS algorithm. From the proposed diagnostic plots, we can conclude that o_{46} fits into the model almost perfectly.

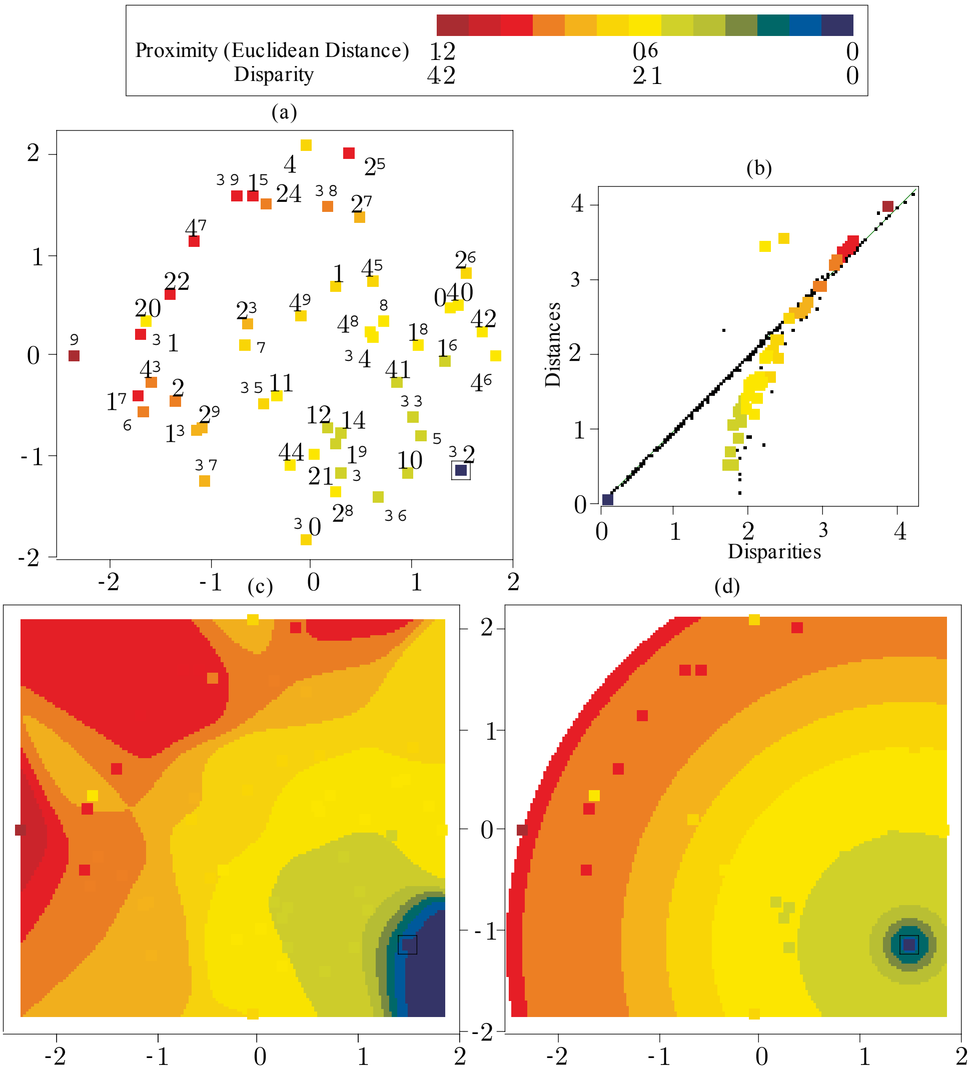

Figure 11. Interactive diagnostic plots for MDS, simulation study : O_{32}. (a) Conditional configuration plot; (b) Conditional linear fit plot; (c) Two-dimensional color-smearing plot; (d) One-dimensional color-smearing plot.

Diagnosis on a stress-contributor. There are three potential stress contributors in Figure 9. We select o_{32} to illustrate the technique. Figure 11a indicates that no observation is really close to o_{32} in the original set of distances (proximities), since there are no dots with colors to the right end of the color spectrum (dark blue). Those points on the lower right portion of the configuration space were placed too close to o_{32} relative to the actual distances (proximities). We can also identify the two points, o_4 and o_{20}, on the upper left corner as out of position. These observations also have a value of 0.5 in the third dimension, x_3. The MDS algorithm has put them too distant from o_{32} on the configuration space.

On 2- and 1-dimensional color-smearing plots, Figures 11c and 11d, the scale of color patterns does not follow that on the color spectrum bar. The misplaced points can also be identified easily via visualization.

The pattern on the plot of linear fit in Figure 11b is even more dramatic than that in the color-smearing plot. All pairs of distance/disparity related to o_{32} are off the perfect fit line, indicating that this observation definitely does not fit into the MDS model.

Diagnosis with the linked residual plot. The residual plot with the brushing windows and the configuration plot with the connecting lines are placed in Figure 12a and b. There are only three significant positive residuals (in red). The corresponding three red lines connect objects o_4, o_{20} and o_{32}, indicating that only the distances among these three objects are over-represented - they are pushed too far away from each other in the configuration space. On the other hand, the blue residual points and the blue connecting lines indicate that the distances between the three stress contributors and their neighboring objects are all under-represented.

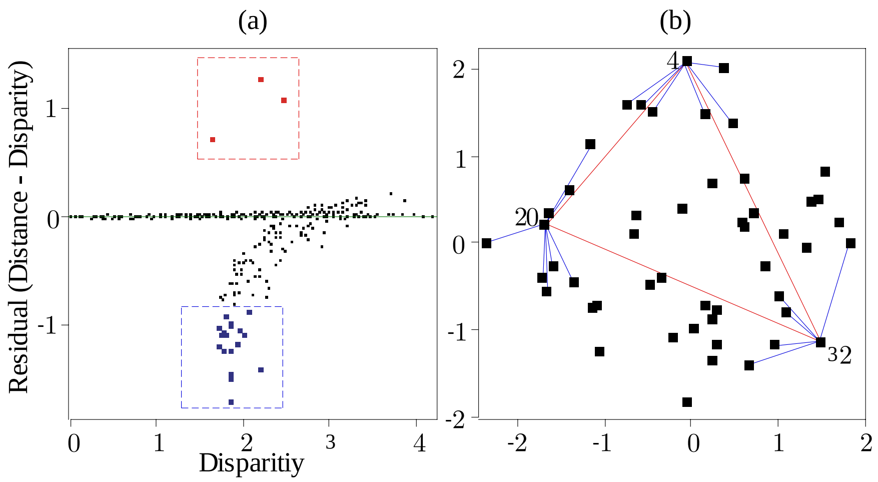

Figure 12. Residual plot with a link function, simulation study. (a) Residual plots (b) Linked configuration plot. The distances among the three stress contributors (Objects 4, 20, 32) are over represented (in red). The distances between the three stress contributors and the corresponding neighboring objects are under represented (in blue).

6. General Guidance on Using the Proposed Diagnosing System

Classical diagnostic methods provide the users an overall confidence about interpreting the MDS output configuration. We have introduced tools for diagnosing an MDS modeling procedure in a more informative way. The plots in our diagnosing system can be roughly divided into three levels.

6.1. Level I: decomposed stress proportion plot and the residual plot

After obtaining the overall performance from the classical indices, users may want to further understand the distribution of the stress structure. This can be done in two complementary procedures. The decomposed stress proportion plot illustrates the proportion of contribution to total stress of each object in a descending order. A smooth linear trend of descent implies no special structure in the stress distribution. An elbow (steep drop) pattern indicates that objects above the elbow (DL2 in Figure 4, and o_{20}, o_{32}, o_4 in Figure 9) contribute relatively more to total stress than do objects below the elbow. These objects need to be included in higher level diagnostic plots for further exploring the structure of stress related to them.

In another direction, the brushing function of the residual plot can be applied to identify the source (pair of relationship) of a particular stress (residual) component.

6.2. Level II: conditional diagnostic plots

While Level I diagnostic plots show the size of stress of individual objects and the source of individual residuals, they do not provide the relative stress structure of each object. The conditional diagnostic plots can display an intermediate level of information. When an object is identified as a potential problem in the stress decomposed plot, a click on it will paint the related n points (among all $C(n, 2)$ points) in the diagnostic plots with colors representing the corresponding n proximities. Important pieces of information can be obtained from these conditional diagnostic plots: relative range of these n proximities (disparities) for the object under examination to all $C(n, 2)$ proximities (disparities); relative positions of highlighted points above or below the perfect fit line.

6.3. Level III: conditional configuration plot with color smearing

The configuration plot is the most important output in an MDS modeling procedure. The usefulness of the interpretation of the configuration structure relies on the reliability of the configuration space. It is possible that there exist some regions in the configuration space that are less stable than other regions. It is important to identify such regions, and the possible patterns of them, while interpreting the configuration plot. The conditional configuration plot with color smearing can augment the information given in Levels I and II with extra information on the directions and regions of problem source through visualization. Users need to pay more attention to the following two pieces of information while examining a particular conditional configuration plot with color smearing: (1) the color pattern representing the proximities should radiate from the clicked point (conditioned object) in a monotonic way in any direction; (2) the degree of monotonic descent or ascent in colors should match the pattern on the color spectrum (bar). That is, the color spectrum can be used as a rule or a compass to evaluate the rate of descent or ascent of color patterns from the center (conditioned point).

In a classical MDS diagnosing procedure, if some objects are identified as the source of high stress scores, two actions can be carried out to resolve the problem: (1) add extra dimensions to relocate these objects in more suitable regions in a higher-dimensional configuration space; (2) exclude these objects from further modeling process. Both actions can reduce the size of stress but they also introduce difficulties in interpreting and (or) visualizing the final configuration.

7. Discussion

Similar to the model fitting in regression analysis, MDS model fitting requires some diagnostic tools to construct a good model for the data set under consideration. As seen in the simulation example, one can easily reach a misleading conclusion based on classical MDS model fitting. By using the proposed diagnosing environment, one can not only identify the potential stress contributors but also build a clearer picture of the overall structure embedded in the set of original proximities.

For a research project like our psychopathological research program, the psychiatrists were dissatisfied by the initial results given by the classical MDS analysis. They sought a more thorough understanding of the global grouping pattern and individual relationship structure of symptoms. Our proposed method partly fulfilled their needs.

In this paper, it takes many color pages of static plots to obtain the desired understanding of the relationship structure. On a computer screen, only a few mouse clicks will provide a comprehensive knowledge of the data structure under consideration. We used the ALSCAL program with a single proximity matrix and two-way measurements to illustrate the proposed concept. These techniques can be easily modified and adapted to other MDS combinations.

MDS is a useful initial data analysis tool for many types of multivariate data. From the decomposed stress proportion plot and the linked residual plot, to dynamic diagnostic plots, to conditional configuration plots with color-smearing, we present a complete and comprehensive system for diagnosing MDS model fitting.

Appendix
The Andreasen's Positive and Negative Symptom Table

	SAPS
AH1	Auditory Hallucinations
AH2	Voices Commenting
AH3	Voices Conversing
AH4	Somatic or Tactile Hallucinations
AH5	Olfactory Hallucinations
AH6	Visual Hallucinations
DL1	Persecutory Delusions
DL2	Delusion of Jealousy
DL3	Delusion of Sin or Guilt
DL4	Grandiose Delusions
DL5	Religious Delusions
DL6	Somatic Delusions
DL7	Ideas and Delusions of Reference
DL8	Delusions of Being Controlled
DL9	Delusions of Mind Reading
DL10	Thought Broadcasting
DL11	Thought Insertion
DL12	Thought Withdrawal
BEH1	Clothing and Appearance
BEH2	Social and Sexual Behavior
BEH3	Aggressive and Agitated Behavior
BEH4	Repetitive or Stereotyped Behavior
TH1	Derailment
TH2	Tangentiality
TH3	Incoherence
TH4	Illogicality
TH5	Circumstantiality
TH6	Pressure of Speech
TH7	Distractible Speech
TH8	Clanging

	SANS
NA1	Unchanging Facial Expression
NA2	Decreased Spontaneous Movements
NA3	Paucity of Expressive Gestures
NA4	Poor Eye Contact
NA5	Affective Nonresponsivity
NA6	Inappropriate Affect
NA7	Lack of Vocal Inflections
NB1	Poverty of Speech
NB2	Poverty of Content of Speech
NB3	Blocking
NB4	Increased Latency of Response
NC1	Grooming and Hygiene
NC2	Impersistence at Work or School
NC3	Physical Anergia
ND1	Recreational Interest and Activities
ND2	Sexual Interest and Activity
ND3	Ability to Feel Intimacy and Closeness
ND4	Relation With Friends and Peers
NE1	Social Inattentiveness
NE2	Inattentiveness During MSE

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